Ivan Markovsky

Low-Rank Approximation

Algorithms, Implementation, Applications

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Preface

Mathematical models are obtained from first principles (natural laws, interconnection, *etc.*) and experimental data. Modeling from first principles is common in natural sciences, while modeling from data is common in engineering. In engineering, often experimental data is available and a simple approximate model is preferred to a complicated detailed one. Indeed, although optimal prediction and control of a complex (high-order, nonlinear, time-varying) system is currently difficult to achieve, robust analysis and design methods, based on a simple (low-order, linear, time-invariant) approximate model, may achieve sufficiently high performance. This book addresses the problem of *data approximation by low-complexity models.*

A unifying theme of the book is low-rank approximation: a prototypical data modeling problem. The rank of a matrix constructed from the data corresponds to the complexity of a linear model that fits the data exactly. The data matrix being full rank implies that there is no exact low complexity linear model for that data. In this case, the aim is to find an approximate model. One approach for approximate modeling, considered in the book, is to find small (in some specified sense) modification of the data that renders the modified data exact. The exact model for the modified data is an optimal (in the specified sense) approximate model for the original data. The corresponding computational problem is low-rank approximation. It allows the user to trade off accuracy vs complexity by varying the rank of the approximation.

The distance measure for the data modification is a user choice that specifies the desired approximation criterion or reflects prior knowledge about the accuracy of the data. In addition, the user may have prior knowledge about the system that generates the data. Such knowledge can be incorporated in the modeling problem by imposing constraints on the model. For example, if the model is known (or postulated) to be a linear time-invariant dynamical system, the data matrix has Hankel structure and the approximating matrix should have the same structure. This leads to a Hankel structured low-rank approximation problem.

A tenet of the book is: the estimation accuracy of the basic low-rank approximation method can be improved by exploiting prior knowledge, *i.e.*, by adding constraints that are known to hold for the data generating system. This path of development leads to weighted, structured, and other constrained low-rank approximation problems. The theory and algorithms of these new classes of problems are interesting in their own right and being application driven are practically relevant.

Stochastic estimation and deterministic approximation are two complementary aspects of data modeling. The former aims to find from *noisy data*, generated by a low-complexity system, an estimate of that data generating system. The latter aims to find from *exact data*, generated by a high complexity system, a low-complexity approximation of the data generating system. In applications both the stochastic estimation and deterministic approximation aspects are likely to be present. The data is likely to be imprecise due to measurement errors and is likely to be generated by a complicated phenomenon that is not exactly representable by a model in the considered model class. The development of data modeling methods in system identification and signal processing, however, has been dominated by the stochastic estimation point of view. If considered, the approximation error is represented in the mainstream data modeling literature as a random process. This is not natural because the approximation error is by definition deterministic and even if considered as a random process, it is not likely to satisfy standard stochastic regularity conditions such as zero mean, stationarity, ergodicity, and Gaussianity.

An exception to the stochastic paradigm in data modeling is the behavioral approach, initiated by J. C. Willems in the mid 80's. Although the behavioral approach is motivated by the deterministic approximation aspect of data modeling, it does not exclude the stochastic estimation approach. In this book, we use the behavioral approach as a *language* for defining different modeling problems and presenting their solutions. We emphasize the importance of deterministic approximation in data modeling, however, we formulate and solve stochastic estimation problems as low-rank approximation problems.

Many well known concepts and problems from systems and control, signal processing, and machine learning reduce to low-rank approximation. Generic examples in system theory are model reduction and system identification. The principal component analysis method in machine learning is equivalent to low-rank approximation, which suggests that related dimensionality reduction, classification, and information retrieval problems can be phrased as low-rank approximation problems. Sylvester structured low-rank approximation has applications in computations with polynomials and is related to methods from computer algebra.

The developed ideas lead to algorithms, which are implemented in software. The algorithms clarify the ideas and the software implementation clarifies the algorithms. Indeed, the software is the ultimate unambiguous description of how the ideas are put to work. In addition, the provided software allows the reader to reproduce the examples in the book and to modify them. The exposition reflects the sequence

$$\text{theory} \mapsto \text{algorithms} \mapsto \text{implementation}.$$

Correspondingly, the text is interwoven with code that generates the numerical examples being discussed.

Prerequisites and practice problems

A common feature of the current research activity in all areas of science and engineering is the narrow specialization. In this book, we pick applications in the broad area of data modeling, posing and solving them as low-rank approximation problems. This unifies seemingly unrelated applications and solution techniques by emphasising their common aspects (*e.g.*, complexity–accuracy trade-off) and abstracting from the application specific details, terminology, and implementation details. Despite of the fact that applications in systems and control, signal processing, machine learning, and computer vision are used as examples, the only real prerequisites for following the presentation is knowledge of linear algebra.

The book is intended to be used for self study by researchers in the area of data modeling and by advanced undergraduate / graduate level students as a complementary text for a course on system identification or machine learning. In either case, the expected knowledge is undergraduate level linear algebra. In addition, MATLAB code is used, so that familiarity with MATLAB programming language is required.

Passive reading of the book gives a broad perspective on the subject. Deeper understanding, however, requires active involvement, such as supplying missing justification of statements and specific examples of the general concepts, application and modification of presented ideas, and solution of the provided exercises and practice problems. There are two types of practice problems: analytical, asking for a proof of a statement clarifying or expanding the material in the book, and computational, asking for experiments with real or simulated data of specific applications. Most of the problems are easy to medium difficulty. A few problems (marked with stars) can be used as small research projects.

The code in the book, available from

http://extra.springer.com/

has been tested with MATLAB 7.9, running under Linux, and uses the Optimization Toolbox 4.3, Control System Toolbox 8.4, and Symbolic Math Toolbox 5.3. A version of the code that is compatible with Octave (a free alternative to MATLAB) is also available from the book's web page.

Software tools used for typesetting the book

The book is typeset using LaTeX and a number of extension packages. Diagrams are created using the PSTricks and `xy` packages and the standalone `xfig` program. All editing is done in the GNU Emacs editor, using org-mode and latex-mode. MATLAB code, presented in a literate programming style is an integral part of the text. This is achieved by the Norman Ramsey's `noweb` system.

The process of compiling the book involves a number of steps automated by a GNU Make file. First the LaTeX source code and the MATLAB functions and scripts are extracted from `noweb`'s source files. The obtained scripts are then executed

in MATLAB in order to generate the figures and numerical results. Finally, LaTeX, bibTeX, `dvips`, and `ps2pdf` are run on the files created in the previous steps to generate the final pdf file of the book. The described process guarantees that the code in the text is the actual code that has generated the results shown in the book.

A laptop and a desktop computers were used for working on the book. Keeping the files synchronized between the two computers was done using the Unison file synchronizer.

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Southampton, *Ivan Markovsky*
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Contents

Chapter 1
Introduction

The very art of mathematics is to say the same thing another way.

Unknown

1.1 Classical and behavioral paradigms for data modeling

Fitting linear models to data can be achieved, both conceptually and algorithmically, by solving approximately a system of linear equations

$$AX \approx B, \tag{LSE}$$

where the matrices A and B are constructed from the given data and the matrix X parametrizes the model. In this *classical paradigm*, the main tools are the ordinary linear least squares method and its variations—regularized least squares, total least squares, robust least squares, *etc*. The least squares method and its variations are mainly motivated by their applications for data fitting, but they invariably consider solving approximately an overdetermined system of equations.

The underlying premise in the classical paradigm is that existence of an exact linear model for the data is equivalent to existence of solution X to a system $AX = B$. Such a model is a linear map: the variables corresponding to the A matrix are inputs (or causes) and the variables corresponding to the B matrix are outputs (or consequences) in the sense that they are determined by the inputs and the model. Note that in the classical paradigm the input/output partition of the variables is postulated a priori. Unless the model is required to have the a priori specified input/output partition, imposing such structure in advance is ad hoc and leads to undesirable theoretical and numerical features of the modeling methods derived.

An alternative to the classical paradigm that does not impose an a priori fixed input/output partition is the *behavioral paradigm.* In the behavioral paradigm, fitting linear models to data is equivalent to the problem of approximating a matrix D, constructed from the data, by a matrix $\widehat{D}$ of lower rank. Indeed, existence of an exact linear model for D is equivalent to D being rank deficient. Moreover, the rank of D is related to the complexity of the model. This fact is the tenet of the book and is revisited in the following chapters in the context of applications from systems and control, signal processing, computer algebra, and machine learning. Also its implication to the development of numerical algorithms for data fitting is explored.

To see that existence of a low complexity exact linear model is equivalent to rank deficiency of the data matrix, let the columns $d_1, \dots, d_N$ of D be the observations and the elements $d_{1j}, \dots, d_{\mathtt{q}j}$ of d_j be the observed variables. We assume that there are at least as many observations as observed variables, *i.e.*, $\mathtt{q} \leq N$. A linear model for D declares that there are linear relations among the variables, *i.e.*, there are vectors r_k, such that

$$r_k^\top d_j = 0, \qquad \text{for } j = 1, \dots, N.$$

If there are $\mathtt{p}$ independent linear relations, then D has rank less than or equal to $\mathtt{m} := \mathtt{q} - \mathtt{p}$ and the observations belong to at most $\mathtt{m}$-dimensional subspace $\mathscr{B}$ of $\mathbb{R}^{\mathtt{q}}$. We identify the model for D, defined by the linear relations $r_1, \dots, r_{\mathtt{p}} \in \mathbb{R}^{\mathtt{q}}$, with the set $\mathscr{B} \subset \mathbb{R}^{\mathtt{q}}$. Once a model $\mathscr{B}$ is obtained from the data, all possible input/output partitions can be enumerated, which is an analysis problem for the identified model. Therefore, the choice of an input/output partition in the behavioral paradigm to data modeling can be incorporated, if desired, in the modeling problem and thus need not be hypothesized as necessarily done in the classical paradigm.

The classical and behavioral paradigms for data modeling are related but not equivalent. Although existence of solution of the system $AX = B$ implies that the matrix $\begin{bmatrix} A & B \end{bmatrix}$ is low rank, it is not true that $\begin{bmatrix} A & B \end{bmatrix}$ having a sufficiently low rank implies that the system $AX = B$ is solvable. This lack of equivalence causes ill-posed (or numerically ill-conditioned) data fitting problems in the classical paradigm, which have no solution (or are numerically difficult to solve). In terms of the data fitting problem, ill-conditioning of the problem (LSE) means that the a priori fixed input/output partition of the variables is not corroborated by the data. In the behavioral setting without the a priori fixed input/output partition of the variables, ill-conditioning of the data matrix D implies that the data approximately satisfies linear relations, so that nearly rank deficiency is a good feature of the data.

The classical paradigm is included in the behavioral paradigm as a special case because approximate solution of an overdetermined system of equations (LSE) is a possible approach to achieve low-rank approximation. Alternatively, low-rank approximation can be achieved by approximating the data matrix with a matrix that has at least $\mathtt{p}$-dimensional null space, or at most $\mathtt{m}$-dimensional column space. Parametrizing the null space and the column space by sets of basis vectors, the alternative approaches are:

1. *kernel representation* there is a full row rank matrix $R \in \mathbb{R}^{\mathtt{p} \times \mathtt{q}}$, such that

$$RD = 0,$$

2. *image representation* there are matrices $P \in \mathbb{R}^{\mathtt{q} \times \mathtt{m}}$ and $L \in \mathbb{R}^{\mathtt{m} \times N}$, such that

$$D = PL.$$

The approaches using kernel and image representations are equivalent to the original low-rank approximation problem. Next, the use of $AX = B$, kernel, and image representations is illustrated on the most simple data fitting problem—line fitting.

1.2 Motivating example for low-rank approximation

Given a (multi)set of points $\{d_1,\dots,d_N\} \subset \mathbb{R}^2$ in the plane, the aim of the line fitting problem is to find a line passing through the origin that "best" matches the given points. The classical approach for line fitting is to define

$$\operatorname{col}(a_j,b_j) := \begin{bmatrix} a_j \\ b_j \end{bmatrix} := d_j$$

(":=" stands for "by definition", see page 263 for a list of notation) and solve approximately the overdetermined system

$$\operatorname{col}(a_1,\dots,a_N)x = \operatorname{col}(b_1,\dots,b_N) \tag{lse}$$

by the least squares method. Let x_{ls} be the least squares solution to (lse). Then the least squares fitting line is

$$\mathscr{B}_{\text{ls}} := \{\, d = \operatorname{col}(a,b) \in \mathbb{R}^2 \mid ax_{\text{ls}} = b \,\}.$$

Geometrically, $\mathscr{B}_{\text{ls}}$ minimizes the sum of the squared *vertical distances* from the data points to the fitting line.

The left plot in Figure 1.1 shows a particular example with $N = 10$ data points. The data points $d_1,\dots,d_{10}$ are the circles in the figure, the fit $\mathscr{B}_{\text{ls}}$ is the solid line, and the fitting errors $e := ax_{\text{ls}} - b$ are the dashed lines. Visually one expects the best fit to be the vertical axis, so minimizing vertical distances does not seem appropriate in this example.

Note that by solving (lse), a (the first components of the d) is treated differently from b (the second components): b is assumed to be a *function* of a. This is an arbitrary choice; the data can be fitted also by solving approximately the system

$$\operatorname{col}(a_1,\dots,a_N) = \operatorname{col}(b_1,\dots,b_N)x, \tag{lse$'$}$$

in which case a is assumed to be a function of b. Let x'_{ls} be the least squares solution to (lse$'$). It gives the fitting line

$$\mathscr{B}'_{\text{ls}} := \{\, d = \operatorname{col}(a,b) \in \mathbb{R}^2 \mid a = bx'_{\text{ls}} \,\},$$

which minimizes the sum of the squared *horizontal distances* (see the right plot in Figure 1.1). The line $\mathscr{B}'_{\text{ls}}$ happens to achieve the desired fit in the example.

In the classical approach for data fitting, *i.e.*, solving approximately a system of linear equations in the least squares sense, the choice of the model representation affects the fitting criterion.

This feature of the classical approach is undesirable: it is more natural to specify a desired fitting criterion independently of how the model happens to be parametrized. In many data modeling methods, however, a model representation is a priori fixed and implicitly corresponds to a particular fitting criterion.

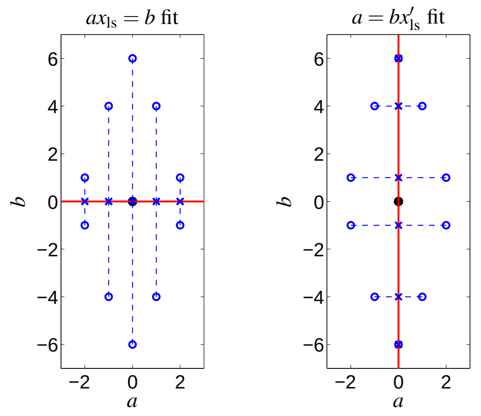

Fig. 1.1 Least squares fits (solid lines) minimizing vertical (left plot) and horizontal (right plot) distances.

The total least squares method is an alternative to least squares method for solving approximately an overdetermined system of linear equations. In terms of data fitting, the total least squares method minimizes the sum of the squared *orthogonal distances* from the data points to the fitting line. Using the system of equations (lse), line fitting by the total least squares method leads to the problem

$$\begin{aligned} &\text{minimize} \quad \text{over } x \in \mathbb{R}, \begin{bmatrix} \widehat{a}_1 \\ \vdots \\ \widehat{a}_N \end{bmatrix} \in \mathbb{R}^N, \text{ and } \begin{bmatrix} \widehat{b}_1 \\ \vdots \\ \widehat{b}_N \end{bmatrix} \in \mathbb{R}^N \quad \sum_{j=1}^{N} \left\| d_j - \begin{bmatrix} \widehat{a}_j \\ \widehat{b}_j \end{bmatrix} \right\|_2^2 \\ &\text{subject to} \quad \widehat{a}_j x = \widehat{b}_j, \quad \text{for } j = 1,\dots,N. \end{aligned} \tag{tls}$$

However, for the data in Figure 1.1 the total least squares problem has no solution. Informally, the approximate solution is $x_{\text{tls}} = \infty$, which corresponds to a fit by a vertical line. Formally,

the total least squares problem (tls) may have no solution and therefore fail to give a model.

The use of (lse) in the definition of the total least squares line fitting problem restricts the fitting line to be a graph of a function $ax = b$ for some $x \in \mathbb{R}$. Thus, the vertical line is a priori excluded as a possible solution. In the example, the line minimizing the sum of the squared orthogonal distances happens to be the vertical line. For this reason, x_{tls} does not exist.

Any line $\mathscr{B}$ passing through the origin can be represented as an image and a kernel, *i.e.*, there exist matrices $P \in \mathbb{R}^{2\times 1}$ and $R \in \mathbb{R}^{1\times 2}$, such that

$$\mathscr{B} = \text{image}(P) := \{\, d = P\ell \in \mathbb{R}^2 \mid \ell \in \mathbb{R} \,\}$$

and

$$\mathscr{B} = \ker(R) := \{\, d \in \mathbb{R}^2 \mid Rd = 0 \,\}.$$

Using the image representation of the model, the line fitting problem of minimizing the sum of the squared orthogonal distances is

$$\begin{aligned} &\text{minimize} \quad \text{over } P \in \mathbb{R}^{2\times 1} \text{ and } \begin{bmatrix}\ell_1 & \cdots & \ell_N\end{bmatrix} \in \mathbb{R}^{1\times N} \quad \sum_{j=1}^{N} \|d_j - \widehat{d}_j\|_2^2 \\ &\text{subject to} \quad \widehat{d}_j = P\ell_j, \quad \text{for } j = 1,\dots,N. \end{aligned} \tag{lra$'_P$}$$

With

$$D := \begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix}, \qquad \widehat{D} := \begin{bmatrix} \widehat{d}_1 & \cdots & \widehat{d}_N \end{bmatrix},$$

and $\|\cdot\|_{\text{F}}$ the *Frobenius norm*,

$$\|E\|_{\text{F}} := \big\|\operatorname{vec}(E)\big\|_2 = \Big\| \begin{bmatrix} e_{11} & \cdots & e_{\mathtt{q}1} & \cdots & e_{1N} & \cdots & e_{\mathtt{q}N} \end{bmatrix}^\top \Big\|_2, \quad \text{for all } E \in \mathbb{R}^{\mathtt{q}\times N}$$

(lra$'_P$) is more compactly written as

$$\begin{aligned} &\text{minimize} \quad \text{over } P \in \mathbb{R}^{2\times 1} \text{ and } L \in \mathbb{R}^{1\times N} \quad \|D - \widehat{D}\|_{\text{F}}^2 \\ &\text{subject to} \quad \widehat{D} = PL. \end{aligned} \tag{lra$_P$}$$

Similarly, using a kernel representation, the line fitting problem, minimizing the sum of squares of the orthogonal distances is

$$\begin{aligned} &\text{minimize} \quad \text{over } R \in \mathbb{R}^{1\times 2},\ R \neq 0, \text{ and } \widehat{D} \in \mathbb{R}^{2\times N} \quad \|D - \widehat{D}\|_{\text{F}}^2 \\ &\text{subject to} \quad R\widehat{D} = 0. \end{aligned} \tag{lra$_R$}$$

Contrary to the total least squares problem (tls), problems (lra$_P$) and (lra$_R$) always have (nonunique) solutions. In the example, solutions are, *e.g.*, $P^* = \operatorname{col}(0,1)$ and $R^* = \begin{bmatrix}1 & 0\end{bmatrix}$, which describe the vertical line

$$\mathscr{B}^* := \text{image}(P^*) = \ker(R^*).$$

The constraints

$$\widehat{D} = PL, \text{ with } P \in \mathbb{R}^{2\times 1},\ L \in \mathbb{R}^{1\times N} \quad \text{and} \quad R\widehat{D} = 0, \text{ with } R \in \mathbb{R}^{1\times 2},\ R \neq 0$$

are equivalent to the constraint $\operatorname{rank}(\widehat{D}) \leq 1$, which shows that the points $\{\, \widehat{d}_1, \dots, \widehat{d}_N \,\}$ being fitted exactly by a line passing through the origin is equivalent to

$$\operatorname{rank}\big(\begin{bmatrix}\widehat{d}_1 & \cdots & \widehat{d}_N\end{bmatrix}\big) \leq 1.$$

Thus, (lra$_P$) and (lra$_R$) are instances of one and the same

abstract problem: approximate the data matrix D by a low rank matrix $\widehat{D}$.

In Chapter 2, the observations made in the line fitting example are generalized to modeling of $\mathtt{q}$-dimensional data. The underlying goal is:

Given a set of points in $\mathbb{R}^{\mathtt{q}}$ (the data), find a subspace of $\mathbb{R}^{\mathtt{q}}$ of bounded dimension (a model) that has the least (2-norm) distance to the data points.

Such a subspace is a (2-norm) optimal fitting *model*. General *representations* of a subspace in $\mathbb{R}^{\mathtt{q}}$ are the kernel or the image of a matrix. The classical least squares and total least squares formulations of the data modeling problem exclude some subspaces. The equations $AX = B$ and $A = BX'$, used in the least squares and total least squares problem formulations to represent the subspace, might fail to represent the optimal solution, while the kernel and image representations do not have such deficiency. This suggests that the kernel and image representations are better suited for data modeling.

The equations $AX = B$ and $A = BX'$ were introduced from an algorithmic point of view—by using them, the data fitting problem is turned into the standard problem of solving approximately an overdetermined system of linear equations. An interpretation of these equations in the data modeling context is that in the model represented by the equation $AX = B$, the variable A is an input and the variable B is an output. Similarly, in the model represented by the equation $A = BX'$, A is an output and B is an input. The input/output interpretation has an intuitive appeal because it implies a causal dependence of the variables: the input is causing the output.

Representing the model by an equation $AX = B$ and $A = BX'$, as done in the classical approach, one a priori assumes that the optimal fitting model has a certain input/output structure. The consequences are:

- existence of exceptional (nongeneric) cases, which complicate the theory,
- ill-conditioning caused by "nearly" exceptional cases, which leads to lack of numerical robustness of the algorithms, and
- need of regularization, which leads to a change of the specified fitting criterion.

These aspects of the classical approach are generally considered as inherent to the data modeling problem. By choosing the alternative image and kernel model representations, the problem of solving approximately an overdetermined system of equations becomes a low-rank approximation problem, where the nongeneric cases (and the related issues of ill-conditioning and need of regularization) are avoided.

1.3 Overview of applications

In this section, examples of low-rank approximation drawn from different application areas are listed. The fact that a matrix constructed from exact data is low rank and the approximate modeling problem is low-rank approximation is sometimes well known (*e.g.*, in realization theory, model reduction, and approximate greatest common divisor). In other cases (*e.g.*, natural language processing and conic section fitting), the link to low-rank approximation is less well known and is not exploited.

Common pattern in data modeling

The motto of the book is:

> Behind every data modeling problem there is a (hidden) low-rank approximation problem: the model imposes relations on the data which render a matrix constructed from exact data rank deficient.

Although an exact data matrix is low rank, a matrix constructed from observed data is generically full rank due to measurement noise, unaccounted effects, and assumptions about the data generating system that are not satisfied in practice. Therefore, generically, the observed data does not have an exact low complexity model. This leads to the problem of approximate modeling, which can be formulated as a low-rank approximation problem as follows. Modify the data as little as possible, so that the matrix constructed from the modified data has a specified low rank. The modified data matrix being low rank implies that there is an exact model for the modified data. This model is by definition an approximate model for the given data. The transition from exact to approximate modeling is an important step in building a coherent theory for data modeling and is emphasized in this book.

In all applications, the exact modeling problem is discussed before the practically more important approximate modeling problem. This is done because 1) exact modeling is simpler than approximate modeling, so that it is the right starting place, and 2) exact modeling is a part of optimal approximate modeling and suggests ways of solving such problems suboptimally. Indeed, small modifications of exact modeling algorithms lead to effective approximate modeling algorithms. Well known examples of the transition from exact to approximate modeling in systems theory are the progressions from realization theory to model reduction and from deterministic subspace identification to approximate and stochastic subspace identification.

The estimator consistency question in stochastic estimation problems corresponds to exact data modeling because asymptotically the true data generating system is recovered from observed data. Estimation with finite sample size, however, necessarily involves approximation. Thus in stochastic estimation theory there is also a step of transition from exact to approximate, see Figure 1.2.

$$\begin{tikzcd}
\text{exact deterministic} \arrow[r] \arrow[d] & \text{approximate deterministic} \arrow[d] \\
\text{exact stochastic} \arrow[r] & \text{approximate stochastic}
\end{tikzcd}$$

Fig. 1.2 Transitions among exact deterministic, approximate deterministic, exact stochastic, and approximate stochastic modeling problems. The arrows show progression from simple to complex.

> The applications can be read in any order or skipped without loss of continuity.

Applications in systems and control

Deterministic system realization and model reduction

Realization theory addresses the problem of finding a state representation of a linear time-invariant dynamical system defined by a transfer function or impulse response representation. The key result in realization theory is that a sequence

$$H = \big(H(0), H(1), \dots, H(t), \dots\big)$$

is an impulse response of a discrete-time linear time-invariant system of order $\mathtt{n}$ if and only if the two sided infinite Hankel matrix

$$\mathscr{H}(H) := \begin{bmatrix} H(1) & H(2) & H(3) & \cdots \\ H(2) & H(3) & \iddots & \\ H(3) & \iddots & & \\ \vdots & & & \end{bmatrix},$$

constructed from H has rank $\mathtt{n}$, *i.e.*,

$$\operatorname{rank}\big(\mathscr{H}(H)\big) = \text{order of a minimal realization of } H.$$

Therefore, existence of a finite dimensional realization of H (exact low complexity linear time-invariant model for H) is equivalent to rank deficiency of a Hankel matrix constructed from the data. A minimal state representation can be obtained from a rank revealing factorization of $\mathscr{H}(H)$.

When there is no exact finite dimensional realization of the data or the exact realization is of high order, one may want to find an approximate realization of a specified low order $\mathtt{n}$. These, respectively, approximate realization and model reduction problems naturally lead to *Hankel structured low-rank approximation.*

The deterministic system realization and model reduction problems are further considered in Sections 2.2, 3.1, and 4.2.

Stochastic system realization

Let y be the output of an nth order linear time-invariant system, driven by white noise (a stochastic system) and let $\mathbf{E}$ be the expectation operator. The sequence

$$R = \big(R(0), R(1), \dots, R(t), \dots\big)$$

defined by

$$R(\tau) := \mathbf{E}\big(y(t)y^\top(t-\tau)\big)$$

is called the *autocorrelation* sequence of y. Stochastic realization theory is concerned with the problem of finding a state representation of a stochastic system that could have generated the observed output y, *i.e.*, a linear time-invariant system driven by white noise, whose output correlation sequence is equal to R.

An important result in stochastic realization theory is that R is the output correlation sequence of an $\mathtt{n}$th order stochastic system if and only if the Hankel matrix $\mathscr{H}(R)$ constructed from R has rank $\mathtt{n}$, *i.e.*,

$$\operatorname{rank}\big(\mathscr{H}(R)\big) = \text{order of a minimal stochastic realization of } R.$$

Therefore, stochastic realization of a random process y is equivalent to deterministic realization of its autocorrelation sequence R. When it exists, the finite dimensional stochastic realizations can be obtained from a rank revealing factorization of the matrix $\mathscr{H}(R)$.

In practice, only a finite number of finite length realizations of the output y are available, so that the autocorrelation sequence is *estimated* from y. With an estimate $\widehat{R}$ of the autocorrelation R, the Hankel matrix $\mathscr{H}(\widehat{R})$ is almost certainly full rank, which implies that a finite dimensional stochastic realization can not be found. Therefore, the problem of finding an approximate stochastic realization occurs. This problem is again Hankel structured low-rank approximation.

System identification

Realization theory considers a *system representation problem*: pass from one representation of a system to another. Alternatively, it can be viewed as a special exact identification problem: find from impulse response data (a special trajectory of the system) a state space representation of the data generating system. The exact identification problem (also called deterministic identification problem) is to find from a general response of a system, a representation of that system. Let

$$w = \operatorname{col}(u,y), \qquad \text{where} \quad u = \big(u(1),\dots,u(T)\big) \quad \text{and} \quad y = \big(y(1),\dots,y(T)\big)$$

be an input/output trajectory of a discrete-time linear time-invariant system of order $\mathtt{n}$ with $\mathtt{m}$ inputs and $\mathtt{p}$ outputs and let $\mathtt{n}_{\max}$ be a given upper bound on $\mathtt{n}$. Then the Hankel matrix

$$\mathscr{H}_{\mathtt{n}_{\max}+1}(w) := \begin{bmatrix} w(1) & w(2) & \cdots & w(T-\mathtt{n}_{\max}) \\ w(2) & w(3) & \cdots & w(T-\mathtt{n}_{\max}+1) \\ \vdots & \vdots & & \vdots \\ w(\mathtt{n}_{\max}+1) & w(\mathtt{n}_{\max}+1) & \cdots & w(T) \end{bmatrix} \qquad (\mathscr{H}_i)$$

with $\mathtt{n}_{\max}+1$ block rows, constructed from the trajectory w, is rank deficient:

$$\operatorname{rank}\big(\mathscr{H}_{\mathtt{n}_{\max}+1}(w)\big) \le \operatorname{rank}\big(\mathscr{H}_{\mathtt{n}_{\max}+1}(u)\big) + \text{order of the system.} \qquad \text{(SYSID)}$$

Conversely, if the Hankel matrix $\mathscr{H}_{\mathtt{n}_{\max}+1}(w)$ has rank $(\mathtt{n}_{\max}+1)\mathtt{m}+\mathtt{n}$ and the matrix $\mathscr{H}_{2\mathtt{n}_{\max}+1}(u)$ is full row rank (*persistency of excitation* of u), then w is a trajectory of a controllable linear time-invariant system of order $\mathtt{n}$. Under the above assumptions, the data generating system can be identified from a rank revealing factorization of the matrix $\mathscr{H}_{\mathtt{n}_{\max}+1}(w)$.

When there are measurement errors or the data generating system is not a low complexity linear time-invariant system, the data matrix $\mathscr{H}_{\mathtt{n}_{\max}+1}(w)$ is generically full rank. In such cases, an approximate low-complexity linear time-invariant model for w can be derived by finding a Hankel structured low-rank approximation of $\mathscr{H}_{\mathtt{n}_{\max}+1}(w)$. Therefore, the Hankel structured low-rank approximation problem can be applied also for approximate system identification. Linear time-invariant system identification is a main topic of the book and appears frequently in the following chapters.

Similarly, to the analogy between deterministic and stochastic system realization, there is an analogy between deterministic and stochastic system identification. The latter analogy suggests an application of Hankel structured low-rank approximation to stochastic system identification.

Applications in computer algebra

Greatest common divisor of two polynomials

The greatest common divisor of the polynomials

$$p(z) = p_0 + p_1 z + \cdots + p_n z^n \qquad \text{and} \qquad q(z) = q_0 + q_1 z + \cdots + q_m z^m$$

is a polynomial c of maximal degree that divides both p and q, *i.e.*, a maximal degree polynomial c, for which there are polynomials r and s, such that

$$p = rc \qquad \text{and} \qquad q = sc.$$

Define the Sylvester matrix of the polynomials p and q

$$\mathscr{R}(p,q) := \begin{bmatrix} p_0 & & & q_0 & & \\ p_1 & p_0 & & q_1 & q_0 & \\ \vdots & p_1 & \ddots & \vdots & q_1 & \ddots \\ p_n & \vdots & \ddots \; p_0 & q_m & \vdots & \ddots \; q_0 \\ & p_n & p_1 & & q_m & q_1 \\ & & \ddots \; \vdots & & & \ddots \; \vdots \\ & & p_n & & & q_m \end{bmatrix} \in \mathbb{R}^{(n+m)\times(n+m)}. \qquad (\mathscr{R})$$

(By convention, in this book, all missing entries in a matrix are assumed to be zeros.) A well known fact in algebra is that the degree of the greatest common divisor of p and q is equal to the rank deficiency (co-rank) of $\mathscr{R}(p,q)$, *i.e.*,

$$\operatorname{degree}(c) = n + m - \operatorname{rank}\big(\mathscr{R}(p,q)\big). \qquad \text{(GCD)}$$

Suppose that p and q have a greatest common divisor of degree $\mathtt{d} > 0$, but the coefficients of the polynomials p and q are imprecise, resulting in perturbed polynomials p_d and q_d. Generically, the matrix $\mathscr{R}(p_\mathrm{d}, q_\mathrm{d})$, constructed from the perturbed polynomials, is full rank, implying that the greatest common divisor of p_d and q_d has degree zero. The problem of finding an *approximate common divisor* of p_d and q_d with degree $\mathtt{d}$, can be formulated as follows. Modify the coefficients of p_d and q_d, as little as possible, so that the resulting polynomials, say, $\widehat{p}$ and $\widehat{q}$ have a greatest common divisor of degree $\mathtt{d}$. This problem is a Sylvester structured low-rank approximation problem. Therefore, *Sylvester structured low-rank approximation* can be applied for computing an approximate common divisor with a specified degree. The approximate greatest common divisor $\widehat{c}$ for the perturbed polynomials p_d and q_d is the exact greatest common divisor of $\widehat{p}$ and $\widehat{q}$.

The approximate greatest common divisor problem is considered in Section 3.2.

Applications in signal processing

Array signal processing

An array of antennas or sensors is used for direction of arrival estimation and adaptive beamforming. Consider $\mathtt{q}$ antennas in a fixed configuration and a wave propagating from distant sources, see Figure 1.3.

Consider, first, the case of a single source. The source intensity ℓ_1 (the signal) is a function of time. Let $w(t) \in \mathbb{R}^{\mathtt{q}}$ be the response of the array at time t (w_i being the response of the ith antenna). Assuming that the source is far from the array (relative to the array's length), the array's response is proportional to the source intensity

$$w(t) = p_1 \ell_1(t - \tau_1),$$

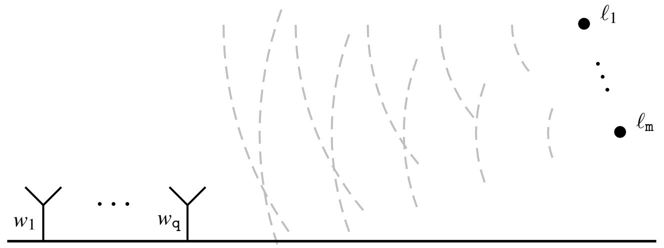

Fig. 1.3 Antenna array processing setup.

where τ_1 is the time needed for the wave to travel from the source to the array and $p_1 \in \mathbb{R}^{\mathtt{q}}$ is the array's response to the source emitting at a unit intensity. The vector p_1 depends only on the array geometry and the source location and is therefore constant in time. Measurements of the antenna at time instants $t = 1,\dots,T$ give a data matrix

$$D := \begin{bmatrix} w(1) & \cdots & w(T) \end{bmatrix} = p_1 \underbrace{\begin{bmatrix} \ell_1(1-\tau) & \cdots & \ell_1(T-\tau) \end{bmatrix}}_{\ell_1} = p_1 \ell_1,$$

which has rank equal to one.

Consider now $\mathtt{m} < \mathtt{q}$ distant sources emitting with intensities $\ell_1,\dots,\ell_\mathtt{m}$. Let p_k be the response of the array to the kth source emitting alone with unit intensity. Assuming that the array responds linearly to a mixture of sources, we have

$$D = \begin{bmatrix} w(1) & \cdots & w(T) \end{bmatrix} = \sum_{k=1}^{\mathtt{m}} p_k \underbrace{\begin{bmatrix} \ell_k(1-\tau_k) & \cdots & \ell_k(T-\tau_k) \end{bmatrix}}_{\ell_k} = PL,$$

where $P := \begin{bmatrix} p_1 & \cdots & p_\mathtt{m} \end{bmatrix}$, $L := \operatorname{col}(\ell_1,\dots,\ell_\mathtt{m})$, and τ_k is the delay of the wave coming from the kth source. This shows that the rank of D is less than or equal to the number of sources $\mathtt{m}$. If the number of sources $\mathtt{m}$ is less than the number of antennas $\mathtt{q}$ and $\mathtt{m}$ is less than the number of samples T, the sources intensities $\ell_1,\dots,\ell_\mathtt{m}$ are linearly independent, and the unit intensity array patterns $p_1,\dots,p_\mathtt{m}$ are linearly independent, then we have that

$$\operatorname{rank}(D) = \text{the number of sources transmitting to the array.}$$

Moreover, the factors P and L in a rank revealing factorization PL of D carry information about the source locations.

With noisy observations, the matrix D is generically a full rank matrix. Then, assuming that the array's geometry is known, low-rank approximation can be used to estimate the number of sources and their locations.

Applications in chemometrics

Multivariate calibration

A basic problem in chemometrics, called multivariate calibration, is identification of the number and type of chemical components from spectral measurements of mixtures of these components. Let $p_k \in \mathbb{R}^{\mathtt{q}}$ be the spectrum of the kth component at $\mathtt{q}$ predefined frequencies. Under a linearity assumption, the spectrum of a mixture of $\mathtt{m}$ components with concentrations $\ell_1,\dots,\ell_{\mathtt{m}}$ is $d = P\ell$, where $P := \begin{bmatrix} p_1 & \cdots & p_{\mathtt{m}} \end{bmatrix}$ and $\ell = \operatorname{col}(\ell_1,\dots,\ell_{\mathtt{m}})$. Given N mixtures of the components with vectors of concentrations $\ell^{(1)},\dots,\ell^{(N)}$, the matrix of the corresponding spectra $d_1,\dots,d_N$ is

$$D := \begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix} = \sum_{k=1}^{\mathtt{m}} p_k \underbrace{\begin{bmatrix} \ell_k^{(1)} & \cdots & \ell_k^{(N)} \end{bmatrix}}_{\ell_k} = PL. \qquad \text{(RRF)}$$

Therefore, the rank of D is less than or equal to the number of components $\mathtt{m}$. Assuming that $\mathtt{q} > \mathtt{m}$, $N > \mathtt{m}$, the spectral responses $p_1,\dots,p_{\mathtt{m}}$ of the components are linearly independent, and the concentration vectors $\ell_1,\dots,\ell_{\mathtt{m}}$ are linearly independent, we have

$$\operatorname{rank}(D) = \text{the number of chemical components in the mixtures.}$$

The factors P and L in a rank revealing factorization PL of D carry information about the components' spectra and the concentrations of the components in the mixtures. Noisy spectral observations lead to a full rank matrix D, so that low-rank approximation can be used to estimate the number of chemical components, their concentrations, and spectra.

Applications in psychometrics

Factor analysis

The psychometric data is test scores and biometrics of a group of people. The test scores can be organized in a data matrix D, whose rows correspond to the scores and the columns correspond to the group members. Factor analysis is a popular method that explains the data as a linear combination of a small number of abilities of the group members. These abilities are called *factors* and the weights by which they are combined in order to reproduce the data are called *loadings*. Factor analysis is based on the assumption that the exact data matrix is low rank with rank being equal to the number of factors. Indeed, the factor model can be written as $D = PL$, where the columns of P correspond to the factors and the rows of L correspond to the loadings. In practice, the data matrix is full rank because the factor model is an

idealization of the way test data is generated. Despite the fact that the factor model is a simplification of the reality, it can be used as an approximation of the way humans perform on tests. low-rank approximation then is a method for deriving optimal in a specified sense approximate psychometric factor models.

The factor model, explained above, is used to assess candidates at the US universities. An important element of the acceptance decision in US universities for undergraduate study is the Scholastic Aptitude Test, and for postgraduate study, the Graduate Record Examination. These tests report three independent scores: writing, mathematics, and critical reading for the Scholastic Aptitude Test; and verbal, quantitative, and analytical for the Graduate Record Examination. The three scores assess what are believed to be the three major factors for, respectively, undergraduate and postgraduate academic performance. In other words, the premise on which the tests are based is that the ability of a prospective student to do undergraduate and postgraduate study is predicted well by a combination of the three factors. Of course, in different areas of study, the weights by which the factors are taken into consideration are different. Even in pure subjects, such as mathematics, however, the verbal as well as quantitative and analytical ability play a role.

> Many graduate-school advisors have noted that an applicant for a mathematics fellowship with a high score on the verbal part of the Graduate Record Examination is a better bet as a Ph.D. candidate than one who did well on the quantitative part but badly on the verbal.
>
> Halmos (1985, page 5)

Applications in machine learning

Natural language processing

Latent semantic analysis is a method in natural language processing for document classification, search by keywords, synonymy and polysemy detection, *etc*. Latent semantic analysis is based on low-rank approximation and fits into the pattern of the other methods reviewed here:

1. An exact data matrix is rank deficient with rank related to the complexity of the data generating model.
2. A noisy data matrix is full rank and, for the purpose of approximate modeling, it is approximated by a low rank matrix.

Consider N documents, involving $\mathtt{q}$ terms and $\mathtt{m}$ concepts. If a document belongs to the kth concept only, it contains the ith term with frequency p_{ik}, resulting in the vector of term frequencies $p_k := \operatorname{col}(p_{1k},\dots,p_{\mathtt{q}k})$, related to the kth concept. The latent semantic analysis model assumes that if a document involves a mixture of the concepts with weights $\ell_1,\dots,\ell_{\mathtt{m}}$ (ℓ_k indicates the relevance of the kth concept to the document), then the vector of term frequencies for that document is

$$d = P\ell, \qquad \text{where} \quad P := \begin{bmatrix} p_1 & \cdots & p_{\mathtt{m}} \end{bmatrix} \quad \text{and} \quad \ell = \operatorname{col}(\ell_1,\dots,\ell_{\mathtt{m}}).$$

Let d_j be the vector of term frequencies, related to the jth document and let $\ell_k^{(j)}$ be the relevance of the kth concept to the jth document. Then, according to the latent semantic analysis model, the term–document frequencies for the N documents form a data matrix, satisfying (RRF). Therefore, the rank of the data matrix is less than or equal to the number of concepts $\mathtt{m}$. Assuming that $\mathtt{m}$ is smaller than the number of terms $\mathtt{q}$, $\mathtt{m}$ is smaller than the number of documents N, the term frequencies $p_1, \dots, p_{\mathtt{m}}$ are linearly independent, and the relevance of concepts $\ell_1, \dots, \ell_{\mathtt{m}}$ are linearly independent, we have that

$$\operatorname{rank}(D) = \text{the number of concepts related to the documents.}$$

The factors P and L in a rank revealing factorization PL of D carry information about the relevance of the concepts to the documents and the term frequencies related to the concepts.

The latent semantic analysis model is not satisfied exactly in practice because the notion of (small number of) concepts related to (many) documents is an idealization. Also the linearity assumption is not likely to hold in practice. In reality the term–document frequencies matrix D is full rank indicating that the number of concepts is equal to either the number of terms or the number of documents. low-rank approximation, however, can be used to find a small number of concepts that explain approximately the term–documents frequencies via the model (RRF). Subsequently, similarity of documents can be evaluated in the concepts space, which is a low dimensional vector space. For example, the j_1th and j_2th documents are related if they have close relevance $\ell_k^{(j_1)}$ and $\ell_k^{(j_2)}$ to all concepts $k = 1, \dots, \mathtt{m}$. This gives a way to classify the documents. Similarly, terms can be clustered in the concepts space by looking at the rows of the P matrix. Nearby rows of P correspond to terms that are related to the same concepts. (Such terms are likely to be synonymous.) Finally, a search for documents by keywords can be done by first translating the keywords to a vector in the concepts space and then finding a nearby cluster of documents to this vector. For example, if there is a single keyword, which is the ith term, then the ith row of the P matrix shows the relevant combination of concepts for this search.

Recommender system

The main issue underlying the abstract low-rank approximation problem and the applications reviewed up to now is data approximation. In the recommender system problem, the main issue is the one of *missing data*: given ratings of some items by some users, infer the missing ratings. Unique recovery of the missing data is impossible without additional assumptions. The underlying assumption in many recommender system problems is that the complete matrix of the ratings is of low rank.

Consider $\mathtt{q}$ items and N users and let d_{ij} be the rating of the ith item by the jth user. As in the psychometrics example, it is assumed that there is a "small" number $\mathtt{m}$ of "typical" (or characteristic, or factor) users, such that all user ratings can be obtained as linear combinations of the ratings of the typical users. This implies that

the complete matrix $D = \begin{bmatrix} d_{ij} \end{bmatrix}$ of the ratings has rank $\mathtt{m}$, *i.e.*,

$$\operatorname{rank}(D) = \text{number of "typical" users.}$$

Then exploiting the prior knowledge that the number of "typical" users is small, the missing data recovery problem can be posed as the following matrix completion problem

$$\begin{array}{lll} \text{minimize} & \text{over } \widehat{D} & \operatorname{rank}(\widehat{D}) \\ \text{subject to} & \widehat{D}_{ij} = D_{ij} & \text{for all } (i,j), \text{ where } D_{ij} \text{ is given.} \end{array} \qquad \text{(MC)}$$

This gives a procedure for solving the exact modelling problem (the given elements of D are assumed to be exact). The corresponding solution method can be viewed as the equivalent of the rank revealing factorization problem in exact modeling problems, for the case of complete data.

Of course, the rank minimization problem (MC) is much harder to solve than the rank revealing factorization problem. Moreover, theoretical justification and additional assumptions (about the number and distribution of the given elements of D) are needed for a solution $\widehat{D}$ of (MC) to be unique and to coincide with the complete true matrix D. It turns out, however, that under certain specified assumptions exact recovery is possible by solving the convex optimization problem obtained by replacing $\operatorname{rank}(\widehat{D})$ in (MC) with the nuclear norm

$$\|\widehat{D}\|_* := \text{sum of the singular values of } \widehat{D}.$$

The importance of the result is that under the specified assumptions the hard problem (MC) can be solved efficiently and reliably by convex optimization methods.

In real-life application of recommender systems, however, the additional problem of data approximation occurs. In this case the constraint $\widehat{D}_{ij} = D_{ij}$ of (MC) has to be relaxed, *e.g.*, replacing it by

$$\widehat{D}_{ij} = D_{ij} + \Delta D_{ij},$$

where ΔD_{ij} are corrections, accounting for the data uncertainty. The corrections are additional optimization variables. Taking into account the prior knowledge that the corrections are small, a term $\lambda \|\Delta D\|_{\mathrm{F}}$ is added in the cost function. The resulting matrix approximation problem is

$$\begin{array}{lll} \text{minimize} & \text{over } \widehat{D} \text{ and } \Delta D & \operatorname{rank}(\widehat{D}) + \lambda \|\Delta D\|_{\mathrm{F}} \\ \text{subject to} & \widehat{D}_{ij} = D_{ij} + \Delta D_{ij} & \text{for all } (i,j), \text{ where } D_{ij} \text{ is given.} \end{array} \qquad \text{(AMC)}$$

In a stochastic setting the term $\lambda \|\Delta D\|_{\mathrm{F}}$ corresponds to the assumption that the true data D is perturbed with noise that is zero mean, Gaussian, independent, and with equal variance.

Again the problem can be relaxed to a convex optimization problem by replacing rank with nuclear norm. The choice of the λ parameter reflects the trade-off between complexity (number of identified "typical" users) and accuracy (size of the correction ΔD) and depends in the stochastic setting on the noise variance.

Nuclear norm and low-rank approximation methods for estimation of missing values are developed in Sections 3.3 and 5.1.

Multidimensional scaling

Consider a set of N points in the plane

$$\mathscr{X} := \{x_1, \dots, x_N\} \subset \mathbb{R}^2$$

and let d_{ij} be the squared distance from x_i to x_j, *i.e.*,

$$d_{ij} := \|x_i - x_j\|_2^2.$$

The $N \times N$ matrix $D = \begin{bmatrix} d_{ij} \end{bmatrix}$ of the pair-wise distances, called in what follows the distance matrix (for the set of points $\mathscr{X}$), has rank at most 4. Indeed,

$$d_{ij} = (x_i - x_j)^\top (x_i - x_j) = x_i^\top x_i - 2x_i^\top x_j + x_j^\top x_j,$$

so that

$$D = \underbrace{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \begin{bmatrix} x_1^\top x_1 & \cdots & x_N^\top x_N \end{bmatrix}}_{\text{rank} \leq 1} - 2 \underbrace{\begin{bmatrix} x_1^\top \\ \vdots \\ x_N^\top \end{bmatrix} \begin{bmatrix} x_1 & \cdots & x_N \end{bmatrix}}_{\text{rank} \leq 2} + \underbrace{\begin{bmatrix} x_1^\top x_1 \\ \vdots \\ x_N^\top x_N \end{bmatrix} \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}}_{\text{rank} \leq 1}. \qquad (*)$$

The localization problem from pair-wise distances is: given the distance matrix D, find the locations $\{x_1, \dots, x_N\}$ of the points up to a rigid transformation, *i.e.*, up to translation, rotation, and reflection of the points. Note that rigid transformations preserve the pair-wise distances, so that the distance matrix D alone is not sufficient to locate the points uniquely.

With exact data, the problem can be posed and solved as a rank revealing factorization problem $(*)$. With noisy measurements, however, the matrix D is generically full rank. In this case, the relative (up to rigid transformation) point locations can be *estimated* by approximating D by a rank-4 matrix $\widehat{D}$. In order to be a valid distance matrix, however, $\widehat{D}$ must have the structure

$$\widehat{D} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \begin{bmatrix} \widehat{x}_1^\top \widehat{x}_1 & \cdots & \widehat{x}_N^\top \widehat{x}_N \end{bmatrix} - 2\widehat{X}^\top \widehat{X} + \begin{bmatrix} \widehat{x}_1^\top \widehat{x}_1 \\ \vdots \\ \widehat{x}_N^\top \widehat{x}_N \end{bmatrix} \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}, \qquad \text{(MDS)}$$

for some $\widehat{X} = \begin{bmatrix} \widehat{x}_1 & \cdots & \widehat{x}_N \end{bmatrix}$, *i.e.*, the estimation problem is a *bilinearly structured low-rank approximation problem.*

Microarray data analysis

The measurements of a microarray experiment are collected in a $\mathtt{q} \times N$ real matrix D—rows correspond to genes and columns correspond to time instances. The element d_{ij} is the *expression level* of the ith gene at the jth moment of time. The rank of D is equal to the number of *transcription factors* that regulate the gene expression levels

$$\text{rank}(D) = \text{number of transcription factors.}$$

In a rank revealing factorization $D = PL$, the jth column of L is a vector of intensities of the transcription factors at time j, and the ith row of P is a vector of sensitivities of the ith gene to the transcription factors. For example, p_{ij} equal to zero means that the jth transcription factor does not regulate the ith gene.

An important problem in bioinformatics is to discover what transcription factors regulate a particular gene and what their time evaluations are. This problem amounts to computing an (approximate) factorization PL of the matrix D. The need of approximation comes from:

1. inability to account for all relevant transcription factors (therefore accounting only for a few dominant ones), and
2. measurement errors occurring in the collection of the data.

Often it is known a priori that certain transcription factors do not regulate certain genes. This implies that certain elements of the sensitivity matrix P are known to be zeros. In addition, the transcription factor activities are modeled to be nonnegative, smooth, and periodic functions of time. Where transcription factors down regulate a gene, the elements of P have to be negative to account for this. In Section 5.4, this prior knowledge is formalized as constraints in a low rank matrix approximation problem and optimization methods for solving the problem are developed.

Applications in computer vision

Conic section fitting

In the applications reviewed so far, the low-rank approximation problem was applied to *linear* data modeling. Nonlinear data modeling, however, can also be formulated as a low-rank approximation problem. The key step—"linearizing" the problem—involves preprocessing the data by a nonlinear function defining the model structure. In the machine learning literature, where nonlinear data modeling is a common practice, the nonlinear function is called the *feature map* and the resulting modeling methods are referred to as *kernel methods*.

As a specific example, consider the problem of fitting data by a conic section, *i.e.*, given a set of points in the plane

$$\{d_1, \dots, d_N\} \subset \mathbb{R}^2, \qquad \text{where} \quad d_j = \text{col}(x_j, y_j),$$

find a conic section

$$\mathscr{B}(A,b,c) := \{\, d \in \mathbb{R}^2 \mid d^\top A d + b^\top d + c = 0 \,\}. \qquad (\mathscr{B}(A,b,c))$$

that fits them. Here A is a 2×2 symmetric matrix, b is a 2×1 vector, and c is a scalar. A, b, and c are parameters defining the conic section. In order to avoid a trivial case $\mathscr{B} = \mathbb{R}^2$, it is assumed that at least one of the parameters A, b, or c is nonzero. The representation ($\mathscr{B}(A,b,c)$) is called implicit representation, because it imposes a relation (implicit function) on the elements x and y of d.

Defining the parameter vector

$$\theta := \begin{bmatrix} a_{11} & 2a_{12} & b_1 & a_{22} & b_2 & c \end{bmatrix},$$

and the extended data vector

$$d_{\text{ext}} := \operatorname{col}(x^2, xy, x, y^2, y, 1), \qquad (d_{\text{ext}})$$

we have

$$d \in \mathscr{B}(\theta) = \mathscr{B}(A,b,c) \quad \iff \quad \theta d_{\text{ext}} = 0.$$

(In the machine learning terminology, the map $d \mapsto d_{\text{ext}}$, defined by (d_{ext}), is the feature map for the conic section model.) Consequently, all data points $d_1, \ldots, d_N$ are fitted by the model if

$$\theta \underbrace{\begin{bmatrix} d_{\text{ext},1} & \cdots & d_{\text{ext},N} \end{bmatrix}}_{D_{\text{ext}}} = 0 \quad \iff \quad \operatorname{rank}(D_{\text{ext}}) \leq 5. \qquad \text{(CSF)}$$

Therefore, for $N > 5$ data points, exact fitting is equivalent to rank deficiency of the extended data matrix D_{ext}. For $N < 5$ data points, there is nonunique exact fit independently of the data. For $N = 5$ different points, the exact fitting conic section is unique, see Figure 1.4.

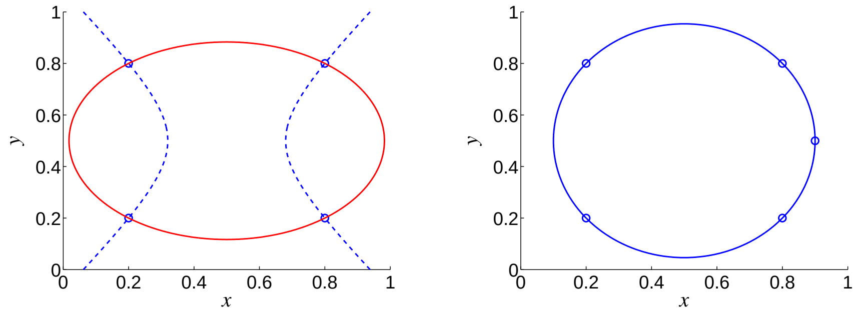

Fig. 1.4 Conic section fitting. Left: $N = 4$ points (circles) have nonunique fit (two fits are shown in the figure with solid and dashed lines). Right: $N = 5$ different points have a unique fit (solid line).

With $N > 5$ noisy data points, the extended data matrix D_{ext} is generically full rank, so that an exact fit does not exists. A problem called geometric fitting is to minimize the sum of squared distances from the data points to the conic section. The problem is equivalent to *quadratically structured low-rank approximation*.

Generalization of the conic section fitting problem to algebraic curve fitting and solution methods for the latter are presented in Chapter 6.

Exercise 1.1. Find and plot another conic section that fits the points

$$d_1 = \begin{bmatrix} 0.2 \\ 0.2 \end{bmatrix}, \quad d_2 = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix}, \quad d_3 = \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix}, \quad \text{and} \quad d_4 = \begin{bmatrix} 0.8 \\ 0.8 \end{bmatrix},$$

in Figure 1.4, left. □

Exercise 1.2. Find the parameters $(A, b, 1)$ in the representation ($\mathscr{B}(A,b,c)$) of the ellipse in Figure 1.4, right. The data points are:

$$d_1 = \begin{bmatrix} 0.2 \\ 0.2 \end{bmatrix}, \quad d_2 = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix}, \quad d_3 = \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix}, \quad d_4 = \begin{bmatrix} 0.8 \\ 0.8 \end{bmatrix}, \quad \text{and} \quad d_5 = \begin{bmatrix} 0.9 \\ 0.5 \end{bmatrix}, \qquad \square$$

(Answer: $A = \left[\begin{smallmatrix} 3.5156 & 0 \\ 0 & 2.7344 \end{smallmatrix}\right]$, $b = \left[\begin{smallmatrix} -3.5156 \\ -2.7344 \end{smallmatrix}\right]$)

Fundamental matrix estimation

A scene is captured by two cameras at fixed locations (stereo vision) and N matching pairs of points

$$\{u_1, \ldots, u_N\} \subset \mathbb{R}^2 \quad \text{and} \quad \{v_1, \ldots, v_N\} \subset \mathbb{R}^2$$

are located in the resulting images. Corresponding points u and v of the two images satisfy what is called an *epipolar constraint*

$$\begin{bmatrix} v^\top & 1 \end{bmatrix} F \begin{bmatrix} u \\ 1 \end{bmatrix} = 0, \qquad \text{for some } F \in \mathbb{R}^{3\times 3}, \text{ with } \operatorname{rank}(F) = 2. \qquad \text{(EPI)}$$

The 3×3 matrix $F \neq 0$, called the *fundamental matrix*, characterizes the relative position and orientation of the cameras and does not depend on the selected pairs of points. Estimation of F from data is a necessary calibration step in many computer vision methods.

The epipolar constraint (EPI) is linear in F. Indeed, defining

$$d_{\text{ext}} := \begin{bmatrix} u_x v_x & u_x v_y & u_x & u_y v_x & u_y v_y & u_y & v_x & v_y & 1 \end{bmatrix}^\top \in \mathbb{R}^9, \qquad (d'_{\text{ext}})$$

where $u = \operatorname{col}(u_x, u_y)$ and $v = \operatorname{col}(v_x, v_y)$, (EPI) can be written as

$$\operatorname{vec}^\top(F) d_{\text{ext}} = 0.$$

Note that, as in the application for conic section fitting, the original data (u, v) is mapped to an extended data vector d_{ext} via a nonlinear function (a feature map). In this case, however, the function is *bilinear*.

Taking into account the epipolar constraints for all data points, we obtain the matrix equation

$$\operatorname{vec}^{\top}(F) D_{\text{ext}} = 0, \qquad \text{where} \quad D_{\text{ext}} := \begin{bmatrix} d_{\text{ext},1} & \cdots & d_{\text{ext},N} \end{bmatrix}. \tag{FME}$$

The rank constraint imposed on F implies that F is a nonzero matrix. Therefore, by (FME), for $N \geq 8$ data points, the extended data matrix D_{ext} is rank deficient. Moreover, the fundamental matrix F can be reconstructed up to a scaling factor from a vector in the left kernel of D_{ext}.

Noisy data with $N \geq 8$ data points generically gives rise to a full rank extended data matrix D_{ext}. The estimation problem is a *bilinearly structured low-rank approximation* problem with an additional constraint that $\operatorname{rank}(F) = 2$.

Summary of applications

Table 1.1 summarized the reviewed applications: given data, data matrix constructed from the original data, structure of the data matrix, and meaning of the rank of the data matrix in the context of the application. More applications are mentioned in the notes and references section in the end of the chapter.

1.4 Overview of algorithms

The rank constraint in the low-rank approximation problem corresponds to the constraint in the data modeling problem that the data is fitted exactly by a linear model of bounded complexity. Therefore, the question of representing the rank constraint in the low-rank approximation problem corresponds to the question of choosing the model representation in the data fitting problem. Different representations lead to

- *optimization problems*, the relation among which may not be obvious;
- *algorithms*, which may have different convergence properties and efficiency; and
- *numerical software*, which may have different numerical robustness.

The virtues of the abstract, representation free, low-rank approximation problem formulation, are both *conceptual:* it clarifies the equivalence among different parameter optimization problems, and *practical:* it shows various ways of formulating one and the same high level data modeling problem as parameter optimization problems. On the conceptual level, the low-rank approximation problem formulation shows what one aims to achieve without a reference to implementation details. In particular, the model representation is such a detail, which is not needed for a

Table 1.1 Meaning of the rank of the data matrix in the applications.

application	data	data matrix	structure	rank =	ref.
approximate realization	impulse response H	$\mathscr{H}(H)$	Hankel	system's order	Sec. 2.2 Sec. 3.1 Sec. 4.2
stochastic realization	autocorrelation function R	$\mathscr{H}(R)$	Hankel	system's order	—
system identification	trajectory w of the system	$\mathscr{H}_{\mathtt{n}_{\max}+1}(w)$	Hankel	(SYSID)	Sec. 2.3 Sec. 4.3
approximate GCD	polynomials p_{d} and q_{d}	$\mathscr{R}(p_{\text{d}}, q_{\text{d}})$	Sylvester	(GCD)	Sec. 3.2
array processing	array response $\big(w(1), \ldots, w(T)\big)$	$\begin{bmatrix} w(1) & \cdots & w(T) \end{bmatrix}$	unstructured	# of signal sources	—
multivariate calibration	spectral responses $\{d_1, \ldots, d_N\} \subset \mathbb{R}^{\mathtt{q}}$	$\begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix}$	unstructured	# of chemical components	—
factor analysis	test scores d_{ij}	$[d_{ij}]$	unstructured	# of factors	—
natural language processing	term–document frequencies d_{ij}	$[d_{ij}]$	unstructured	# of concepts	—
recommender system	some ratings d_{ij}	$[d_{ij}]$	unstructured missing data	# of tastes	Sec. 3.3 Sec. 5.1
multidimensional scaling	pair-wise distances d_{ij}	$[d_{ij}]$	(MDS)	$\dim(x) + 2$	—
microarray data analysis	gene expression levels d_{ij}	$[d_{ij}]$	unstructured	# of transcript. factors	Sec. 5.4
conic section fitting	points $\{d_1, \ldots, d_N\} \subset \mathbb{R}^2$	(d_{ext}), (CSF)	quadratic	5	Ch. 6
fundamental matrix estimation	points $u_j, v_j \in \mathbb{R}^2$	(d'_{ext}), (FME)	bilinear	6	—

high level formulation of data modeling problems. As discussed next, however, the representation is unavoidable when one solves the problem analytically or numerically.

On the practical level, the low rank problem formulation allows one to translate the abstract data modeling problem to different concrete parametrized problems by choosing the model representation. Different representations naturally lend themselves to different analytical and numerical methods. For example, a controllable linear time-invariant system can be represented by a transfer function, state space, convolution, *etc.* representations. The analysis tools related to these representations are rather different and, consequently, the obtained solutions differ despite of the fact that they solve the same abstract problem. Moreover, the parameter optimization problems, resulting from different model representations, lead to algorithms and numerical implementations, whose robustness properties and computational efficiency differ. Although, often in practice, there is no universally "best" algorithm or software implementation, having a wider set of available options is an advantage.

Independent of the choice of the rank representation only a few special low-rank approximation problems have analytic solutions. So far, the most important special case with an analytic solution is the unstructured low-rank approximation in the Frobenius norm. The solution in this case can be obtained from the singular value decomposition of the data matrix (Eckart–Young–Mirsky theorem). Extensions of this basic solution are problems known as generalized and restricted low-rank approximation, where some columns or, more generally submatrices of the approximation, are constrained to be equal to given matrices. The solutions to these problems are given by, respectively, the generalized and restricted singular value decompositions. Another example of low-rank approximation problem with analytic solution is the circulant structured low-rank approximation, where the solution is expressed in terms of the discrete Fourier transform of the data.

In general, low-rank approximation problems are NP-hard. There are three fundamentally different solution approaches for the general low-rank approximation problem:

- heuristic methods based on convex relaxations,
- local optimization methods, and
- global optimization methods.

From the class of heuristic methods the most popular ones are the subspace methods. The approach used in the subspace type methods is to relax the difficult low-rank approximation problem to a problem with an analytic solution in terms of the singular value decomposition, *e.g.*, ignore the structure constraint of a structured low-rank approximation problem. The subspace methods are found to be very effective in model reduction, system identification, and signal processing. The class of the subspace system identification methods is based on the unstructured low-rank approximation in the Frobenius norm (*i.e.*, singular value decomposition) while the original problems are Hankel structured low-rank approximation.

The methods based on local optimization split into two main categories:

- *alternating projections* and
- *variable projections*

type algorithms. Both alternating projections and variable projections exploit the bilinear structure of the low-rank approximation problems.

In order to explain the ideas underlining the alternating projections and variable projections methods, consider the optimization problem

$$\text{minimize} \quad \text{over } P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}} \text{ and } L \in \mathbb{R}^{\mathtt{m}\times N} \quad \|D - PL\|_{\mathrm{F}}^2 \tag{LRA$_P$}$$

corresponding to low-rank approximation with an image representation of the rank constraint. The term PL is bilinear in the optimization variables P and L, so that for a fixed P, (LRA$_P$) becomes a linear least squares problem in L and vice verse, for a fixed L, (LRA$_P$) becomes a linear least squares problem in P. This suggests

an iterative algorithm starting from an initial guess for P and L and alternatively solves the problem with one of the variables fixed. Since each step is a projection operation the method has the name alternating projections. It is globally convergent to a locally optimal solution of (LRA$_P$) with a linear convergence rate.

The bilinear nature of (LRA$_P$) implies that for a fixed P the problem can be solved in closed form with respect to L. This gives us an equivalent cost function depending on P. Subsequently, the original problem can be solved by minimizing the equivalent cost function over P. Of course, the latter problem is a nonlinear optimization problem. Standard local optimization methods can be used for this purpose. The elimination of the L variable from the problem has the advantage of reducing the number of optimization variables, thus simplifying the problem. Evaluation of the cost function for a given P is a projection operation. In the course of the nonlinear minimization over P, this variable changes, thus the name of the method—variable projections.

In the statistical literature, the alternating projections algorithm is given the interpretation of *expectation maximization*. The problem of computing the optimal approximation $\widehat{D} = PL$, given P is the expectation step and the problem of computing P, given L is the maximization step of the expectation maximization procedure.

1.5 Literate programming

At first, I thought programming was primarily analogous to musical composition—to the creation of intricate patterns, which are meant to be performed. But lately I have come to realize that a far better analogy is available: Programming is best regarded as the process of creating *works of literature*, which are meant to be read.

Knuth (1992, page ix)

The ideas presented in the book are best expressed as algorithms for solving data modeling problems. The algorithms, in turn, are practically useful when implemented in ready-to-use software. The gap between the theoretical discussion of data modeling methods and the practical implementation of these methods is bridged by using a literate programming style. The software implementation (MATLAB code) is interwoven in the text, so that the full implementation details are available in a human readable format and they come in the appropriate context of the presentation.

A literate program is composed of interleaved code segments, called chunks, and text. The program can be split into chunks in any way and the chunks can be presented in any order, deemed helpful for the understanding of the program. This allows us to focus on the logical structure of the program rather than the way a computer executes it. The actual computer executable code is *tangled* from a *web* of the code chunks by skipping the text and putting the chunks in the right order. In addition, literate programming allows us to use a powerful typesetting system such as LaTeX (rather than plain text) for the documentation of the code.

The noweb system for literate programming is used. Its main advantage over alternative systems is independence of the programming language being used.

Next, some typographic conventions are explained. The code is typeset in `small true type` font and consists of a number of code chunks. The code chunks begin with tags enclosed in angle brackets (*e.g.*, ⟨*code tag*⟩) and are sequentially numbered by the page number and a letter identifying them on the page. Thus the chunk's identification number (given to the left of the tag) is also used to locate the chunk in the text. For example,

25a ⟨*Print a figure* 25a⟩≡

```
function print_fig(file_name)
xlabel('x'), ylabel('y'), title('t'), set(gca, 'fontsize', 25)
eval(sprintf('print -depsc %s.eps', file_name));
```

Defines:
`print_fig`, used in chunks 103a, 116b, 128, 129g, 165c, 195a, 215, and 223c.

(a function exporting the current figure to an encapsulated postscript file with a specified name, using default labels and font size) has identification number 25a, locating the code as being on page 25.

If a chunk is included in, is a continuation of, or is continued by other chunk(s), its definition has references to the related chunk(s). The sintax convention for doing this is best explained by an example.

Example: block Hankel matrix constructor

Consider the implementation of the (block) Hankel matrix constructor

$$\mathscr{H}_{i,j}(w) := \begin{bmatrix} w(1) & w(2) & \cdots & w(j) \\ w(2) & w(3) & \cdots & w(j+1) \\ \vdots & \vdots & & \vdots \\ w(i) & w(i+1) & \cdots & w(j+i-1) \end{bmatrix}, \qquad (\mathscr{H}_{i,j})$$

where

$$w = \big(w(1),\ldots,w(T)\big), \qquad \text{with} \quad w(t) \in \mathbb{R}^{\mathtt{q}\times N}.$$

The definition of the function, showing its input and output arguments, is

25b ⟨*Hankel matrix constructor* 25b⟩≡ 26b▷

```
function H = blkhank(w, i, j)
```

Defines:
`blkhank`, used in chunks 78b, 81, 90c, 111b, 116a, 118b, 119b, 122b, 127b, 129b, and 213.

(The reference to the right of the identification tag shows that the definition is continued in chunk number 26b.) The third input argument of `blkhank`—the number of block columns `j` is optional. Its default value is maximal number of block columns

$$j = T - i + 1.$$

26a ⟨*optional number of (block) columns* 26a⟩≡ (26)

```
if nargin < 3 | isempty(j), j = T - i + 1; end
if j <= 0, error('Not enough data.'), end
```

(The reference to the right of the identification tag now shows that this chunk is included in other chunks.)

Two cases are distinguished, depending on whether w is a vector ($N = 1$) or matrix ($N > 1$) valued trajectory.

26b ⟨*Hankel matrix constructor* 25b⟩+≡ ◁25b

```
if length(size(w)) == 3
  ⟨matrix valued trajectory w 26c⟩
else
  ⟨vector valued trajectory w 26f⟩
end
```

(The reference to the right of the identification tag shows that this chunk is a continuation of chunk 25b and is not followed by other chunks. Its body includes chunks 26c and 26f.)

- If w is a matrix valued trajectory, the input argument `w` should be a 3 dimensional tensor, constructed as follows:

$$\mathtt{w}(:,:,\mathtt{t}) = w(t) \qquad (\mathtt{w})$$

26c ⟨*matrix valued trajectory w* 26c⟩≡ (26b) 26d▷

```
[q, N, T]  = size(w);
⟨optional number of (block) columns 26a⟩
```

(This chunk is both included and followed by other chunks.) In this case, the construction of the block Hankel matrix $H_{i,j}(w)$ is done explicitly by a double loop:

26d ⟨*matrix valued trajectory w* 26c⟩+≡ (26b) ◁26c

```
H = zeros(i * q, j * N);
for ii = 1:i
  for jj = 1:j
    H(((ii - 1) * q + 1):(ii * q), ...
      ((jj - 1) * N + 1):(jj * N)) = w(: ,:, ii + jj - 1);
  end
end
```

- If w is a vector valued trajectory , the input argument `w` should be a matrix formed as follows $\mathtt{w}(:,\mathtt{t}) = w(t)$, however, since T must be greater than or equal to the number of variables $\mathtt{q} := \dim\big(w(t)\big)$, when `w` has more rows than columns, the input is treated as $\mathtt{w}(\mathtt{t},:) = w^\top(t)$.

26e ⟨*reshape w and define* `q`*, T* 26e⟩≡ (26f 82 89 118a 119a 121b 122a)

```
[q, T] = size(w); if T < q, w = w'; [q, T] = size(w); end
```

26f ⟨*vector valued trajectory w* 26f⟩≡ (26b) 27▷

```
⟨reshape w and define q, T 26e⟩
⟨optional number of (block) columns 26a⟩
```

The reason to consider the case of a vector valued w separately is that in this case the construction of the Hankel matrix $\mathscr{H}_{i,j}(w)$ can be done with a single loop along the block rows.

27 ⟨*vector valued trajectory w* 26f⟩+≡ (26b) ◁26f

```
  H = zeros(i * q, j);
  for ii = 1:i
    H(((ii - 1) * q + 1):(ii * q), :) = w(:, ii:(ii + j - 1));
  end
```

Since in typical situations when `blkhank` is used (system identification problems), $i \ll j$ and MATLAB, being an interpreted language, executes `for` loops slowly, the reduction to a single `for` loop along the block rows of the matrix leads to significant decrease of the execution time compared to the implementation with two nested `for` loops in the general case.

Exercise 1.3. Download and install `noweb` from

`www.cs.tufts.edu/~nr/noweb/`

Exercise 1.4. Write a literate program for constructing the Sylvester matrix $\mathscr{R}(p,q)$, defined in ($\mathscr{R}$) on page 11. Use your program to find the degree `d` of the greatest common divisor of the polynomials

$$p(z) = 1 + 3z + 5z^2 + 3z^3 \qquad \text{and} \qquad q(z) = 3 + 5z + 3z^2 + z^3.$$

(Answer: $\mathtt{d} = 1$)

1.6 Notes and references

Classical and behavioral paradigms for data modeling

Methods for solving overdetermined systems of linear equations (*i.e.*, data modeling methods using the classical input/output representation paradigm) are reviewed in Appendix A. The behavioral paradigm for data modeling was put forward by Jan C. Willems in the early 80's. It became firmly established with the publication of the three part paper (Willems, 1986, 1987). Other landmark publications on the behavioral paradigm are (Willems, 1989, 1991, 2007), and the book (Polderman and Willems, 1998).

The numerical linear algebra problem of low-rank approximation is a computational tool for data modeling, which fits the behavioral paradigm as "a hand fits a glove". Historically the low-rank approximation problem is closely related to the singular value decomposition, which is a method for computing low-rank approximations and is a main tool in many algorithms for data modeling. A historical account of the development of the singular value decomposition is given in (Stewart, 1993). The Eckart–Young–Mirsky matrix low-rank approximation theorem is proven in (Eckart and Young, 1936).

Applications

For details about the realization and system identification problems, see Sections 2.2, 3.1, and 4.3. Direction of arrival and adaptive beamforming problems are discussed in (Krim and Viberg, 1996; Kumaresan and Tufts, 1983). low-rank approximation methods (alternating least squares) for estimation of mixture concentrations in chemometrics are proposed in (Wentzell et al, 1997). An early reference on the approximate greatest common divisor problem is (Karmarkar and Lakshman, 1998). Efficient optimization based methods for approximate greatest common divisor computation are discussed in Section 3.2. Other computer algebra problems that reduce to structured low-rank approximation are discussed in (Botting, 2004).

Many problems for information retrieval in machine learning, see, *e.g.*, (Bishop, 2006; Fierro and Jiang, 2005; Shawe-Taylor and Cristianini, 2004), are low-rank approximation problems and the corresponding solution techniques developed in the machine learning community are methods for solving low-rank approximation problems. For example, clustering problems have been related to low-rank approximation problems in (Ding and He, 2004; Kiers, 2002; Vichia and Saporta, 2009). Machine learning problems, however, are often posed in a stochastic estimation setting which obscures their deterministic approximation interpretation. For example, principal component analysis (Jackson, 2003; Jolliffe, 2002) and unstructured low-rank approximation with Frobenius norm are equivalent optimization problems. The principal component analysis problem, however, is motivated in a statistical setting and for this reason may be considered as a different problem. In fact, principal component analysis provides another (statistical) interpretation of the low-rank approximation problem.

The conic section fitting problem has extensive literature, see Chapter 6 and the tutorial paper (Zhang, 1997). The kernel principal component analysis method is developed in the machine learning and statistics literature (Schölkopf et al, 1999). Despite of the close relation between kernel principal component analysis and conic section fitting, the corresponding literature are disjoint.

Closely related to the estimation of the fundamental matrix problem in two-view computer vision is the shape from motion problem (Ma et al, 2004; Tomasi and Kanade, 1993).

Matrix factorization techniques have been used in the analysis of microarray data in (Alter and Golub, 2006) and (Kim and Park, 2007). Alter and Golub (2006) propose a principal component projection to visualize high dimensional gene expression data and show that some known biological aspects of the data are visible in a two dimensional subspace defined by the first two principal components.

Distance problems

The low-rank approximation problem aims at finding the "smallest" correction of a given matrix that makes the corrected matrix rank deficient. This is a special case of a distance problems: find the "nearest" matrix with a specified property to a given matrix. For an overview of distance problems, see (Higham, 1989). In (Byers, 1988), an algorithm for computing the distance of a stable matrix (Hurwitz matrix in the case of continuous-time and Schur matrix in the case of discrete-time linear time-invariant dynamical system) to the set of unstable matrices is presented. Stability radius for structured perturbations and its relation to the algebraic Riccati equation is presented in (Hinrichsen and Pritchard, 1986).

Structured linear algebra

Related to the topic of distance problems is the grand idea that the whole linear algebra (solution of systems of equations, matrix factorization, *etc*.) can be generalized to uncertain data. The uncertainty is described as structured perturbation on the data and a solution of the problem is obtained by correcting the data with a correction of the smallest size that renders the problem solvable for the corrected data. Two of the first references on the topic of structured linear algebra are (Chandrasekaran et al, 1998; El Ghaoui and Lebret, 1997).

Structured pseudospectra

Let $\lambda(A)$ be the set of eigenvalues of $A \in \mathbb{C}^{n\times n}$ and $\mathscr{M}$ be a set of structured matrices

$$\mathscr{M} := \{\, \mathscr{S}(p) \mid p \in \mathbb{R}^{n_p} \,\},$$

with a given structure specification $\mathscr{S}$. The ε-structured pseudospectrum (Graillat, 2006; Trefethen and Embree, 1999) of A is defined as the set

$$\lambda_\varepsilon(A) := \{\, z \in \mathbb{C} \mid z \in \lambda(\widehat{A}),\ \widehat{A} \in \mathscr{M}, \text{ and } \|A - \widehat{A}\|_2 \leq \varepsilon \,\}.$$

Using the structured pseudospectra, one can determine the structured distance of A to singularity as the minimum of the following optimization problem:

$$\text{minimize} \quad \text{over } \widehat{A} \quad \|A - \widehat{A}\|_2 \quad \text{subject to} \quad \widehat{A} \text{ is singular and } \widehat{A} \in \mathscr{M}.$$

This is a special structured low-rank approximation problem for squared data matrix and rank reduction by one. Related to structured pseudospectra is the structured condition number problem for a system of linear equations, see (Rump, 2003).

Statistical properties

Related to low-rank approximation are the *orthogonal regression* (Gander et al, 1994), *errors-in-variables* (Gleser, 1981), and *measurement errors* methods in the statistical literature (Carroll et al, 1995; Cheng and Van Ness, 1999). Classic papers on the univariate errors-in-variables problem are (Adcock, 1877, 1878; Koopmans, 1937; Madansky, 1959; Pearson, 1901; York, 1966). Closely related to the errors-in-variables framework for low-rank approximation is the probabilistic principal component analysis framework of (Tipping and Bishop, 1999).

Reproducible research

"An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures."
Buckheit and Donoho (1995)

The reproducible research concept is at the core of all sciences. In applied fields such as data modeling, however, algorithms' implementation, availability of data, and reproducibility of the results obtained by the algorithms on data are often neglected. This leads to a situation, described in (Buckheit and Donoho, 1995) as a scandal. See also (Kovacevic, 2007).

A quick and easy way of making computational results obtained in MATLAB reproducible is to use the function `publish`. Better still, the code and the obtained results can be presented in a literate programming style.

Literate programming

The creation of the literate programming is a byproduct of the TEX project, see (Knuth, 1984, 1992). The original system, called `web` is used for documentation of the TEX program (Knuth, 1986) and is for the Pascal language. Later a version `cweb` for the C language was developed. The `web` and `cweb` systems are followed by many other systems for literate programming that target specific languages. Unfortunately this leads to numerous literate programming dialects.

The `noweb` system for literate programming, created by N. Ramsey in the mid 90's, is not bound to any specific programming language and text processing system. A tutorial introduction is given in (Ramsey, 1994). The `noweb` syntax is also adopted in the babel part of Emacs org-mode (Dominik, 2010)—a package for keeping structured notes that includes support for organization and automatic evaluation of computer code.

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Part I
Linear modeling problems

Chapter 2
From data to models

. . . whenever we have two different representations of the same thing we can learn a great deal by comparing representations and translating descriptions from one representation into the other. Shifting descriptions back and forth between representations can often lead to insights that are not inherent in either of the representations alone.

Abelson and diSessa (1986, page 105)

Summary: In Chapter 1, the equivalence between line fitting and rank-one matrix approximation was considered. This chapter extends the equivalence to general linear static and dynamic linear time-invariant data modeling problems. First, three linear static model representations—kernel, image, and input/output—are defined and the connections among them are shown. Then, representations of linear time-invariant dynamic models are defined. Finally, exact and approximate modeling problems are related to low-rank approximation problems. In the general case of linear dynamic modeling, the problem is Hankel structured low-rank approximation.

2.1 Linear static model representations

A linear static model with $\mathtt{q}$ variables is a subspace of $\mathbb{R}^{\mathtt{q}}$. We denote the set of linear static models with $\mathtt{q}$ variables by $\mathscr{L}_0^{\mathtt{q}}$. Three basic representations of a linear static model $\mathscr{B} \subseteq \mathbb{R}^{\mathtt{q}}$ are the kernel, image, and input/output ones:

- kernel representation

$$\mathscr{B} = \ker(R) := \{\, d \in \mathbb{R}^{\mathtt{q}} \mid Rd = 0 \,\}, \qquad (\text{KER}_0)$$

  with parameter $R \in \mathbb{R}^{\mathtt{p}\times\mathtt{q}}$,
- image representation

$$\mathscr{B} = \operatorname{image}(P) := \{\, d = P\ell \in \mathbb{R}^{\mathtt{q}} \mid \ell \in \mathbb{R}^{\mathtt{m}} \,\}, \qquad (\text{IMAGE}_0)$$

  with parameter $P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}$, and
- input/output representation

$$\mathscr{B}_{\text{i/o}}(X,\Pi) := \{\, d = \Pi \operatorname{col}(u,y) \in \mathbb{R}^{\mathtt{q}} \mid u \in \mathbb{R}^{\mathtt{m}},\ y = X^\top u \,\}, \qquad (\text{I/O}_0)$$

  with parameters $X \in \mathbb{R}^{\mathtt{m}\times\mathtt{p}}$ and a $\mathtt{q}\times\mathtt{q}$ permutation matrix Π.

If the parameter Π in an input/output representation is not specified, then by default it is assumed to be the identity matrix $\Pi = I_{\mathtt{q}}$, *i.e.*, the first $\mathtt{m}$ variables are assumed inputs and the other $\mathtt{p} := \mathtt{q} - \mathtt{m}$ variables are outputs.

In the representation (IMAGE$_0$), the columns of P are *generators* of the model $\mathscr{B}$, *i.e.*, they span or generate the model. In the representation (KER$_0$), the rows of R are *annihilators* of $\mathscr{B}$, *i.e.*, they are orthogonal to the elements of $\mathscr{B}$. The parameters R and P are not unique, because

1. linearly dependent generators and annihilators can be added, respectively, to an existing set of annihilators and generators of $\mathscr{B}$ keeping the model the same, and

2. a set of generators or annihilators can be changed by an invertible transformation, without changing the model, *i.e.*,

$$\ker(R) = \ker(UR), \qquad \text{for all } U \in \mathbb{R}^{\mathtt{p}\times\mathtt{p}}, \text{ such that } \det(U) \neq 0;$$

   and

$$\operatorname{image}(P) = \operatorname{image}(PV), \qquad \text{for all } V \in \mathbb{R}^{\mathtt{m}\times\mathtt{m}}, \text{ such that } \det(V) \neq 0.$$

The smallest possible number of generators, *i.e.*, $\operatorname{col\,dim}(P)$, such that (IMAGE$_0$) holds is invariant of the representation and is equal to $\mathtt{m} := \dim(\mathscr{B})$—the dimension of $\mathscr{B}$. Integers, such as $\mathtt{m}$ and $\mathtt{p} := \mathtt{q} - \mathtt{m}$ that are invariant of the representation, characterize properties of the model (rather than of the representation) and are called *model invariants*. The integers $\mathtt{m}$ and $\mathtt{p}$ have data modeling interpretation as number of inputs and number of outputs, respectively. Indeed, $\mathtt{m}$ variables are free (unassigned by the model) and the other $\mathtt{p}$ variables are determined by the model and the inputs. The number of inputs and outputs of the model $\mathscr{B}$ are denoted by $\mathtt{m}(\mathscr{B})$ and $\mathtt{p}(\mathscr{B})$, respectively.

The model class of linear static models with $\mathtt{q}$ variables, at most $\mathtt{m}$ of which are inputs is denoted by $\mathscr{L}_{\mathtt{m},0}^{\mathtt{q}}$. With $\operatorname{col\,dim}(P) = \mathtt{m}$, the columns of P form a basis for $\mathscr{B}$. The smallest possible $\operatorname{row\,dim}(R)$, such that $\ker(R) = \mathscr{B}$ is invariant of the representation and is equal to the number of outputs of $\mathscr{B}$. With $\operatorname{row\,dim}(R) = \mathtt{p}$, the rows of R form a basis for the orthogonal complement $\mathscr{B}^\perp$ of $\mathscr{B}$. Therefore, without loss of generality we can assume that $P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}$ and $R \in \mathbb{R}^{\mathtt{p}\times\mathtt{q}}$.

Exercise 2.1. Show that for $\mathscr{B} \in \mathscr{L}_0^{\mathtt{q}}$,

- $\min_{P,\ \operatorname{image}(P)=\mathscr{B}} \operatorname{col\,dim}(P)$ is equal to $\dim(\mathscr{B})$ and
- $\min_{R,\ \ker(R)=\mathscr{B}} \operatorname{row\,dim}(R)$ is equal to $\mathtt{q} - \dim(\mathscr{B})$. □

In general, many input/output partitions of the variables d are possible. Choosing an input/output partition amounts to choosing a full rank $\mathtt{p}\times\mathtt{p}$ submatrix of R or a full rank $\mathtt{m}\times\mathtt{m}$ submatrix of P. In some data modeling problems, there is no a priori reason to prefer one partition of the variables over another. For such problems, the classical setting posing the problem as an overdetermined system of linear equations $AX \approx B$ is not a natural starting point.

Transition among input/output, kernel, and image representations

The transition from one model representation to another gives insight into the properties of the model. These *analysis problems* need to be solved before the more complicated modeling problems are considered. The latter can be viewed as *synthesis problems* since the model is created or synthesised from data and prior knowledge.

If the parameters R, P, and (X,Π) describe the same system $\mathscr{B}$, then they are related. We show the relations that the parameters must satisfy as well as code that does the transition from one representation to another. Before we describe the transition among the parameters, however, we need an efficient way to store and multiply by permutation matrices and a tolerance for computing rank numerically.

Input/output partition of the variables

In the input/output model representation $\mathscr{B}_{\mathrm{i/o}}(X,\Pi)$, the partitioning of the variables $d \in \mathbb{R}^{\mathtt{q}}$ into inputs $u \in \mathbb{R}^{\mathtt{m}}$ and outputs $y \in \mathbb{R}^{\mathtt{p}}$ is specified by a permutation matrix Π,

$$d \underset{\Pi}{\overset{\Pi^{-1}=\Pi^\top}{\rightleftarrows}} \operatorname{col}(u,y) \quad , \qquad d = \Pi \begin{bmatrix} u \\ y \end{bmatrix}, \quad \begin{bmatrix} u \\ y \end{bmatrix} = \Pi^\top d.$$

In the software implementation, however, it is more convenient (as well as more memory and computation efficient) to specify the partitioning by a vector

$$\pi := \Pi \operatorname{col}(1,\dots,\mathtt{q}) \in \{1,\dots,\mathtt{q}\}^{\mathtt{q}}.$$

Clearly, the vector π contains the same information as the matrix Π and one can reconstruct Π from π by permuting the rows of the identity matrix. (In the code `io` is the variable corresponding to the vector π and `Pi` is the variable corresponding to the matrix Π.)

39a ⟨$\pi \mapsto \Pi$ 39a⟩≡ (40a)
```
  Pi = eye(length(io)); Pi = Pi(io,:);
```

Permuting the elements of a vector is done more efficiently by direct reordering of the elements, instead of a matrix-vector multiplication. If `d` is a variable corresponding to a vector d, then `d(io)` corresponds to the vector Πd.

The default value for Π is the identity matrix I, corresponding to first $\mathtt{m}$ variables of d being inputs and the remaining $\mathtt{p}$ variables outputs, $d = \left[\begin{smallmatrix} u \\ y \end{smallmatrix}\right]$.

39b ⟨*default input/output partition* 39b⟩≡ (41 43b)
```
  if ~exist('io') || isempty(io), io = 1:q; end
```

In case the inverse permutation $\Pi^{-1} = \Pi^\top$ is needed, the corresponding "permutation vector" is

$$\pi' = \Pi^\top \operatorname{col}(1,\dots,\mathtt{q}) \in \{1,\dots,\mathtt{q}\}^{\mathtt{q}}.$$

In the code `inv_io` is the variable corresponding to the vector π' and the transition from the original variables `d` to the partitioned variables `uy = [u; y]` via `io` and `inv_io` is done by the following indexing operations:

$$\mathtt{d} \underset{\mathtt{io}}{\overset{\mathtt{io\_inv}}{\rightleftarrows}} \mathtt{uy} \quad , \qquad \mathtt{d} = \mathtt{uy(io)}, \quad \mathtt{uy} = \mathtt{d(io\_inv)}.$$

40a ⟨*inverse permutation* 40a⟩≡ (44a)
```
  ⟨π ↦ Π 39a⟩, inv_io = (1:length(io)) * Pi;
```

Tolerance for rank computation

In the computation of an input/output representation from a given kernel or image representation of a model (as well as in the computation of the models' complexity), we need to find the rank of a matrix. Numerically this is an ill-posed problem because arbitrary small perturbations of the matrix's elements may (generically will) change the rank. A solution to this problem is to replace rank with "numerical rank" defined as follows

$$\operatorname{num rank}(A,\varepsilon) := \text{number of singular values of } A \text{ greater than } \varepsilon, \qquad (\text{num rank})$$

where $\varepsilon \in \mathbb{R}_+$ is a user defined tolerance. Note that

$$\operatorname{num rank}(A,0) = \operatorname{rank}(A),$$

i.e., by taking the tolerance to be equal to zero, the numerical rank reduces to the theoretical rank. A nonzero tolerance ε makes the numerical rank robust to perturbations of size (measured in the induced 2-norm) less than ε. Therefore, ε reflects the size of the expected errors in the matrix. The default tolerance is set to a small value, which corresponds to numerical errors due to a double precision arithmetic. (In the code `tol` is the variable corresponding to ε.)

40b ⟨*default tolerance* `tol` 40b⟩≡ (43 44c 78c)
```
  if ~exist('tol') || isempty(tol), tol = 1e-12; end
```

Note 2.2. The numerical rank definition (num rank) is the solution of an unstructured rank minimization problem: find a matrix $\widehat{A}$ of minimal rank, such that $\|A-\widehat{A}\|_2 < \varepsilon$.

From input/output representation to kernel or image representations

Consider a linear static model $\mathscr{B} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},0}$, defined by an input/output representation $\mathscr{B}_{\mathrm{i/o}}(X,\Pi)$. From $y = X^\top u$, we have

$$\begin{bmatrix} X^\top & -I \end{bmatrix} \operatorname{col}(u,y) = 0$$

or since $d = \Pi \left[\begin{smallmatrix} u \\ y \end{smallmatrix}\right]$,

$$\underbrace{\begin{bmatrix}X^\top & -I\end{bmatrix}\Pi^\top}_{R}\underbrace{\Pi\begin{bmatrix}u\\y\end{bmatrix}}_{d}=0.$$

Therefore, the matrix

$$R=\begin{bmatrix}X^\top & -I\end{bmatrix}\Pi^\top \qquad ((X,\Pi)\mapsto R)$$

is a parameter of a kernel representations of $\mathscr{B}$, *i.e.*,

$$\mathscr{B}_{\text{i/o}}(X,\Pi)=\ker\Big(\begin{bmatrix}X^\top & -I\end{bmatrix}\Pi^\top\Big)=\mathscr{B}.$$

Moreover, the representation is minimal because R is full row rank.

Similarly, a minimal image representation is derived from the input/output representation as follows. From $y=X^\top u$,

$$\begin{bmatrix}u\\y\end{bmatrix}=\begin{bmatrix}I\\X^\top\end{bmatrix}u,$$

so that, using $d=\Pi\left[\begin{smallmatrix}u\\y\end{smallmatrix}\right]$,

$$d=\Pi\begin{bmatrix}u\\y\end{bmatrix}=\Pi\begin{bmatrix}I\\X^\top\end{bmatrix}u=:Pu.$$

Therefore, the matrix

$$P=\Pi\begin{bmatrix}I\\X^\top\end{bmatrix} \qquad ((X,\Pi)\mapsto P)$$

is a parameter of an image representations of $\mathscr{B}$, *i.e.*,

$$\mathscr{B}_{\text{i/o}}(X,\Pi)=\operatorname{image}\left(\Pi\begin{bmatrix}I\\X^\top\end{bmatrix}\right)=\mathscr{B}.$$

The representation is minimal because P is full column rank.

Formulae $((X,\Pi)\mapsto R)$ and $((X,\Pi)\mapsto P)$ give us a straight forward way of transforming a given input/output representation to minimal kernel and minimal image representations.

41a $\langle (X,\Pi)\mapsto R$ 41a$\rangle\equiv$
```
function r = xio2r(x, io)
r = [x', -eye(size(x, 2))]; q = size(r, 2);
⟨default input/output partition 39b⟩, r = r(:, io);
```
Defines:
`xio2r`, used in chunk 46b.

41b $\langle (X,\Pi)\mapsto P$ 41b$\rangle\equiv$
```
function p = xio2p(x, io)
p = [eye(size(x, 1)); x']; q = size(p, 1);
⟨default input/output partition 39b⟩, p = p(io, :);
```
Defines:
`xio2p`, used in chunk 46b.

From image to minimal kernel and from kernel to minimal image representation

The relation

$$\ker(R)=\operatorname{image}(P)=\mathscr{B}\in\mathscr{L}^{\mathtt{q}}_{\mathtt{m},0} \quad\Longrightarrow\quad RP=0 \qquad (R\leftrightarrow P)$$

gives a link between the parameters P and R. In particular, a minimal image representation $\operatorname{image}(P)=\mathscr{B}$ can be obtained from a given kernel representation $\ker(R)=\mathscr{B}$ by computing a basis for the null space of R. Conversely, a minimal kernel representation $\ker(R)=\mathscr{B}$ can be obtained from a given image representation $\operatorname{image}(P)=\mathscr{B}$ by computing a basis for the left null space of P.

42a $\langle R\mapsto P$ 42a$\rangle\equiv$
```
function p = r2p(r), p = null(r);
```
Defines:
`r2p`, used in chunk 46.

42b $\langle P\mapsto R$ 42b$\rangle\equiv$
```
function r = p2r(p), r = null(p')';
```
Defines:
`p2r`, used in chunk 46b.

Converting an image or kernel representation to a minimal one

The kernel and image representations obtained from `xio2r`, `xio2p`, `p2r`, and `r2p` are minimal. In general, however, a given kernel or image representations can be non-minimal, *i.e.*, R may have redundant rows and P may have redundant columns. The kernel representation, defined by R, is minimal if and only if R is full row rank. Similarly, the image representation, defined by P, is minimal if and only if P is full column rank.

The problems of converting kernel and image representations to minimal ones are equivalent to the problem of finding a full rank matrix that has the same kernel or image as a given matrix. A numerically reliable way to solve this problem is to use the singular value decomposition.

Consider a model $\mathscr{B}\in\mathscr{L}^{\mathtt{q}}_{\mathtt{m},0}$ with parameters $R\in\mathbb{R}^{g\times\mathtt{q}}$ and $P\in\mathbb{R}^{\mathtt{q}\times g}$ of respectively kernel and image representations. Let

$$R=U\Sigma V^\top$$

be the singular value decomposition of R and let $\mathtt{p}$ be the rank of R. With the partitioning,

$$V=:\begin{bmatrix}V_1 & V_2\end{bmatrix}, \qquad \text{where} \quad V_1\in\mathbb{R}^{\mathtt{q}\times\mathtt{p}},$$

we have that

$$\operatorname{image}(R^\top)=\operatorname{image}(V_1).$$

Therefore,

$$\ker(R) = \ker(V_1^\top) \qquad \text{and } V_1 \text{ is full rank,}$$

so that $V_1^\top$ is a parameter of a minimal kernel representation of $\mathscr{B}$.

Similarly, let

$$P = U\Sigma V^\top$$

be the singular value decomposition of P. With the partitioning,

$$U =: \begin{bmatrix} U_1 & U_2 \end{bmatrix}, \qquad \text{where} \quad U_1 \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}},$$

we have that

$$\text{image}(P) = \text{image}(U_1).$$

Since U_1 is full rank, it is a parameter of a minimal image representation of $\mathscr{B}$.

In the numerical implementation, the rank is replaced by the numerical rank with respect to a user defined tolerance `tol`.

43a ⟨*$R \mapsto$ minimal R* 43a⟩≡
```
function r = minr(r, tol)
[p, q] = size(r); ⟨default tolerance tol 40b⟩
[u, s, v] = svd(r, 'econ'); pmin = sum(diag(s) > tol);
if pmin < p, r = v(:, 1:pmin)'; end
```
Defines:
`minr`, used in chunks 44a and 45b.

Exercise 2.3. Write a function `minp` that implements the transition $P \mapsto$ minimal P. □

From kernel or image to input/output representation

The transformations from kernel to input/output and from image to input/output representations are closely related. They involve as a sub-problem the problem of finding input/output partitions of the variables in the model. Because of this, they are more complicated than the inverse transformations, considered above.

Assume first that the input/output partition is given. This amounts to knowing the permutation matrix $\Pi \in \mathbb{R}^{\mathtt{q}\times\mathtt{q}}$ in (I/O$_0$).

43b ⟨*$(R,\Pi) \mapsto X$* 43b⟩≡ 44a▷
```
function x = rio2x(r, io, tol)
q = size(r, 2); ⟨default input/output partition 39b⟩, ⟨default tolerance tol 40b⟩
```
Defines:
`rio2x`, used in chunks 45, 46, and 122a.

Consider given parameters $R \in \mathbb{R}^{\mathtt{p}\times\mathtt{q}}$ of *minimal* kernel representation of a linear static system $\mathscr{B} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},0}$ and define the partitioning

$$R\Pi =: \begin{bmatrix} R_u & R_y \end{bmatrix}, \quad \text{where } R_y \in \mathbb{R}^{\mathtt{p}\times\mathtt{p}}.$$

44a ⟨*$(R,\Pi) \mapsto X$* 43b⟩+≡ ◁43b 44b▷
```
r = minr(r, tol); p = size(r, 1); m = q - p;
⟨inverse permutation 40a⟩, rpi = r(:, inv_io);
ru  = rpi(:, 1:m); ry = rpi(:, (m + 1):end);
```
Uses `minr` 43a.

Similarly, for a parameter $P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}$ of *minimal* image representation of $\mathscr{B}$, define

$$\Pi^\top P =: \begin{bmatrix} P_u \\ P_y \end{bmatrix}, \quad \text{where } P_u \in \mathbb{R}^{\mathtt{m}\times\mathtt{m}}.$$

If R_y and P_u are non-singular, it follows from $((X,\Pi) \mapsto R)$ and $((X,\Pi) \mapsto P)$ that

$$X = -(R_y^{-1}R_u)^\top \qquad ((R,\Pi) \mapsto X)$$

and

$$X = (P_y P_u^{-1})^\top \qquad ((P,\Pi) \mapsto X)$$

is the parameter of the input/output representation $\mathscr{B}_{\text{i/o}}(X,\Pi)$ of $\mathscr{B}$, *i.e.*,

$$\ker\Big(\underbrace{\begin{array}{cc} \mathtt{m} & \mathtt{p} \\ \big[R_u & R_y\big] \end{array} \Pi^\top}_{R}\Big) = \mathscr{B}_{\text{i/o}}\big(-(R_y^{-1}R_u)^\top, \Pi\big)$$

and

$$\text{image}\left(\underbrace{\Pi \begin{bmatrix} P_u \\ P_y \end{bmatrix}}_{P} \begin{array}{c} \mathtt{m} \\ \mathtt{p} \end{array}\right) = \mathscr{B}_{\text{i/o}}\big((P_y P_u^{-1})^\top, \Pi\big).$$

44b ⟨*$(R,\Pi) \mapsto X$* 43b⟩+≡ ◁44a
```
[u, s, v] = svd(ry); s = diag(s);
if s(end) < tol
    warning('Computation of X is ill conditioned.'); x = NaN;
else
    x = -( v * diag(1 ./ s) * u' * ru )';
end
```
Singularity of the blocks R_y and P_u implies that the input/output representation with a permutation matrix Π is not possible. In such cases, the function `rio2x` issues a warning message and returns `NaN` value for X.

The function `r2io` uses `rio2x` in order to find all possible input/output partitions for a model specified by a kernel representation.

44c ⟨*$R \mapsto \Pi$* 44c⟩≡ 45a▷
```
function IO = r2io(r, tol)
q = size(r, 2); ⟨default tolerance tol 40b⟩
```
Defines:
`r2io`, used in chunk 45c.

The search is exhaustive over all input/output partitionings of the variables (*i.e.*, all choices of $\mathtt{m}$ elements of the set of variable indexes $\{1,\dots,\mathtt{q}\}$), so that the computation is feasible only for a small number of variables (say less than 6).

45a ⟨$R \mapsto \Pi$ 44c⟩+≡ ◁44c 45b▷
```
  IO = perms(1:q); nio = size(IO, 1);
```
The parameter X for each candidate partition is computed. If the computation of X is ill-conditioned, the corresponding partition is not consistent with the model and is discarded.

45b ⟨$R \mapsto \Pi$ 44c⟩+≡ ◁45a
```
  not_possible = []; warning_state = warning('off');
  r = minr(r, tol);
  for i = 1:nio
      x = rio2x(r, IO(i, :), tol);
      if isnan(x), not_possible = [not_possible, i]; end
  end
  warning(warning_state); IO(not_possible, :) = [];
```
Uses `minr` 43a and `rio2x` 43b.

Example 2.4. Consider the linear static model with three variables and one input

$$\mathscr{B} = \operatorname{image}\left(\begin{bmatrix}1\\0\\0\end{bmatrix}\right) = \ker\left(\begin{bmatrix}0&1&0\\0&0&1\end{bmatrix}\right).$$

Clearly, this model has only two input/output partitions:

$$u = w_1,\ y = \begin{bmatrix}w_2\\w_3\end{bmatrix} \qquad \text{and} \qquad u = w_1,\ y = \begin{bmatrix}w_3\\w_2\end{bmatrix}.$$

Indeed, the function `r2io`

45c ⟨*Test* `r2io` 45c⟩≡
```
  r2io([0 0 1; 0 1 0])
```
Uses `r2io` 44c.

correctly computes the input output partitionings from the parameter R in a kernel representation of the model

```
ans =

     1     2     3
     1     3     2
```
□

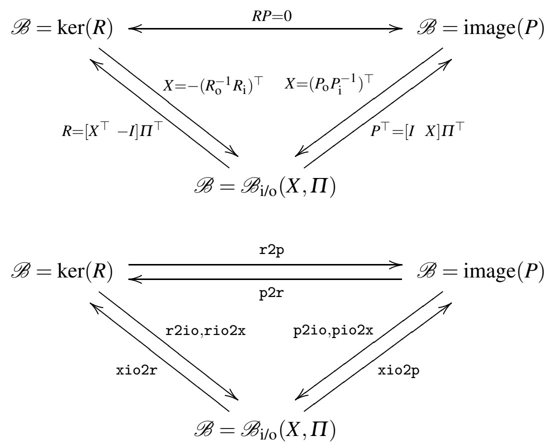
Exercise 2.5. Write functions `pio2x` and `p2io` that implement the transitions

$$(P,\Pi) \mapsto X \quad \text{and} \quad P \mapsto \Pi. \qquad \square$$

Exercise 2.6. Explain how to check that two models, specified by kernel or image representation, are equivalent. □

Summary of transitions among representations

Figure 2.1 summarizes the links among the parameters R, P, and (X,Π) of a linear static model $\mathscr{B}$ and the functions that implement the transitions.



$$\begin{tikzcd}
\mathscr{B}=\ker(R) \arrow[rr, leftrightarrow, "RP=0"] \arrow[dr, shift left, "X=-(R_{\rm o}^{-1}R_{\rm i})^\top"] & & \mathscr{B}=\operatorname{image}(P) \arrow[dl, shift right, "X=(P_{\rm o}P_{\rm i}^{-1})^\top"'] \\
& \mathscr{B}=\mathscr{B}_{\rm i/o}(X,\Pi) \arrow[ul, shift left, "R=[X^\top\ -I]\Pi^\top"] \arrow[ur, shift right, "P^\top=[I\ \ X]\Pi^\top"'] &
\end{tikzcd}$$

$$\begin{tikzcd}
\mathscr{B}=\ker(R) \arrow[rr, shift left, "\texttt{r2p}"] \arrow[dr, shift left, "\texttt{r2io,rio2x}"] & & \mathscr{B}=\operatorname{image}(P) \arrow[ll, shift left, "\texttt{p2r}"] \arrow[dl, shift right, "\texttt{p2io,pio2x}"'] \\
& \mathscr{B}=\mathscr{B}_{\rm i/o}(X,\Pi) \arrow[ul, shift left, "\texttt{xio2r}"] \arrow[ur, shift right, "\texttt{xio2p}"'] &
\end{tikzcd}$$

Fig. 2.1 Relations and functions for the transitions among linear static model parameters.

Numerical example

In order to test the functions for transition among the kernel, image, and input/output model representations, we choose, a random linear static model, specified by a kernel representation,

46a ⟨*Test model transitions* 46a⟩≡ 46b▷
```
  m = 2; p = 3; R = rand(p, m + p); P = r2p(R);
```
Uses `r2p` 42a.

and traverse the diagram in Figure 2.1 clock-wise and anti clock-wise

46b ⟨*Test model transitions* 46a⟩+≡ ◁46a 46c▷
```
  R_ = xio2r(pio2x(r2p(R))); P_ = xio2p(rio2x(p2r(P)));
```
Uses `p2r` 42b, `r2p` 42a, `rio2x` 43b, `xio2p` 41b, and `xio2r` 41a.

As a verification of the software, we check that after traversing the loop, equivalent models are obtained.

46c ⟨*Test model transitions* 46a⟩+≡ ◁46b
```
  norm(rio2x(R) - rio2x(R_)), norm(pio2x(P) - pio2x(P_))
```
Uses `rio2x` 43b.

The answers are around the machine precision, which confirms that the models are the same.

Linear static model complexity

A linear static model is a finite dimensional subspace. The dimension $\mathtt{m}$ of the subspace is equal to the number of inputs and is invariant of the model representation. The integer constant $\mathtt{m}$ quantifies the *model complexity*: the model is more complex when it has more inputs. The rationale for this definition of model complexity is that inputs are "unexplained" variables by the model, so the more inputs the model has, the less it "explains" the modeled phenomenon. In data modeling the aim is to obtain low-complexity models, a principle generally refered to as *Occam's razor*.

Note 2.7 (Computing the model complexity is a rank estimation problem). Computing the model complexity, implicitly specified by (exact) data, or by a nonminimal kernel or image representation is a rank computation problem; see Section 2.3 and the function `minr`.

2.2 Linear time-invariant model representations

An observation d_j of a static model is a vector of variables. In the dynamic case, the observations depend on time, so that apart from the multivariable aspect, there is also a time evaluation aspect. In the dynamic case, an observation is refered to as a *trajectory*, *i.e.*, it is a vector valued *function* of a scalar argument. The time variable takes its values in the set of integers $\mathbb{Z}$ (*discrete-time* model) or in the set of real numbers $\mathbb{R}$ (*continuous-time* model). We denote the time axis by $\mathscr{T}$.

A dynamic model $\mathscr{B}$ with $\mathtt{q}$ variables is a subset of the trajectory space $(\mathbb{R}^{\mathtt{q}})^{\mathscr{T}}$ — the set of all functions from the time axis $\mathscr{T}$ to the variable space $\mathbb{R}^{\mathtt{q}}$.

In this book, we consider the special class of finite dimensional linear time-invariant dynamical models. By definition, a model $\mathscr{B}$ is *linear* if it is a subspace of the data space $(\mathbb{R}^{\mathtt{q}})^{\mathscr{T}}$. In order to define the *time-invariance* property, we introduce the *shift operator* σ^τ. Acting on a signal w, σ^τ produces a signal $\sigma^\tau w$, which is the backwards shifted version of w by τ time units, *i.e.*,

$$(\sigma^\tau w)(t) := w(t+\tau), \qquad \text{for all } t \in \mathscr{T}.$$

Acting on a set of trajectories, σ^τ shifts all trajectories in the set, *i.e.*,

$$\sigma^\tau \mathscr{B} := \{\, \sigma^\tau w \mid w \in \mathscr{B} \,\}.$$

A model $\mathscr{B}$ is shift-invariant if it is invariant under any shift in time, *i.e.*,

$$\sigma^\tau \mathscr{B} = \mathscr{B}, \qquad \text{for all } \tau \in \mathscr{T}.$$

The model $\mathscr{B}$ is *finite dimensional* if it is a closed subset (in the topology of pointwise convergence). Finite dimensionality is equivalent to the property that at any time t the future behavior of the model is deterministically independent of the past behavior, given a finite dimensional vector, called a *state* of the model. Intuitively, the state is the information (or memory) of the past that is needed in order to predict the future. The smallest state dimension is an invariant of the system, called the *order*. We denote the set of finite dimensional linear time-invariant models with $\mathtt{q}$ variables and order at most $\mathtt{n}$ by $\mathscr{L}^{\mathtt{q},\mathtt{n}}$ and the *order* of $\mathscr{B}$ by $\mathtt{n}(\mathscr{B})$.

A finite dimensional linear time-invariant model $\mathscr{B} \in \mathscr{L}^{\mathtt{q},\mathtt{n}}$ admits a representation by a difference or differential equation

$$\begin{aligned} R_0 w + R_1 \lambda w + \cdots + R_1 \lambda^{\mathtt{l}} w &= \underbrace{\left(R_0 + R_1 \lambda + \cdots + R_1 \lambda^{\mathtt{l}}\right)}_{R(\lambda)} w \\ &= R(\lambda) w = 0, \end{aligned} \tag{DE}$$

where λ is the unit shift operator σ in the discrete-time case and the differential operator $\frac{\mathrm{d}}{\mathrm{d}t}$ in the continuous-time case. Therefore, the model $\mathscr{B}$ is the kernel

$$\mathscr{B} := \ker\big(R(\lambda)\big) = \{\, w \mid \text{(DE) holds} \,\}, \tag{KER}$$

of the difference or differential operator $R(\lambda)$. The smallest degree $\mathtt{l}$ of a polynomial matrix

$$R(z) := R_0 + R_1 z + \cdots + R_1 z^{\mathtt{l}} \in \mathbb{R}^{g \times \mathtt{q}}[z],$$

in a kernel representation (KER) of $\mathscr{B}$, is invariant of the representation and is called the *lag* $\mathtt{l}(\mathscr{B})$ of $\mathscr{B}$.

The order of the system is the total degree of the polynomial matrix R in a kernel representation of the system. Therefore, we have the following link between the order and the lag of a linear time-invariant model:

$$\mathtt{n}(\mathscr{B}) \leq \mathtt{p}(\mathscr{B})\mathtt{l}(\mathscr{B}).$$

As in the static case, the smallest possible number of rows g of the polynomial matrix R in a kernel representation (KER) of a finite dimensional linear time-invariant system $\mathscr{B}$ is the invariant $\mathtt{p}(\mathscr{B})$ — number of outputs of $\mathscr{B}$. Finding an input/output partitioning for a model specified by a kernel representation amounts to selection of a nonsingular $\mathtt{p} \times \mathtt{p}$ submatrix of R. The resulting input/output representation is:

$$\mathscr{B} = \mathscr{B}_{\mathrm{i/o}}(P, Q, \Pi) := \ker\left(\Pi \begin{bmatrix} Q(\lambda) & P(\lambda) \end{bmatrix}\right), \tag{I/O}$$

with parameters the polynomial matrices

$$Q \in \mathbb{R}^{\mathtt{p} \times \mathtt{m}}[z] \qquad \text{and} \qquad P \in \mathbb{R}^{\mathtt{p} \times \mathtt{p}}[z], \quad \text{such that } \det(P) \neq 0,$$

and the permutation matrix Π.

In general, the representation (I/O) involves higher order shifts or derivatives. A first order representation

$$\mathscr{B} = \mathscr{B}_{\text{i/s/o}}(A,B,C,D,\Pi) := \{ w = \Pi \operatorname{col}(u,y) \mid \text{there is } x, \text{ such that } \lambda x = Ax + Bu \text{ and } y = Cx + Du \}, \qquad \text{(I/S/O)}$$

with an auxiliary variable x, however, is always possible. The representation (I/S/O) displays not only the input/output structure of the model but also its state structure and is refered to as an input/state/output representation of the model. The parameters of an input/state/output representation are the matrices

$$A \in \mathbb{R}^{\mathtt{n}\times\mathtt{n}}, \quad B \in \mathbb{R}^{\mathtt{n}\times\mathtt{m}}, \quad C \in \mathbb{R}^{\mathtt{p}\times\mathtt{n}}, \quad D \in \mathbb{R}^{\mathtt{p}\times\mathtt{m}},$$

and a permutation matrix Π. The parameters are non unique due to

- nonuniqueness in the choice of the input/output partition,
- existence of redundant states (nonminimality of the representation), and
- change of state space basis

$$\mathscr{B}_{\text{i/s/o}}(A,B,C,D) = \mathscr{B}_{\text{i/s/o}}(T^{-1}AT, T^{-1}B, CT, D), \quad \text{for any nonsingular matrix } T \in \mathbb{R}^{\mathtt{n}\times\mathtt{n}}. \qquad \text{(CB)}$$

An input/state/output representation $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ is called *minimal* when the state dimension $\mathtt{n}$ is as small as possible. The minimal state dimension is an invariant of the system and is equal to the order $\mathtt{n}(\mathscr{B})$ of the system.

A system $\mathscr{B}$ is *autonomous* if for any trajectory $w \in \mathscr{B}$ the "past"

$$w_- := \big(\dots, w(-2), w(-1)\big)$$

of w completely determines its "future"

$$w_+ := \big(w(0), w(1), \dots\big).$$

It can be shown that a system $\mathscr{B}$ is autonomous if and only if it has no inputs. An autonomous finite dimensional linear time-invariant system is parametrized by the pair of matrices A and C via the state space representation

$$\mathscr{B}_{\text{i/s/o}}(A,C) := \{ w = y \mid \text{there is } x, \text{ such that } \sigma x = Ax \text{ and } y = Cx \}.$$

The dimension $\dim(\mathscr{B})$ of an autonomous linear model $\mathscr{B}$ is equal to the order $\mathtt{n}(\mathscr{B})$.

In a way the opposite of an autonomous model is a controllable system. The model $\mathscr{B}$ is *controllable* if for any trajectories w_p and w_f of $\mathscr{B}$, there is $\tau > 0$ and a third trajectory $w \in \mathscr{B}$, which coincides with w_p in the past, *i.e.*, $w(t) = w_\text{p}(t)$, for all $t < 0$, and coincides with w_f in the future, *i.e.*, $w(t) = w_\text{f}(t)$, for all $t \geq \tau$. The subset of controllable systems of the set of linear time-invariant systems $\mathscr{L}^{\mathtt{q}}$ is denoted by $\mathscr{L}^{\mathtt{q}}_{\text{ctrb}}$. A summary of properties of a dynamical system is given in Table 2.1.

Apart from the kernel, input/output, and input/state/output representation, a controllable finite dimensional linear time-invariant model admits the following representations:

Table 2.1 Summary of model $\mathscr{B} \subset (\mathbb{R}^{\mathtt{q}})^{\mathscr{T}}$ properties.

property		definition
linearity	—	$w, v \in \mathscr{B} \implies \alpha w + \beta v \in \mathscr{B}$, for all $\alpha, \beta \in \mathbb{R}$
time-invariance	—	$\sigma^\tau \mathscr{B} = \mathscr{B}$, for all $\tau \in \mathscr{T}$
finite dimensionality	—	$\mathscr{B}$ is a closed set; equivalently $\mathtt{n}(\mathscr{B}) < \infty$
autonomy	—	the past of any trajectory completely determines its future; equivalently $\mathtt{m}(\mathscr{B}) = 0$
controllability	—	the past of any trajectory can be concatenated to the future of any other trajectory by a third trajectory if a transition period is allowed

- *image representation*

$$\mathscr{B} = \operatorname{image}\big(P(\lambda)\big) := \{ w \mid w = P(\lambda)\ell, \text{ for some } \ell \}, \qquad \text{(IMAGE)}$$

with parameter the polynomial matrix $P(z) \in \mathbb{R}^{\mathtt{q}\times g}[z]$,
- *convolution representation*

$$\mathscr{B} = \mathscr{B}_{\text{i/o}}\big(H, \Pi\big) := \{ w = \Pi \operatorname{col}(u,y) \mid y = H \star u \}, \qquad \text{(CONV)}$$

where $\star$ is the convolution operator

$$y(t) = (H \star u)(t) := \sum_{\tau=0}^{\infty} H(\tau) u(t-\tau), \qquad \text{in discrete-time, or}$$

$$y(t) = (H \star u)(t) := \int_0^\infty H(\tau) u(t-\tau) \mathrm{d}\tau, \qquad \text{in continuous-time,}$$

with parameters the signal $H : \mathscr{T} \to \mathbb{R}^{\mathtt{p}\times\mathtt{m}}$ and a permutation matrix Π; and
- *transfer function*,

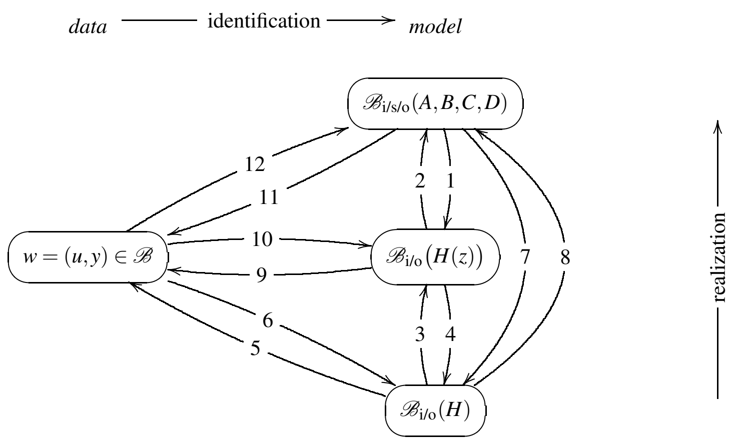
$$\mathscr{B} = \mathscr{B}_{\text{i/o}}\big(H, \Pi\big) := \{ w = \Pi \operatorname{col}(u,y) \mid \mathscr{F}(y) = H(z) \mathscr{F}(u) \}, \qquad \text{(TF)}$$

where $\mathscr{F}$ is the Z-transform in discrete-time and the Laplace transform in continuous-time, with parameters the rational matrix $H \in \mathbb{R}^{\mathtt{p}\times\mathtt{m}}(s)$ (the transfer function) and a permutation matrix Π.

Transitions among the parameters H, $H(z)$, and (A,B,C,D) are classical problems, see Figure 2.2. Next, we review the transition from impulse response H to parameters (A,B,C,D) of an input/state/output representation, which plays an important role in deriving methods for Hankel structured low-rank approximation.

System realization

The problem of passing from a convolution representation to an input/state/output representation is called (impulse response) realization.


data
identification
model
$\mathscr{B}_{\mathrm{i/s/o}}(A,B,C,D)$
$w=(u,y)\in\mathscr{B}$
$\mathscr{B}_{\mathrm{i/o}}(H(z))$
$\mathscr{B}_{\mathrm{i/o}}(H)$
1
2
3
4
5
6
7
8
9
10
11
12
realization

1. $H(z) = C(Iz-A)^{-1}B + D$
2. realization of a transfer function
3. Z or Laplace transform of $H(t)$
4. inverse transform of $H(z)$
5. convolution $y_{\mathrm{d}} = H \star u_{\mathrm{d}}$
6. exact identification
7. $H(0) = D$, $H(t) = CA^{t-1}B$ (discrete-time), $H(t) = Ce^{At}B$ (continuous-time), for $t>0$
8. realization of an impulse response
9. simulation with input u_{d} and $x(0)=0$
10. exact identification
11. simulation with input u_{d} and $x(0) = x_{\mathrm{ini}}$
12. exact identification

Fig. 2.2 Data, input/output model representations, and links among them.

Definition 2.8 (Realization). A linear time-invariant system $\mathscr{B}$ with $\mathtt{m}$ inputs and $\mathtt{p}$ outputs and an input/output partition, specified by a permutation matrix Π, is a *realization* of (or realizes) an impulse response $H:\mathscr{T}\to\mathbb{R}^{\mathtt{p}\times\mathtt{m}}$ if $\mathscr{B}$ has a convolution representation $\mathscr{B}=\mathscr{B}_{\mathrm{i/o}}(H,\Pi)$. A realization $\mathscr{B}$ of H is *minimal* if its order $\mathtt{n}(\mathscr{B})$ is the smallest over all realization of H. □

In what follows, we fix the input/output partition Π to the default one

$$w = \operatorname{col}(u,y)$$

and use the notation

$$H := \begin{bmatrix} h_1 & \cdots & h_{\mathtt{m}} \end{bmatrix} \qquad \text{and} \qquad I_{\mathtt{m}} := \begin{bmatrix} e_1 & \cdots & e_{\mathtt{m}} \end{bmatrix}.$$

An equivalent definition of impulse response relization that makes explicit the link of the realization problem to data modeling is the following one.

Definition 2.9 (Realization, as a data modeling problem). The system $\mathscr{B}$ realizes H if the set of input/output trajectories (e_i,h_i), for $i=1,\dots,\mathtt{m}$ are impulse responses of $\mathscr{B}$, *i.e.*,

$$(e_i\delta, 0\wedge h_i)\in\mathscr{B}, \qquad \text{for} \quad i=1,\dots,\mathtt{m},$$

where δ is the delta function and $\wedge$ is the concatenation map (at time 0)

$$w = w_{\mathrm{p}}\wedge w_{\mathrm{f}}, \qquad w(t) := \begin{cases} w_{\mathrm{p}}(t), & \text{if } t<0 \\ w_{\mathrm{f}}(t), & \text{if } t\geq 0 \end{cases} \qquad \square$$

Note 2.10 (Discrete-time vs continuous-time system realization). There are some differences between the discrete and continuous-time realization theory. Next, we consider the discrete-time case. It turns out, however, that the discrete-time algorithms can be used for realization of continuous-time systems by applying them on the sequence of the Markov parameter $\big(H(0), \frac{\mathrm{d}}{\mathrm{d}t}H(0),\dots\big)$ of the system.

The sequence

$$H = \big(H(0),H(1),H(2),\dots,H(t),\dots\big), \qquad \text{where} \quad H(t)\in\mathbb{R}^{\mathtt{p}\times\mathtt{m}}$$

is a one sided infinite matrix-values time series. Acting on H, the shift operator σ, removes the first sample, *i.e.*,

$$\sigma H = \big(H(1),H(2),\dots,H(t),\dots\big).$$

A sequence H might not be realizable by a *finite dimensional* linear time-invariant system, but if it is realizable, a minimal realization is unique.

Theorem 2.11 (Test for realizability). *The sequence $H:\mathbb{Z}_+\to\mathbb{R}^{\mathtt{p}\times\mathtt{m}}$ is realizable by a finite dimensional linear time-invariant system with $\mathtt{m}$ inputs if and only if the two-sided infinite Hankel matrix $\mathscr{H}(\sigma H)$ has a finite rank $\mathtt{n}$. Moreover, the order of a minimal realization is equal to $\mathtt{n}$, and there is a unique system $\mathscr{B}$ in $\mathscr{L}_{\mathtt{m}}^{\mathtt{q},\mathtt{n}}$ that realizes H.*

Proof. ($\Longrightarrow$) Let H be realizable by a system $\mathscr{B}\in\mathscr{L}_{\mathtt{m}}^{\mathtt{q},\mathtt{n}}$ with a minimal input/state/output representation $\mathscr{B}=\mathscr{B}_{\mathrm{i/s/o}}(A,B,C,D)$. Then

$$H(0) = D \qquad \text{and} \qquad H(t) = CA^{t-1}B, \qquad \text{for } t>0.$$

The (i,j) block element of the Hankel matrix $\mathscr{H}(\sigma H)$ is

$$H(i+j-1) = CA^{i+j-2}B = CA^{i-1}A^{j-1}B.$$

Let

$$\mathscr{O}_t(A,C) := \operatorname{col}(C, CA, \dots, CA^{t-1}) \tag{$\mathscr{O}$}$$

be the extended observability matrix of the pair (A,C) and

$$\mathscr{C}_t(A,B) := \begin{bmatrix} B & AB & \cdots & A^{t-1}B \end{bmatrix} \tag{$\mathscr{C}$}$$

be the extended controllability matrix of the pair (A,B). With $\mathscr{O}(A,C)$ and $\mathscr{C}(A,B)$ being the infinite observability and controllability matrices, we have

$$\mathscr{H}(\sigma H) = \mathscr{O}(A,C)\mathscr{C}(A,B) \tag{$\mathscr{O}\mathscr{C}$}$$

Since the representation $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ is assumed to be minimal, $\mathscr{C}(A,B)$ is full row rank and $\mathscr{O}(A,C)$ is full column rank. Therefore, $(\mathscr{O}\mathscr{C})$ is a rank revealing factorization of $\mathscr{H}(\sigma H)$ and

$$\operatorname{rank}\big(\mathscr{H}(\sigma H)\big) = \mathtt{n}(\mathscr{B}).$$

($\Longleftarrow$) In this direction, the proof is constructive and results in an *algorithm* for computation of the minimal realization of H in $\mathscr{L}_{\mathtt{m}}^{\mathtt{q},\mathtt{n}}$, where $\mathtt{n} = \mathit{rank}\big(\mathscr{H}(\sigma H)\big)$. A realization algorithm is presented in Section 3.1. □

Theorem 2.11 shows that

$$\operatorname{rank}\big(\mathscr{H}_{i,j}(\sigma H)\big) = \mathtt{n}(\mathscr{B}), \qquad \text{for } \mathtt{p}i \geq \mathtt{n}(\mathscr{B}) \text{ and } \mathtt{m}j \geq \mathtt{n}(\mathscr{B}).$$

This suggests a method to find the order $\mathtt{n}(\mathscr{B})$ of the minimal realization of H: compute the rank of the *finite* Hankel matrix $\mathscr{H}_{i,j}(\sigma H)$, where $\mathtt{n}_{\max} := \min(\mathtt{p}i, \mathtt{m}j)$ is an upper bound of the order. Algorithms for computing the order and parameters of the minimal realization are presented in Chapter 3.1.

Linear time-invariant model complexity

Associate with a linear time-invariant dynamical system $\mathscr{B}$, we have defined the following system invariants:

$\mathtt{m}(\mathscr{B})$	—	number of inputs,	$\mathtt{n}(\mathscr{B})$	—	order, and
$\mathtt{p}(\mathscr{B})$	—	number of outputs,	$\mathtt{l}(\mathscr{B})$	—	lag.

The complexity of a linear static model $\mathscr{B}$ is the number of inputs $\mathtt{m}(\mathscr{B})$ of $\mathscr{B}$ or, equivalently, the dimension $\dim(\mathscr{B})$ of $\mathscr{B}$. Except for the class of autonomous systems, however, the dimension of a dynamical model is infinite. We define the restriction $\mathscr{B}|_{[1,T]}$ of $\mathscr{B}$ to the interval $[1,T]$,

$$\mathscr{B}|_{[1,T]} := \{\, w \in \mathbb{R}^T \mid \text{there exist } w_{\text{p}} \text{ and } w_{\text{f}}, \text{ such that } (w_{\text{p}}, w, w_{\text{f}}) \in \mathscr{B} \,\}. \quad (\mathscr{B}|_{[1,T]})$$

For a linear time-invariant model $\mathscr{B}$ and for $T > \mathtt{n}(\mathscr{B})$,

$$\dim(\mathscr{B}|_{[1,T]}) = \mathtt{m}(\mathscr{B})T + \mathtt{n}(\mathscr{B}) \leq \mathtt{m}(\mathscr{B})T + \mathtt{l}(\mathscr{B})\mathtt{p}(\mathscr{B}), \qquad (\dim \mathscr{B})$$

which shows that the pairs of natural numbers

$$\big(\mathtt{m}(\mathscr{B}), \mathtt{n}(\mathscr{B})\big) \qquad \text{and} \qquad \big(\mathtt{m}(\mathscr{B}), \mathtt{l}(\mathscr{B})\big)$$

characterize the model's complexity. The elements of the model class $\mathscr{L}_{\mathtt{m},\mathtt{l}}^{\mathtt{q}}$ are linear time-invariant systems of complexity bounded by the pair $(\mathtt{m},\mathtt{l})$ and, similarly, the elements of the model class $\mathscr{L}_{\mathtt{m}}^{\mathtt{q},\mathtt{n}}$ are linear time-invariant systems of complexity

bounded by the pair $(\mathtt{m},\mathtt{n})$. A static model is a special case of a dynamic model when the lag (or the order) is zero. This is reflected in the notation $\mathscr{L}_{\mathtt{m},\mathtt{l}}^{\mathtt{q},\mathtt{n}}$: the linear static model class $\mathscr{L}_{\mathtt{m},0}$ corresponds to the linear time-invariant model class $\mathscr{L}_{\mathtt{m},\mathtt{l}}$ with $\mathtt{l} = 0$.

Note that in the autonomous case, *i.e.*, with $\mathtt{m}(\mathscr{B}) = 0$, $\dim(\mathscr{B}) = \mathtt{n}$. The dimension of the system corresponds to the number of degrees of freedom in selecting a trajectory. In the case of an autonomous system, the trajectory depends only on the initial condition (an $\mathtt{n}(\mathscr{B})$ dimensional vector). In the presence of inputs, the number of degrees of freedom due to the initial condition is increased on each time step by the number of inputs, due to the free variables. Asymptotically as $T \to \infty$, the term $\mathtt{m}T$ in ($\dim \mathscr{B}$) dominates the term $\mathtt{n}$. Therefore, in comparing linear time-invariant system's complexities, by convention, a system with more inputs is more complex than a system with less inputs, irrespective of their state dimensions.

2.3 Exact and approximate data modeling

General setting for data modeling

In order to treat static, dynamic, linear, and nonlinear modeling problems with unified terminology and notation, we need an abstract setting that is general enough to accommodate all envisaged applications. Such a setting is described in this section.

The data $\mathscr{D}$ and a model $\mathscr{B}$ for the data are subsets of a *universal set* $\mathscr{U}$ of possible observations. In static modeling problems, $\mathscr{U}$ is a real $\mathtt{q}$-dimensional vector space $\mathbb{R}^{\mathtt{q}}$, *i.e.*, the observations are real valued vectors. In dynamic modeling problems, $\mathscr{U}$ is a function space $(\mathbb{R}^{\mathtt{q}})^{\mathscr{T}}$, with $\mathscr{T}$ being $\mathbb{Z}$ in the discrete-time case and $\mathbb{R}$ in the continuous-time case.

Note 2.12 (Categorical data and finite automata). In modeling problems with categorical data and finite automata, the universal set $\mathscr{U}$ is discrete and may be finite.

We consider data sets $\mathscr{D}$ consisting of a finite number of observations

$$\mathscr{D} = \{\, w_{\text{d},1}, \ldots, w_{\text{d},N} \,\} \subset \mathscr{U}.$$

In discrete-time dynamic modeling problems, the $w_{\text{d},j}$'s are trajectories, *i.e.*,

$$w_{\text{d},j} = \big(w_{\text{d},j}(1), \ldots, w_{\text{d},j}(T_j)\big), \qquad \text{with } w_{\text{d},j}(t) \in \mathbb{R}^{\mathtt{q}} \text{ for all } t.$$

In dynamic problems, the data $\mathscr{D}$ often consists of a single trajectory $w_{\text{d},1}$, in which case the subscript index 1 is skipped and $\mathscr{D}$ is identified with w_{d}. In static modeling problems, an observation $w_{\text{d},j}$ is a vector and the alternative notation $d_j = w_{\text{d},j}$ is used in order to emphasise the fact that the observations do not depend on time.

Note 2.13 (Given data vs general trajectory). In order to distinguish a general trajectory w of the system from the given data w_{d} (a specific trajectory) we use the subscript "d" in the notation of the given data.

A *model class* $\mathscr{M}$ is a set of sets of $\mathscr{U}$, *i.e.*, $\mathscr{M}$ is an element of the power set $2^{\mathscr{U}}$ of $\mathscr{U}$. We consider the generic model classes of

- linear static models $\mathscr{L}_0$,
- linear time-invariant models $\mathscr{L}$, and
- polynomial static models $\mathscr{P}$ (see Chapter 6).

In some cases, however, subclasses of the generic classes above are of interest. For examples, the controllable and finite impulse response model subclasses of the class of linear time invariant models, and the ellipsoids subclass of the class of second order polynomial models (conic sections).

The complexity $\mathtt{c}$ of a model $\mathscr{B}$ is a vector of positive integers

$$\mathtt{c}(\mathscr{B}) := \begin{cases} \mathtt{m}(\mathscr{B}) = \dim(\mathscr{B}), & \text{if } \mathscr{B} \in \mathscr{L}_0, \\ \big(\mathtt{m}(\mathscr{B}), \mathtt{l}(\mathscr{B})\big) \text{ or } \big(\mathtt{m}(\mathscr{B}), \mathtt{n}(\mathscr{B})\big), & \text{if } \mathscr{B} \in \mathscr{L}, \\ \big(\mathtt{m}(\mathscr{B}), \deg(R)\big), \text{ where } \mathscr{B} = \ker(R), & \text{if } \mathscr{B} \in \mathscr{P}. \end{cases} \qquad (\mathtt{c}(\mathscr{B}))$$

Complexities are compared in this book by the lexicographic ordering, *i.e.*, two complexities are compared by comparing their corresponding elements in the increasing order of the indexes. The first time an index is larger, the corresponding complexity is declared larger. For linear time-invariant dynamic models, this convention and the ordering of the elements in $\mathtt{c}(\mathscr{B})$ imply that a model with more inputs is always more complex than a model with less inputs irrespective of their orders.

The complexity $\mathtt{c}$ of a model class $\mathscr{M}$ is the largest complexity of a model in the model class. Of interest is the restriction of the generic model classes $\mathscr{M}$ to subclasses $\mathscr{M}_{\mathtt{c}_{\max}}$ of models with bounded complexity, *e.g.*, $\mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}_{\max}}$, with $\mathtt{m} < \mathtt{q}$.

Exact data modeling

A model $\mathscr{B}$ is an *exact model* for the data $\mathscr{D}$ if $\mathscr{D} \subset \mathscr{B}$. Otherwise, it is an *approximate model*. An exact model for the data may not exist in a model class $\mathscr{M}_{\mathtt{c}_{\max}}$ of bounded complexity. This is generically the case when the data is noisy and the data set $\mathscr{D}$ is large enough (relative to the model complexity). A practical data modeling problem must involve approximation. Our starting point, however, is the simpler problem of exact data modeling.

Problem 2.14 (Exact data modeling). Given data $\mathscr{D} \subset \mathscr{U}$ and a model class $\mathscr{M}_{\mathtt{c}_{\max}} \in 2^{\mathscr{U}}$, find a model $\widehat{\mathscr{B}}$ in $\mathscr{M}_{\mathtt{c}_{\max}}$ that contains the data and has minimal (in the lexicographic ordering) complexity or assert that such a model does not exist, *i.e.*,

$$\text{minimize} \quad \text{over } \mathscr{B} \in \mathscr{M}_{\mathtt{c}_{\max}} \quad \mathtt{c}(\mathscr{B}) \quad \text{subject to} \quad \mathscr{D} \subset \mathscr{B} \qquad \text{(EM)}$$

The question occurs:

(Existence of exact model) Under what conditions on the data $\mathscr{D}$ and the model class $\mathscr{M}_{\mathtt{c}_{\max}}$ does a solution to problem (EM) exist?

If a solution exists, it is unique. This unique solution is called the *most powerful unfalsified model* for the data $\mathscr{D}$ in the model class $\mathscr{M}_{\mathtt{c}_{\max}}$ and is denoted by $\mathscr{B}_{\mathrm{mpum}}(\mathscr{D})$. (The model class $\mathscr{M}_{\mathtt{c}_{\max}}$ is not a part of the notation $\mathscr{B}_{\mathrm{mpum}}(\mathscr{D})$ and is understood from the context.)

Suppose that the data $\mathscr{D}$ is generated by a model $\mathscr{B}_0$ in the model class $\mathscr{M}_{\mathtt{c}_{\max}}$, *i.e.*,

$$\mathscr{D} \subset \mathscr{B}_0 \in \mathscr{M}_{\mathtt{c}_{\max}}.$$

Then, the exact modeling problem has a solution in the model class $\mathscr{M}_{\mathtt{c}_{\max}}$, however, the solution $\mathscr{B}_{\mathrm{mpum}}(\mathscr{D})$ may not be the data generating model $\mathscr{B}_0$. The question occurs:

(Identifiability) Under what conditions on the data $\mathscr{D}$, the data generating model $\mathscr{B}_0$, and the model class $\mathscr{M}_{\mathtt{c}_{\max}}$, the most powerful unfalsified model $\mathscr{B}_{\mathrm{mpum}}(\mathscr{D})$ in $\mathscr{M}_{\mathtt{c}_{\max}}$ coincides with the data generating model $\mathscr{B}_0$?

Example 2.15 (Exact data fitting by a linear static model). Existence of a linear static model $\widehat{\mathscr{B}}$ of bounded complexity $\mathtt{m}$ for the data $\mathscr{D}$ is equivalent to rank deficiency of the matrix

$$\Phi(\mathscr{D}) := \begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix} \in \mathbb{R}^{\mathtt{q} \times N},$$

composed of the data. (Show this.) Moreover, the rank of the matrix $\Phi(\mathscr{D})$ is equal to the *minimal* dimension of an exact model for $\mathscr{D}$

$$\text{existence of } \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},0}, \text{ such that } \mathscr{D} \subset \widehat{\mathscr{B}} \quad \iff \quad \operatorname{rank}\big(\Phi(\mathscr{D})\big) \leq \mathtt{m}. \qquad (*)$$

The exact model

$$\widehat{\mathscr{B}} = \operatorname{image}\big(\Phi(\mathscr{D})\big) \qquad (**)$$

of minimal dimension

$$\mathtt{c}(\mathscr{B}) = \operatorname{rank}\big(\Phi(\mathscr{D})\big)$$

always exists and is unique.

The equivalence $(*)$ between data modeling and the concept of rank is the basis for application of linear algebra and matrix computations to linear data modeling. Indeed, $(**)$ provides an *algorithm* for exact linear static data modeling. As shown next, exact data modeling has also direct relevance to approximate data modeling.

Approximate data modeling

When an exact model does not exist in the considered model class, an approximate model that is in some sense "close" to the data is aimed at instead. Closeness is measured by a suitably defined criterion. This leads to the following approximate data modeling problem.

Problem 2.16 (Approximate data modeling). Given data $\mathscr{D} \subset \mathscr{U}$, a model class $\mathscr{M}_{\mathtt{c}_{\max}} \in 2^{\mathscr{U}}$, and a measure $f(\mathscr{D},\mathscr{B})$ for the lack of fit of the data $\mathscr{D}$ by a model $\mathscr{B}$, find a model $\widehat{\mathscr{B}}$ in the model class $\mathscr{M}_{\mathtt{c}_{\max}}$ that minimizes the lack of fit, *i.e.*,

$$\text{minimize} \quad \text{over } \mathscr{B} \in \mathscr{M}_{\mathtt{c}_{\max}} \quad f(\mathscr{D},\mathscr{B}). \tag{AM}$$

□

Since an observation w is a point in and the model $\mathscr{B}$ is a subset of the data space $\mathscr{U}$, it is natural to measure the lack of fit between w and $\mathscr{B}$ by the *geometric distance*

$$\operatorname{dist}(w,\mathscr{B}) := \min_{\widehat{w}\in\mathscr{B}} \|w-\widehat{w}\|_2. \tag{dist($w,\mathscr{B}$)}$$

The auxiliary variable $\widehat{w}$ is the best approximation of w in $\mathscr{B}$. Geometrically, it is the orthogonal projection of w on $\mathscr{B}$.

For the set of observations $\mathscr{D}$, we define the distance from $\mathscr{D}$ to $\mathscr{B}$ as

$$\operatorname{dist}(\mathscr{D},\mathscr{B}) := \min_{\widehat{w}_1,\dots,\widehat{w}_N\in\mathscr{B}} \sqrt{\sum_{j=1}^{N} \|w_{\mathrm{d},j}-\widehat{w}_j\|_2^2}. \tag{dist}$$

The set of points

$$\widehat{\mathscr{D}} = \{\widehat{w}_1,\dots,\widehat{w}_N\}$$

in the definition of (dist) is an approximation of the data $\mathscr{D}$ in the model $\mathscr{B}$. Note that problem (dist) is separable, *i.e.*, it decouples into N independent problems (dist($w,\mathscr{B}$)).

Algorithms for computing the geometric distance are discussed in Section 3.2, in the case of linear models, and in Chapter 6, in the case of polynomial models.

Note 2.17 (Invariance of (dist) *to rigid transformation).* The geometric distance $\operatorname{dist}(\mathscr{D},\mathscr{B})$ is invariant to a rigid transformation, *i.e.*, translation, rotation, and reflection of the data points and the model.

An alternative distance measure, called *algebraic distance*, is based on a kernel representation $\mathscr{B} = \ker(R)$ of the model $\mathscr{B}$. Since R is a mapping from $\mathscr{U}$ to $\mathbb{R}^g$, such that

$$w \in \mathscr{B} \quad \iff \quad R(w) = 0,$$

we have that

$$\|R(w)\|_{\mathrm{F}} > 0 \quad \iff \quad w \notin \mathscr{B}.$$

The algebraic "distance" measures the lack of fit between w and $\mathscr{B}$ by the "size" $\|R(w)\|_{\mathrm{F}}$ of the residual $R(w)$. For a data set $\mathscr{D}$, we define

$$\operatorname{dist}'(\mathscr{D},\mathscr{B}) := \sqrt{\sum_{j=1}^{N} \|R(w_{\mathrm{d},j})\|_{\mathrm{F}}^2}, \tag{dist$'$}$$

The algebraic distance depends on the choice of the parameter R in a kernel representation of the model, while the geometric distance is representation invariant. In addition, the algebraic distance is not invariant to a rigid transformation. However, a modification of the algebraic distance that is invariant to a rigid transformation is presented in Section 6.3.

Example 2.18 (Geometric distance for linear and quadratic models). The two plots in Figure 2.3 illustrate the geometric distance (dist) from a set of eight data points

$$\mathscr{D} = \{\, d_i = (x_i, y_i) \mid i = 1,\dots,8 \,\}$$

in the plane to, respectively, linear $\mathscr{B}_1$ and quadratic $\mathscr{B}_2$ models. As its name suggests, $\operatorname{dist}(\mathscr{D},\mathscr{B})$ has geometric interpretation—in order to compute the geometric distance, we project the data points on the models. This is a simple task (linear least squares problem) for linear models but a nontrivial task (nonconvex optimization problem) for nonlinear models. In contrast, the algebraic "distance" (not visualised in the figure) has no simple geometrical interpretation but is easy to compute for linear and nonlinear models alike.

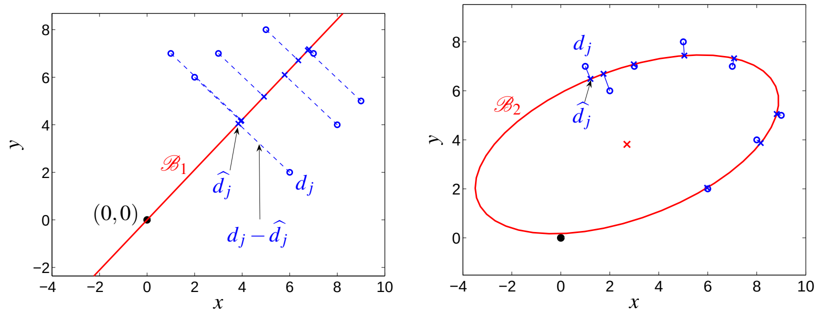


Fig. 2.3 Geometric distance from eight data points to a linear (left) and quadratic (right) models

Note 2.19 (Approximate modeling in the case of exact data). If an exact model $\mathscr{B}$ exists in the model class $\mathscr{M}_{\mathtt{c}_{\max}}$, then $\mathscr{B}$ is a global optimum point of the approximate modeling problem (AM) (irrespective of the approximation criterion f being used). Indeed,

$$\mathscr{D} \subset \mathscr{B} \quad \iff \quad \operatorname{dist}(\mathscr{D},\mathscr{B}) = \operatorname{dist}'(\mathscr{D},\mathscr{B}) = 0.$$

An optimal approximate model, *i.e.*, a solution of (AM), however, need not be unique. In contrast, the most powerful unfalsified model is unique. This is due to the fact that (AM) imposes an upper bound but does not minimize the model complexity, while (EM) minimizes the model complexity. As a result, when

$$\mathtt{c}\big(\mathscr{B}_{\text{mpum}}(\mathscr{D})\big) < \mathtt{c}_{\max},$$

(AM) has a nonunique solution. In the next section, we present a more general approximate data modeling problem formulation that minimizes simultaneously the complexity as well as the fitting error.

The terminology "geometric" and "algebraic" distance comes from the computer vision application of the methods for fitting curves and surfaces to data. In the system identification community, the geometric fitting method is related to the *misfit* approach and the algebraic fitting criterion is related to the *latency* approach. Misfit and latency computation are data smoothing operations. For linear time-invariant systems, the misfit and latency can be computed efficiently by Riccati type recursions. In the statistics literature, the geometric fitting is related to errors-in-variable estimation and the algebraic fitting is related to classical regression estimation, see Table 2.2.

Table 2.2 Correspondence among terms for data fitting criteria in different fields.

computer vision	system identification	statistics	mathematics
geometric fitting	misfit	errors-in-variables	implicit function
algebraic fitting	latency	regression	function

Example 2.20 (Algebraic fit and errors-in-variables modeling). From a statistical point of view, the approximate data modeling problem (AM) with the geometric fitting criterion (dist) yields a maximum likelihood estimator for the true model $\mathscr{B}_0$ in the errors-in-variables setup

$$w_{\text{d},j} = w_{0,j} + \widetilde{w}_j, \tag{EIV}$$

where

$$\mathscr{D}_0 := \{w_{0,1}, \dots, w_{0,N}\} \subset \mathscr{B}_0$$

is the true data and

$$\widetilde{\mathscr{D}} := \{\widetilde{w}_1, \dots, \widetilde{w}_N\}$$

is the measurement noise, which is assumed to be a set of independent, zero mean, Gaussian random vectors, with covariance matrix $\sigma^2 I$. □

Example 2.21 (Algebraic fit by a linear model and regression). A linear model class, defined by the input/output representation $\mathscr{B}_{\text{i/o}}(\Theta)$ and algebraic fitting criterion (dist′), where

$$w := \operatorname{col}(u, y) \qquad \text{and} \qquad R(w) := \Theta^\top u - y$$

lead to the ordinary linear least squares problem

$$\text{minimize} \quad \text{over } \Theta \in \mathbb{R}^{\mathtt{m}\times\mathtt{p}} \quad \big\|\Theta^\top \Phi(u_\text{d}) - \Phi(y_\text{d})\big\|_\text{F}. \tag{LS}$$

The statistical setting for the least squares approximation problem (LS) is the classical regression model

$$R(w_{\text{d},j}) = e_j, \tag{REG}$$

where $e_1, \dots, e_N$ are zero mean independent and identically distributed random variables. Gauss-Markov's theorem states that the least squares approximate solution is the best linear unbiased estimator for the regression model (REG).

Complexity–accuracy trade-off

Data modeling is a mapping from a given data set $\mathscr{D}$, to a model $\mathscr{B}$ in a given model class $\mathscr{M}$:

$$\text{data set } \mathscr{D} \subset \mathscr{U} \xrightarrow{\text{data modeling problem}} \text{model } \mathscr{B} \in \mathscr{M} \in 2^{\mathscr{U}}.$$

A data modeling problem is defined by specifying the model class $\mathscr{M}$ and one or more modeling criteria. Basic criteria in any data modeling problem are:

- "simple" model, measured by the model complexity $\mathtt{c}(\mathscr{B})$, and
- "good" fit of the data by the model, measured by (vector) cost function $F(\mathscr{D}, \mathscr{B})$.

Small complexity $\mathtt{c}(\mathscr{B})$ and small fitting error $F(\mathscr{D}, \mathscr{B})$, however, are contradicting objectives, so that a core issue throughout data modeling is the complexity–accuracy trade-off. A generic data modeling problem is:

Given a data set $\mathscr{D} \in \mathscr{U}$ and a measure F for the fitting error, solve the multiobjective optimization problem:

$$\text{minimize} \quad \text{over } \mathscr{B} \in \mathscr{M} \quad \begin{bmatrix} \mathtt{c}(\mathscr{B}) \\ F(\mathscr{D}, \mathscr{B}) \end{bmatrix}. \tag{DM}$$

Next we consider the special cases of linear static models and linear time-invariant dynamic models with $F(\mathscr{D}, \mathscr{B})$ being $\operatorname{dist}(\mathscr{D}, \mathscr{B})$ or $\operatorname{dist}'(\mathscr{D}, \mathscr{B})$. The model class assumption implies that $\dim(\mathscr{B})$ is a complexity measure in both static and dynamic cases.

Two possible scalarizations: low-rank approximation and rank minimization

The data set $\mathscr{D}$, can be parametrized by a real vector $p \in \mathbb{R}^{n_p}$. (Think of the vector p as a representation of the data in the computer memory.) For a linear model $\mathscr{B}$ and exact data $\mathscr{D}$, there is a relation between the model complexity and the rank of a data matrix $\mathscr{S}(p)$:

$$\mathtt{c}\big(\mathscr{B}_{\text{mpum}}(\mathscr{D})\big) = \operatorname{rank}\big(\mathscr{S}(p)\big). \tag{$*$}$$

The mapping

$$\mathscr{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times n}$$

from the data parameter vector p to the data matrix $\mathscr{S}(p)$ depends on the application. For example, $\mathscr{S}(p) = \Phi(\mathscr{D})$ is unstructured in the case of linear static modeling (see Example 2.15) and $\mathscr{S}(p) = \mathscr{H}(w_{\mathrm{d}})$ is Hankel structured in the case of autonomous linear time-invariant dynamic model identification,

Let p be the parameter vector for the data $\mathscr{D}$ and $\widehat{p}$ be the parameter vector for the data approximation $\widehat{\mathscr{D}}$. The geometric distance $\operatorname{dist}(\mathscr{D},\mathscr{B})$ can be expressed in terms of the parameter vectors p and $\widehat{p}$ as

$$\text{minimize} \quad \text{over } \widehat{p} \quad \|p-\widehat{p}\|_2 \quad \text{subject to} \quad \widehat{\mathscr{D}} \subset \mathscr{B}.$$

Moreover, the norm in the parameter space $\mathbb{R}^{n_p}$ can be chosen as weighted 1-, 2-, and ∞-(semi)norms:

$$\begin{aligned}
\|\widetilde{p}\|_{w,1} &:= \|w \odot \widetilde{p}\|_1 := \textstyle\sum_{i=1}^{n_p} |w_i \widetilde{p}_i|, \\
\|\widetilde{p}\|_{w,2} &:= \|w \odot \widetilde{p}\|_2 := \sqrt{\textstyle\sum_{i=1}^{n_p} (w_i \widetilde{p})^2}, \\
\|\widetilde{p}\|_{w,\infty} &:= \|w \odot \widetilde{p}\|_\infty := \max_{i=1,\dots,n_p} |w_i \widetilde{p}_i|,
\end{aligned} \tag{$\|\cdot\|_w$}$$

where w is a vector with nonnegative elements, specifying the weights, and $\odot$ is the element-wise (Hadamard) product.

Using the data parametrization $(*)$ and one of the distance measures $(\|\cdot\|_w)$, the data modeling problem (DM) becomes the biobjective matrix approximation problem:

$$\text{minimize} \quad \text{over } \widehat{p} \quad \begin{bmatrix} \operatorname{rank}\big(\mathscr{S}(\widehat{p})\big) \\ \|p-\widehat{p}\| \end{bmatrix}. \tag{DM'}$$

Two possible ways to scalarize the biobjective problem (DM') are:

1. misfit minimization subject to a bound r on the model complexity

$$\text{minimize} \quad \text{over } \widehat{p} \quad \|p-\widehat{p}\| \quad \text{subject to} \quad \operatorname{rank}\big(\mathscr{S}(\widehat{p})\big) \le r. \tag{SLRA}$$

2. model complexity minimization subject to a bound ε on the fitting error

$$\text{minimize} \quad \text{over } \widehat{p} \quad \operatorname{rank}\big(\mathscr{S}(\widehat{p})\big) \quad \text{subject to} \quad \|p-\widehat{p}\| \le \varepsilon. \tag{RM}$$

Problem (SLRA) is a structured low-rank approximation problem and (RM) is a rank minimization problem.

By varying the parameters r and ε from zero to infinity, both problems sweep the trade-off curve (set of Pareto optimal solutions) of (DM'). Note, however, that r ranges over the natural numbers and only small values are of practical interest. In addition, in applications often a "suitable" value for r can be chosen a priori or is even a part of the problem specification. In contrast, ε is a positive real number and is data dependent, so that a "suitable" value is not readily available. These considerations, suggest that the structured low-rank approximation problem is a more convenient scalarization of (DM') for solving practical data modeling problems.

Convex relaxation algorithms for solving (DM') are presented in Section 3.3.

2.4 Unstructured low-rank approximation

Linear static data modeling leads to unstructured low-rank approximation. Vice verse, unstructured low-rank approximation problems can be given the interpretation (or motivation) of linear static data modeling problems. As argued in Section 1.1, these are equivalent problems. The data modeling view of the problem makes link to applications. The low-rank approximation view of the problem makes link to computational algorithms for solving the problem.

Problem 2.22 (Unstructured low-rank approximation). Given a matrix $D \in \mathbb{R}^{\mathtt{q}\times N}$, with $\mathtt{q} \le N$, a matrix norm $\|\cdot\|$, and an integer $\mathtt{m}$, $0 < \mathtt{m} < \mathtt{q}$, find a matrix

$$\widehat{D}^* := \arg\min_{\widehat{D}} \|D-\widehat{D}\| \quad \text{subject to} \quad \operatorname{rank}(\widehat{D}) \le \mathtt{m}. \tag{LRA}$$

□

The matrix $\widehat{D}^*$ is an optimal rank-$\mathtt{m}$ (or less) approximation of D with respect to the given norm $\|\cdot\|$.

The special case of (LRA) with $\|\cdot\|$ being the weighted 2-norm

$$\|\Delta D\|_W := \sqrt{\operatorname{vec}^\top(\Delta D) W \operatorname{vec}(\Delta D)}, \qquad \text{for all } \Delta D \tag{$\|\cdot\|_W$}$$

where $W \in \mathbb{R}^{\mathtt{q}N\times\mathtt{q}N}$ is a positive definite matrix, is called *weighted low-rank approximation problem*. In turn, special cases of the weighted low-rank approximation problem are obtained when the weight matrix W has diagonal, block diagonal, or some other structure.

- *Element-wise weighting:*

$$W = \operatorname{diag}(w_1,\dots,w_{\mathtt{q}N}), \qquad \text{where} \quad w_i > 0, \text{ for } i = 1,\dots,\mathtt{q}N.$$

- *Column-wise weighting:*

$$W = \operatorname{diag}(W_1, \dots, W_N), \qquad \text{where} \quad W_j \in \mathbb{R}^{\mathtt{q} \times \mathtt{q}},\ W_j > 0,\ \text{for } j = 1, \dots, N.$$

- *Column-wise weighting with equal weight matrix for all columns:*

$$W = \operatorname{diag}(W_\mathrm{l}, \dots, W_\mathrm{l}), \qquad \text{where} \quad W_\mathrm{l} \in \mathbb{R}^{\mathtt{q} \times \mathtt{q}},\ W_\mathrm{l} > 0.$$

- *Row-wise weighting:*

$$\bar{W} = \operatorname{diag}(W_1, \dots, W_\mathtt{q}), \qquad \text{where} \quad W_i \in \mathbb{R}^{N \times N},\ W_i > 0,\ \text{for } i = 1, \dots, \mathtt{q},$$

and $\bar{W}$ is a matrix, such that

$$\|\Delta D\|_W = \|\Delta D^\top\|_{\bar{W}}, \qquad \text{for all } \Delta D.$$

- *Row-wise weighting with equal weight matrix for all rows:*

$$\bar{W} = \operatorname{diag}(\underbrace{W_\mathrm{r}, \dots, W_\mathrm{r}}_{\mathtt{q}}), \qquad \text{where} \quad W_\mathrm{r} \in \mathbb{R}^{N \times N},\ W_\mathrm{r} > 0.$$

Figure 2.4 shows the hierarchy of weighted low-rank approximation problems, according to the structure of the weight matrix W. Exploiting the structure of the weight matrix allows more efficient solution of the corresponding weighted low-rank approximation problems compared to the general problem with unstructured W.

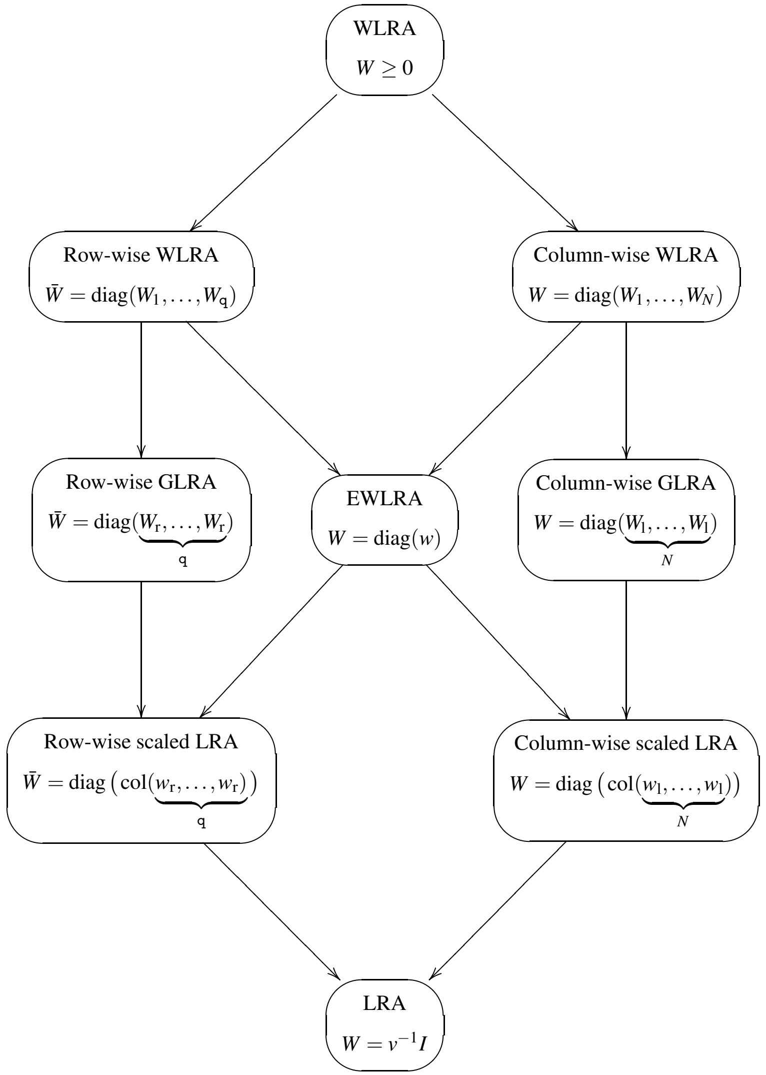
As shown in the next section left/right weighting with equal matrix for all rows/columns corresponds to approximation criteria $\|\sqrt{W_\mathrm{l}}\Delta D\|_\mathrm{F}$ and $\|\Delta D\sqrt{W_\mathrm{r}}\|_\mathrm{F}$. The approximation problem with criterion $\|\sqrt{W_\mathrm{l}}\Delta D\sqrt{W_\mathrm{r}}\|_\mathrm{F}$ is called *two-sided weighted* and is also known as the generalized low-rank approximation problem. This latter problem allows analytic solution in terms of the singular value decomposition of the data matrix.

Special cases with known analytic solutions

An extreme special case of the weighted low-rank approximation problem is the "unweighted" case, *i.e.*, weight matrix a multiple of the identity $W = v^{-1}I$, for some $v > 0$. Then, $\|\cdot\|_W$ is proportional to the Frobenius norm $\|\cdot\|_\mathrm{F}$ and the low-rank approximation problem has an analytic solution in terms of the singular value decomposition of D. The results is known as the Eckart–Young–Mirsky theorem or the matrix approximation lemma. In view of its importance, we refer to this case as the *basic low-rank approximation problem*.

Theorem 2.23 (Eckart–Young–Mirsky). *Let*

$$D = U\Sigma V^\top$$


WLRA
$W \geq 0$
Row-wise WLRA
$\bar{W} = \operatorname{diag}(W_1, \dots, W_\mathtt{q})$
Column-wise WLRA
$W = \operatorname{diag}(W_1, \dots, W_N)$
Row-wise GLRA
$\bar{W} = \operatorname{diag}(\underbrace{W_\mathrm{r}, \dots, W_\mathrm{r}}_{\mathtt{q}})$
EWLRA
$W = \operatorname{diag}(w)$
Column-wise GLRA
$W = \operatorname{diag}(\underbrace{W_\mathrm{l}, \dots, W_\mathrm{l}}_{N})$
Row-wise scaled LRA
$\bar{W} = \operatorname{diag}\big(\operatorname{col}(\underbrace{w_\mathrm{r}, \dots, w_\mathrm{r}}_{\mathtt{q}})\big)$
Column-wise scaled LRA
$W = \operatorname{diag}\big(\operatorname{col}(\underbrace{w_\mathrm{l}, \dots, w_\mathrm{l}}_{N})\big)$
LRA
$W = v^{-1}I$

LRA	— low-rank approximation	GLRA	— generalized low-rank approximation
WLRA	— weighted low-rank approximation	EWLRA	— element-wise weighted LRA

Fig. 2.4 Hierarchy of weighted low-rank approximation problems according to the structure of the weight matrix W. On the left side are weighted low-rank approximation problems with row-wise weighting and on the right side are weighted low-rank approximation problems with column-wise weighting. The generality of the problem reduces from top to bottom.

be the singular value decomposition of D and partition U, $\Sigma =: \operatorname{diag}(\sigma_1,\dots,\sigma_{\mathtt{q}})$, and V as follows:

$$U =: \begin{array}{cc} \mathtt{m} & \mathtt{q}-\mathtt{m} \\ \end{array} \begin{bmatrix} U_1 & U_2 \end{bmatrix} \mathtt{q}, \quad \Sigma =: \begin{array}{c} \begin{array}{cc}\mathtt{m} & \mathtt{q}-\mathtt{m}\end{array} \\ \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \end{array} \begin{array}{c} \mathtt{m} \\ \mathtt{q}-\mathtt{m} \end{array} \quad \text{and} \quad V =: \begin{array}{cc} \mathtt{m} & \mathtt{q}-\mathtt{m} \\ \end{array} \begin{bmatrix} V_1 & V_2 \end{bmatrix} N,$$

Then the rank-$\mathtt{m}$ matrix, obtained from the truncated singular value decomposition

$$\widehat{D}^* = U_1 \Sigma_1 V_1^\top,$$

is such that

$$\|D-\widehat{D}^*\|_{\mathrm{F}} = \min_{\operatorname{rank}(\widehat{D})\leq \mathtt{m}} \|D-\widehat{D}\|_{\mathrm{F}} = \sqrt{\sigma_{\mathtt{m}+1}^2+\cdots+\sigma_{\mathtt{q}}^2}.$$

The minimizer $\widehat{D}^*$ is unique if and only if $\sigma_{\mathtt{m}+1} \neq \sigma_{\mathtt{m}}$.

The proof is given in Appendix B.

Note 2.24 (Unitarily invariant norms). Theorem 2.23 holds for any norm $\|\cdot\|$ that is invariant under orthogonal transformations, *i.e.*, satisfying the relation

$$\|U\Delta D V\| = \|\Delta D\|, \qquad \text{for any } \Delta D \text{ and for any orthogonal matrices } U \text{ and } V.$$

Note 2.25 (Approximation in the spectral norm). For a matrix ΔD, let $\|\Delta D\|_2$ be the spectral (2-norm induced) matrix norm

$$\|\Delta D\|_2 = \sigma_{\max}(\Delta D).$$

Then

$$\min_{\operatorname{rank}(\widehat{D})=\mathtt{m}} \|D-\widehat{D}\|_2 = \sigma_{\mathtt{m}+1},$$

i.e., the optimal rank-$\mathtt{m}$ spectral norm approximation error is equal to the first neglected singular value. The truncated singular value decomposition yields an optimal approximation with respect to the spectral norm, however, in this case a minimizer is not unique even when the singular values $\sigma_{\mathtt{m}}$ and $\sigma_{\mathtt{m}+1}$ are different.

As defined, the low-rank approximation problem aims at a matrix $\widehat{D}$ that is a solution to the optimization problem (LRA). In data modeling problems, however, of primary interest is the optimal model, *i.e.*, the most powerful unfalsified model for $\widehat{D}^*$. Theorem 2.23 gives the optimal approximating matrix $\widehat{D}^*$ in terms of the singular value decomposition of the data matrix D. Minimal parameters of kernel and image representations of the corresponding optimal model are directly available from the factors of the singular value decomposition of D.

Corollary 2.26. *An optimal in the Frobenius norm approximate model for the data D in the model class $\mathscr{L}_{\mathtt{m},0}$,* i.e., *$\widehat{\mathscr{B}}^* := \mathscr{B}_{\text{mpum}}(\widehat{D}^*)$ is unique if and only if the singular values $\sigma_{\mathtt{m}}$ and $\sigma_{\mathtt{m}+1}$ of D are different, in which case*

$$\widehat{\mathscr{B}}^* = \ker(U_2^\top) = \operatorname{image}(U_1).$$

The proof is left as an exercise.

66 ⟨*low-rank approximation* 66⟩≡
```
function [R, P, dh] = lra(d, r)
[u, s, v] = svd(d); R = u(:, (r + 1):end)'; P = u(:, 1:r);
if nargout > 2, dh = u(:, 1:r) * s(1:r, 1:r) * v(:, 1:r)'; end
```
Defines:
  `lra`, used in chunks 87d, 90c, 102f, 103a, 193b, 194e, and 231a.

Corollary 2.27 (Nested approximations). *The optimal in the Frobenius norm approximate models $\widehat{\mathscr{B}}_{\mathtt{m}}^*$ for the data D in the model classes $\mathscr{L}_{\mathtt{m},0}$, where $\mathtt{m}=1,\dots,\mathtt{q}$ are nested,* i.e.,

$$\widehat{\mathscr{B}}_{\mathtt{q}} \subseteq \widehat{\mathscr{B}}_{\mathtt{q}-1} \subseteq \cdots \subset \widehat{\mathscr{B}}_1.$$

The proof is left as an exercise.

Note 2.28 (Efficient computation using QR factorization when $N \gg \mathtt{q}$). An optimal model $\widehat{\mathscr{B}}^*$ for D depends only on the left singular vectors of D. Since post multiplication of D by an orthogonal matrix Q does not change the left singular vectors $\widehat{\mathscr{B}}^*$ is an optimal model for the data matrix DQ.

For $N \gg \mathtt{q}$, computing the QR factorization

$$D^\top = \begin{bmatrix} R_1 \\ 0 \end{bmatrix} Q^\top, \qquad \text{where } R_1 \text{ is upper triangular,} \tag{QR}$$

and the singular value decomposition of R_1 is a more efficient alternative for finding $\widehat{\mathscr{B}}$ than computing the singular value decomposition of D.

An analytic solution in terms of the singular value decomposition, similar to the one in Theorem 2.23 is not known for the general weighted low-rank approximation problem. Presently the largest class of weighted low-rank approximation problems with analytic solution are those with a weight matrix of the form

$$W = W_{\mathrm{r}} \otimes W_{\mathrm{l}}, \qquad \text{where} \quad W_{\mathrm{l}} \in \mathbb{R}^{\mathtt{q}\times\mathtt{q}} \text{ and } W_{\mathrm{r}} \in \mathbb{R}^{N\times N} \tag{$W_{\mathrm{r}}\otimes W_{\mathrm{l}}$}$$

are positive definite matrices and $\otimes$ is the Kronecker product.

Using the identities

$$\operatorname{vec}(AXB) = (B^\top \otimes A)\operatorname{vec}(X)$$

and

$$(A_1\otimes B_1)(A_2\otimes B_2) = (A_1A_2)\otimes(B_1B_2),$$

we have

$$\begin{aligned}\|D-\widehat{D}\|_{W_\mathrm{r}\otimes W_\mathrm{l}} &= \sqrt{\operatorname{vec}^\top(\Delta D)\big(W_\mathrm{r}\otimes W_\mathrm{l}\big)\operatorname{vec}(\Delta D)}\\ &= \big\|\big(\sqrt{W_\mathrm{r}}\otimes\sqrt{W_\mathrm{l}}\big)\operatorname{vec}(\Delta D)\big\|_2\\ &= \big\|\operatorname{vec}\big(\sqrt{W_\mathrm{l}}\Delta D\sqrt{W_\mathrm{r}}\big)\big\|_2\\ &= \|\sqrt{W_\mathrm{l}}\Delta D\sqrt{W_\mathrm{r}}\|_\mathrm{F}.\end{aligned}$$

Therefore, the low-rank approximation problem (LRA) with norm ($\|\cdot\|_W$) and weight matrix ($W_\mathrm{r}\otimes W_\mathrm{l}$) is equivalent to the two-sided weighted (or generalized) low-rank approximation problem

$$\begin{array}{ll}\text{minimize} & \text{over } \widehat{D} \quad \|\sqrt{W_\mathrm{l}}(D-\widehat{D})\sqrt{W_\mathrm{r}}\|_\mathrm{F}\\ \text{subject to} & \operatorname{rank}(\widehat{D})\le \mathtt{m},\end{array}\qquad \text{(WLRA2)}$$

which has an analytic solution.

Theorem 2.29 (Two-sided weighted low-rank approximation). *Define the modified data matrix*

$$D_\mathrm{m} := \sqrt{W_\mathrm{l}}D\sqrt{W_\mathrm{r}},$$

and let $\widehat{D}_\mathrm{m}^*$ be the optimal (unweighted) low-rank approximation of D_m. Then

$$\widehat{D}^* := \big(\sqrt{W_\mathrm{l}}\big)^{-1}\widehat{D}_\mathrm{m}^*\big(\sqrt{W_\mathrm{r}}\big)^{-1},$$

is a solution of the following two-sided weighted low-rank approximation problem (WLRA2). A solution always exists. It is unique if and only if $\widehat{D}_\mathrm{m}^*$ is unique.

The proof is left as an exercise (Problem P.14).

Exercise 2.30. Using the result in Theorem 2.29, write a function that solves the two-sided weighted low-rank approximation problem (WLRA2).

Data modeling via (LRA)

The following problem is the approximate modeling problem (AM) for the model class of linear static models, *i.e.*, $\mathscr{M}_{\mathtt{c}_\mathrm{max}} = \mathscr{L}_{\mathtt{m},0}$, with the orthogonal distance approximation criterion, *i.e.*, $f(\mathscr{D},\mathscr{B}) = \operatorname{dist}(\mathscr{D},\mathscr{B})$. The norm $\|\cdot\|$ in the definition of dist, however, in the present context is a general vector norm, rather than the 2-norm.

Problem 2.31 (Static data modeling). Given N, $\mathtt{q}$-variable observations

$$\{d_1,\dots,d_N\}\subset\mathbb{R}^\mathtt{q},$$

a matrix norm $\|\cdot\|$, and model complexity $\mathtt{m}$, $0<\mathtt{m}<\mathtt{q}$,

$$\begin{array}{ll}\text{minimize} & \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{D} \quad \|D-\widehat{D}\|\\ \text{subject to} & \operatorname{image}(\widehat{D})\subseteq\widehat{\mathscr{B}} \text{ and } \dim(\widehat{\mathscr{B}})\le\mathtt{m},\end{array}\qquad (\text{AM } \mathscr{L}_{\mathtt{m},0})$$

where $D\in\mathbb{R}^{\mathtt{q}\times N}$ is the data matrix $D := \begin{bmatrix}d_1 & \cdots & d_N\end{bmatrix}$. □

A solution $\widehat{\mathscr{B}}^*$ to (AM $\mathscr{L}_{\mathtt{m},0}$) is an optimal approximate model for the data D with complexity bounded by $\mathtt{m}$. Of course, $\widehat{\mathscr{B}}^*$ depends on the approximation criterion, specified by the given norm $\|\cdot\|$. A justification for the choice of the norm $\|\cdot\|$ is provided in the errors-in-variables setting (see Example 2.20), *i.e.*, the data matrix D is assumed to be a noisy measurement of a true matrix D_0

$$\begin{aligned}&D = D_0+\widetilde{D},\quad \operatorname{image}(D_0)=\mathscr{B}_0,\quad \dim(\mathscr{B}_0)\le\mathtt{m},\\ &\qquad\text{and}\quad \operatorname{vec}(\widetilde{D})\sim \mathrm{N}(0,\sigma^2W^{-1}),\quad\text{where}\quad W\succ 0\end{aligned}\qquad (\text{EIV}_0)$$

and $\widetilde{D}$ is the measurement error that is assumed to be a random matrix with zero mean and normal distribution. The true matrix D_0 is "generated" by a model $\mathscr{B}_0$, with a known complexity bound $\mathtt{m}$. The model $\mathscr{B}_0$ is the object to be estimated in the errors-in-variables setting.

Proposition 2.32 (Maximum likelihood property of optimal static model $\widehat{\mathscr{B}}^*$). *Assume that the data is generated in the errors-in-variables setting (EIV$_0$), where the matrix $W\succ 0$ is known and the scalar σ^2 is unknown. Then a solution $\widehat{\mathscr{B}}^*$ to Problem 2.31 with weighted 2-norm ($\|\cdot\|_W$) is a maximum likelihood estimator for the true model $\mathscr{B}_0$.*

The proof is given in Appendix B.

The main assumption of Proposition 2.32 is

$$\operatorname{cov}(\operatorname{vec}(\widetilde{D})) = \sigma^2W^{-1},\qquad \text{with } W \text{ given}.$$

Note, however, that σ^2 is not given, so that the probability density function of $\widetilde{D}$ is not completely specified. Proposition 2.32 shows that the problem of computing the maximum likelihood estimator in the errors-in-variables setting is equivalent to Problem 2.22 with the weighted norm $\|\cdot\|_W$. Maximum likelihood estimation for density functions other than normal leads to low-rank approximation with norms other than the weighted 2-norm.

2.5 Structured low-rank approximation

Structured low-rank approximation is a low-rank approximation, in which the approximating matrix $\widehat{D}$ is constrained to have some a priori specified structure; typically, the same structure as the one of the data matrix D. Common structures encountered in applications are Hankel, Toeplitz, Sylvester, and circulant as well as their block versions. In order to state the problem in its full generality, we first define a structured matrix. Consider a mapping $\mathscr{S}$ from a parameter space $\mathbb{R}^{n_p}$ to a set of matrices $\mathbb{R}^{m\times n}$. A matrix $\widehat{D} \in \mathbb{R}^{m\times n}$ is called *$\mathscr{S}$-structured* if it is in the image of $\mathscr{S}$, *i.e.*, if there exists a parameter $\widehat{p} \in \mathbb{R}^{n_p}$, such that $\widehat{D} = \mathscr{S}(\widehat{p})$.

Problem SLRA (Structured low-rank approximation). Given a structure specification

$$\mathscr{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times n}, \qquad \text{with } m \leq n,$$

a parameter vector $p \in \mathbb{R}^{n_p}$, a vector norm $\|\cdot\|$, and an integer r, $0 < r < \min(m,n)$,

$$\text{minimize} \quad \text{over } \widehat{p} \quad \|p - \widehat{p}\| \quad \text{subject to} \quad \operatorname{rank}\big(\mathscr{S}(\widehat{p})\big) \leq r. \tag{SLRA}$$

The matrix $\widehat{D}^* := \mathscr{S}(\widehat{p}^*)$ is an optimal rank-r (or less) approximation of the matrix $D := \mathscr{S}(p)$, within the class of matrices with the same structure as D. Problem SLRA is a generalization of Problem 2.22. Indeed, choosing $\mathscr{S}$ to be vec^{-1} (an operation reconstructing a matrix M from the vector $\operatorname{vec}(M)$) and norm $\|\Delta p\|$ to be such that

$$\|\Delta p\| = \|\mathscr{S}(\Delta p)\|, \qquad \text{for all } \Delta p,$$

Problem SLRA is equivalent to Problem 2.22.

Special cases with known analytic solutions

We showed that some weighted unstructured low-rank approximation problems have global analytic solution in terms of the singular value decomposition. Similar result exists for circulant structured low-rank approximation. If the approximation criterion is a unitarily invariant matrix norm, the unstructured low-rank approximation (obtained for example from the truncated singular value decomposition) is unique. In the case of a circulant structure, it turns out that this unique minimizer also has circulant structure, so the structure constraint is satisfied without explicitly enforcing it in the approximation problem.

An efficient computational way of obtaining the circulant structured low-rank approximation is the fast Fourier transform. Consider the scalar case and let

$$P_k := \sum_{j=1}^{n_p} p_j e^{-\mathbf{i}\frac{2\pi}{n_p}kj}$$

be the discrete Fourier transform of p. Denote with $\mathscr{K}$ the subset of $\{1,\dots,n_p\}$ consisting of the indexes of the $\mathtt{m}$ largest elements of $\{|P_1|,\dots,|P_{n_p}|\}$. Assuming that $\mathscr{K}$ is uniquely defined by the above condition, *i.e.*, assuming that

$$k \in \mathscr{K} \text{ and } k' \notin \mathscr{K} \quad \Longrightarrow \quad |P_k| > |P_{k'}|,$$

the solution $\widehat{p}^*$ of the structured low-rank approximation problem with $\mathscr{S}$ a circulant matrix is unique and is given by

$$\widehat{p}^* = \frac{1}{n_p} \sum_{k\in\mathscr{K}} P_k e^{\mathbf{i}\frac{2\pi}{n_p}kj}.$$

Data modeling via (SLRA)

The reason to consider the more general structured low-rank approximation is that $D = \mathscr{S}(p)$ being low rank and Hankel structured is equivalent to p being generated by a linear time-invariant dynamic model. To show this, consider first the special case of a scalar Hankel structure

$$\mathscr{H}_{\mathtt{l}+1}(p) := \begin{bmatrix} p_1 & p_2 & \cdots & p_{n_p-\mathtt{l}} \\ p_2 & p_3 & \cdots & p_{n_p-\mathtt{l}+1} \\ \vdots & \vdots & & \vdots \\ p_{\mathtt{l}+1} & p_{\mathtt{l}+2} & \cdots & p_{n_p} \end{bmatrix}.$$

The approximation matrix

$$\widehat{D} = \mathscr{H}_{\mathtt{l}+1}(\widehat{p})$$

being rank deficient implies that there is a nonzero vector $R = \begin{bmatrix} R_0 & R_1 & \cdots & R_{\mathtt{l}} \end{bmatrix}$, such that

$$R\mathscr{H}_{\mathtt{l}+1}(\widehat{p}) = 0.$$

Due to the Hankel structure, this system of equations can be written as

$$R_0\widehat{p}_t + R_1\widehat{p}_{t+1} + \cdots + R_{\mathtt{l}}\widehat{p}_{t+\mathtt{l}} = 0, \quad \text{for } t = 1,\dots,n_p - \mathtt{l},$$

i.e., a homogeneous constant coefficients difference equation. Therefore, $\widehat{p}$ is a trajectory of an autonomous linear time-invariant system, defined by (KER). Recall that for an autonomous system $\mathscr{B}$,

$$\dim(\mathscr{B}|_{[1,T]}) = \mathtt{n}(\mathscr{B}), \qquad \text{for } T \geq \mathtt{n}(\mathscr{B}).$$

The scalar Hankel low-rank approximation problem is then equivalent to the following dynamic modeling problem. Given T samples of a scalar signal $w_{\mathrm{d}} \in \mathbb{R}^T$, a signal norm $\|\cdot\|$, and a model complexity $\mathtt{n}$,

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{w} \quad \|w_{\mathrm{d}} - \widehat{w}\| \\ &\text{subject to} && \widehat{w} \in \widehat{\mathscr{B}}|_{[1,T]} \text{ and } \dim(\widehat{\mathscr{B}}) \leq \mathtt{n}. \end{aligned} \tag{AM $\mathscr{L}_{0,1}$}$$

A solution $\widehat{\mathscr{B}}^*$ is an optimal approximate model for the signal w_{d} with bounded complexity: order at most $\mathtt{n}$.

In the general case when the data is a vector valued signal with $\mathtt{q}$ variables, the model $\mathscr{B}$ can be represented by a kernel representation, where the parameters R_i are $\mathtt{p} \times \mathtt{q}$ matrices. The block-Hankel structured low-rank approximation problem is equivalent to the approximate linear time-invariant dynamic modeling problem (AM) with model class $\mathscr{M}_{\mathtt{c}_{\max}} = \mathscr{L}_{\mathtt{m},\mathtt{l}}$ and orthogonal distance fitting criterion.

Problem 2.33 (Linear time-invariant dynamic modeling). Given T samples, $\mathtt{q}$ variables, vector signal $w_{\mathrm{d}} \in (\mathbb{R}^{\mathtt{q}})^T$, a signal norm $\|\cdot\|$, and a model complexity $(\mathtt{m},\mathtt{l})$,

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{w} \quad \|w_{\mathrm{d}} - \widehat{w}\| \\ &\text{subject to} \quad \widehat{w} \in \widehat{\mathscr{B}}|_{[1,T]} \text{ and } \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}}. \end{aligned} \tag{AM $\mathscr{L}_{\mathtt{m},\mathtt{l}}$}$$

□

The solution $\widehat{\mathscr{B}}^*$ is an optimal approximate model for the signal w_{d} with complexity bounded by $(\mathtt{m},\mathtt{l})$. Note that problem (AM $\mathscr{L}_{\mathtt{m},\mathtt{l}}$) reduces to

- (AM $\mathscr{L}_{0,\mathtt{l}}$) when $\mathtt{m} = 0$, *i.e.*, when the model is autonomous, and
- (AM $\mathscr{L}_{\mathtt{m},0}$) when $\mathtt{l} = 0$, *i.e.*, when the model is static.

Therefore, (AM $\mathscr{L}_{\mathtt{m},\mathtt{l}}$) is a proper generalization of linear static and dynamic autonomous data modeling problems.

Computing the optimal approximate model $\widehat{\mathscr{B}}^*$ from the solution $\widehat{p}^*$ to Problem SLRA is an exact identification problem. As in the static approximation problem, however, the parameter of a model representation is an optimization variable of the optimization problem, used for Problem SLRA, so that a representation of the model is actually obtained directly from the optimization solver.

Similarly to the static modeling problem, the dynamic modeling problem has a maximum likelihood interpretation in the errors-in-variables setting.

Proposition 2.34 (Maximum likelihood property of an optimal dynamic model). *Assume that the data w_{d} is generated in the errors-in-variables setting*

$$w_{\mathrm{d}} = w_0 + \widetilde{w}, \quad \text{where} \quad w_0 \in \mathscr{B}_0|_{[1,T]} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}} \text{ and } \widetilde{w} \sim \mathrm{N}(0, vI). \tag{EIV}$$

Then an optimal approximate model $\widehat{\mathscr{B}}^*$, solving (AM $\mathscr{L}_{\mathtt{m},\mathtt{l}}$) with $\|\cdot\| = \|\cdot\|_2$ is a maximum likelihood estimator for the true model $\mathscr{B}_0$.

The proof is analogous to the proof of Proposition 2.32 and is skipped.

In Chapter 3, we describe local optimization methods for general affinely structured low-rank approximation problems and show how in the case of Hankel, Toeplitz, and Sylvester structured problem, the matrix structure can be exploited for efficient cost function evaluation.

2.6 Notes and references

The concept of the most powerful unfalsified model is introduced in (Willems, 1986, Definition 4). See also (Antoulas and Willems, 1993; Kuijper, 1997; Kuijper and Willems, 1997; Willems, 1997). Kung's method for approximate system realization is presented in (Kung, 1978).

Modeling by the orthogonal distance fitting criterion (misfit approach) is initiated in (Willems, 1987) and further on developed in (Markovsky et al, 2005b; Roorda, 1995a,b; Roorda and Heij, 1995), where algorithms for solving the problems are developed. A proposal for combination of misfit and latency for linear time-invariant system identification is made in (Lemmerling and De Moor, 2001).

Weighted low-rank approximation methods are developed in (De Moor, 1993; Gabriel and Zamir, 1979; Manton et al, 2003; Markovsky and Van Huffel, 2007; Markovsky et al, 2005a; Srebro, 2004; Wentzell et al, 1997). The analytic solution of circulant structured low-rank approximation problem is derived independently in the optimization community (Beck and Ben-Tal, 2006) and in the systems and control community (Vanluyten et al, 2005).

Equivalence of low-rank approximation and principal component analysis

The principal component analysis method for dimensionality reduction is usually introduced in a stochastic setting as maximisation of the variance of the projected data on a subspace. Computationally, however, the problem of finding the principal components and the corresponding principal vectors is an eigenvalue/eigenvector decomposition problem for the sample covariance matrix

$$\boldsymbol{\Psi}(\mathscr{D}) := \boldsymbol{\Phi}(\mathscr{D})\boldsymbol{\Phi}^\top(\mathscr{D}), \qquad \text{where} \quad \boldsymbol{\Phi}(\mathscr{D}) := \begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix}$$

From this algorithmic point of view, the equivalence of principal component analysis and low-rank approximation problem is a basic linear algebra fact: the space spanned by the first $\mathtt{m}$ principal vectors of $\mathscr{D}$ coincides with the model $\widehat{\mathscr{B}} = \operatorname{image}\big(\boldsymbol{\Phi}(\widehat{\mathscr{D}})\big)$, where $\mathscr{D}$ is a solution of the low-rank approximation problem (LRA).

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Chapter 3
Algorithms

Writing a book is a little more difficult than writing a technical paper, but writing software is a lot more difficult than writing a book.

D. Knuth

Summary: A few special structured low-rank approximation problems have analytic solutions. However, in general, the structured low-rank approximation problem is NP-hard. There are three conceptually different approaches for solving it: convex relaxations, local optimization, and global optimization. System realization methods and methods based on local optimization and convex relaxation, using the nuclear norm heuristic, are presented. The local optimization and convex relaxation method can deal with general affine structure and approximation norm, and allow regularization and inequality constraints on the approximation.

The latest version of the code presented is available from the book's web page.

3.1 Subspace methods

The singular value decomposition is at the core of many algorithms for approximate modeling, most notably the methods based on balanced model reduction, the subspace identification methods, and the MUSIC and ESPRIT methods in signal processing. The reason for this is that the singular value decomposition is a robust and efficient way of computing unstructured low-rank approximation of a matrix in the Frobenius norm. In system identification, signal processing, and computer algebra, however, the low-rank approximation is restricted to the class of matrices with specific (Hankel, Toeplitz, Sylvester) structure. Ignoring the structure constraint renders the singular value decomposition-based methods suboptimal with respect to a desired optimality criterion.

Except for the few special cases, described in Section 2.5, there are no global solution methods for general structured and weighted low-rank approximation problems. The singular value decomposition based methods can be seen as relaxations of the original NP-hard structured weighted low-rank approximation problem, ob-

tained by removing the structure constraint and using the Frobenius norm in the approximation criterion. Another approach is taken in Section 3.3, where convex relaxations of the related rank minimization problem are proposed. Convex relaxation methods give polynomial time suboptimal solutions and are shown to provide globally optimal solutions in certain cases.

Presently, there is no uniformly best method for computing suboptimal structured low-rank approximation. In the context of system identification (*i.e.*, block-Hankel structured low-rank approximation), subspace and local optimization based methods have been compared on practical data sets. In general, the heuristic methods are faster but less accurate than the methods based on local optimization. It is a common practice to use a suboptimal solution obtained by a heuristic method as an initial approximation for an optimization based method. Therefore, the two approaches complement each other.

Realization algorithms

The aim of the realization algorithms is to compute a state space representation $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ of the minimal realization $\mathscr{B}_{\text{mpum}}(H)$ of H, see Section 2.2. Finding the model parameters A,B,C,D can be done by computing a rank revealing factorization of a Hankel matrix constructed from the data. Let

$$\mathscr{H}_{\mathtt{n}+1,\mathtt{n}+1}(\sigma H) = \Gamma\Delta, \quad \text{where} \quad \Gamma \in \mathbb{R}^{\mathtt{p}(\mathtt{n}+1)\times\mathtt{n}} \text{ and } \Delta \in \mathbb{R}^{\mathtt{n}\times\mathtt{m}(\mathtt{n}+1)}$$

be a rank revealing factorization of the finite Hankel matrix $\mathscr{H}_{\mathtt{n}+1,\mathtt{n}+1}(\sigma H)$. The Hankel structure implies that the factors Γ and Δ are observability and controllability matrices, *i.e.*, there are matrices $A \in \mathbb{R}^{\mathtt{n}\times\mathtt{n}}$, $C \in \mathbb{R}^{\mathtt{p}\times\mathtt{n}}$, and $B \in \mathbb{R}^{\mathtt{n}\times\mathtt{m}}$, such that

$$\Gamma = \mathscr{O}_{\mathtt{n}+1}(A,C) \qquad \text{and} \qquad \Delta = \mathscr{C}_{\mathtt{n}+1}(A,B).$$

Then, $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ is the minimal realization of H.

A rank revealing factorization is not unique. For any $\mathtt{n}\times\mathtt{n}$ nonsingular matrix T, a new factorization

$$\mathscr{H}_{\mathtt{n}+1,\mathtt{n}+1}(\sigma H) = \Gamma\Delta = \underbrace{\Gamma T}_{\Gamma'}\underbrace{T^{-1}\Delta}_{\Delta'}$$

is obtained with the same inner dimension. The nonuniqueness of the factorization corresponds to the nonuniqueness of the input/state/output representation of the minimal realization due to a change of the state space bases:

$$\mathscr{B}_{\text{i/s/o}}(A,B,C,D) = \mathscr{B}_{\text{i/s/o}}(T^{-1}AT, T^{-1}B, CT, D).$$

The structure of the observability and controllability matrices is referred to as the *shift structure*. The parameters B and C of an input/state/output representation of the realization are directly available from the first block elements of Γ and Δ, respectively.

77a ⟨$(\Gamma,\Delta)\mapsto(A,B,C)$ 77a⟩≡ (79a) 77b▷
```
  b = C(:, 1:m); c = O(1:p, :);
```
The parameter A is computed from the overdetermined system of linear equations

$$\sigma^{-1}\Gamma A = \sigma\Gamma, \tag{SE$_1$}$$

where, acting on a block matrix, σ and σ^{-1} remove, respectively, the first and the last block elements.

77b ⟨$(\Gamma,\Delta)\mapsto(A,B,C)$ 77a⟩+≡ (79a) ◁77a
```
  a = O(1:end - p, :) \ O((p + 1):end, :);
```

Note 3.1 (Solution of the shift equation). When a unique solution exists, the code in chunk 77a computes the exact solution. When a solution A of (SE$_1$) does not exist, the same code computes a least squares approximate solution. □

Equivalently (in the case of exact data), A can be computed from the Δ factor

$$A\sigma^{-1}\Delta = \sigma\Delta. \tag{SE$_2$}$$

In the case of noisy data (approximate realization problem) or data from a high order system (model reduction problem), (SE$_1$) and (SE$_2$) generically have no exact solutions and their least squares approximate solutions are different.

Implementation

As square as possible Hankel matrix $\mathscr{H}_{i,j}(\sigma H)$ is formed, using all data points, *i.e.*,

$$i = \left\lceil \frac{T\mathtt{m}}{\mathtt{m}+\mathtt{p}} \right\rceil \qquad \text{and} \qquad j = T - i. \tag{i,j}$$

77c ⟨*dimension of the Hankel matrix* 77c⟩≡ (79a 83)
```
  if ~exist('i', 'var') | ~isreal(i) | isempty(i)
    i = ceil(T * m / (m + p));
  end
  if ~exist('j', 'var') | ~isreal(j) | isempty(j)
    j = T - i;
  elseif j > T - i
    error('Not enough data.')
  end
```
The choice (i,j) for the dimension of the Hankel matrix maximazes the order of the realization that can be computed. Indeed, a realization of order n can be computed from the matrix $\mathscr{H}_{i,j}(\sigma H)$ provided

$$\mathtt{n} \le \mathtt{n}_{\max} := \min(\mathtt{p}i - 1, \mathtt{m}j).$$

78a ⟨*check* $\mathtt{n} < \min\big(\mathtt{p}i - 1, \mathtt{m}j\big)$ 78a⟩≡ (79a)
```
  if n > min(i * p - 1, j * m), error('Not enough data'), end
```
The minimal number of samples T of the impulse response that allows identification of a system of order n is

$$T_{\min} := \left\lceil \frac{\mathtt{n}}{\mathtt{p}} \right\rceil + \left\lceil \frac{\mathtt{n}}{\mathtt{m}} \right\rceil + 1. \tag{$T_{\min}$}$$

The key computational step of the realization algorithm is the factorization of the Hankel matrix. In particular, this step involves rank determination. In finite precision arithmetic, however, rank determination is a nontrivial problem. A numerically reliable way of computing rank is the singular value decomposition

$$\mathscr{H}_{i,j}(\sigma H) = U\Sigma V^{\top}.$$

78b ⟨*singular value decomposition of* $\mathscr{H}_{i,j}(\sigma H)$ 78b⟩≡ (79a)
```
  [U, S, V] = svd(blkhank(h(:, :, 2:end), i, j), 0); s = diag(S);
```
Uses `blkhank` 25b.

The order n of the realization is theoretically equal to the rank of the Hankel matrix, which is equal to the number of nonzero singular values $\sigma_1,\dots,\sigma_{\min(i,j)}$. In practice, the system's order is estimated as the numerical rank of the Hankel matrix, *i.e.*, the number of singular values greater than a user specified tolerance.

78c ⟨*order selection* 78c⟩≡ (79a)
```
  ⟨default tolerance tol 40b⟩, n = sum(s > tol);
```
Defining the partitioning

$$U =: \begin{array}{c} \quad \mathtt{n} \quad \\ \begin{bmatrix} U_1 & U_2 \end{bmatrix} \end{array}, \quad \Sigma =: \begin{array}{cc} \mathtt{n} & \\ \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} & \mathtt{n} \end{array}, \quad \text{and} \quad V =: \begin{array}{c} \quad \mathtt{n} \quad \\ \begin{bmatrix} V_1 & V_2 \end{bmatrix} \end{array},$$

the factors Γ and Δ of the rank revealing factorization are chosen as follows

$$\Gamma := U_1\sqrt{\Sigma_1} \qquad \text{and} \qquad \Delta := \sqrt{\Sigma_1}V_1^{\top}. \tag{Γ,Δ}$$

78d ⟨*define* Δ *and* Γ 78d⟩≡ (79a)
```
  sqrt_s = sqrt(s(1:n))';
  O =  sqrt_s(ones(size(U, 1), 1), :) .* U(:, 1:n);
  C = (sqrt_s(ones(size(V, 1), 1), :) .* V(:, 1:n))';
```
This choice leads to a *finite-time balanced* realization of $\mathscr{B}_{\mathrm{i/s/o}}(A,B,C,D)$, *i.e.*, the finite time controllability and observability Gramians

$$\mathscr{O}_i^{\top}(A,C)\mathscr{O}_i(A,C) = \Gamma^{\top}\Gamma \qquad \text{and} \qquad \mathscr{C}_j(A,B)\mathscr{C}_j^{\top}(A,B) = \Delta\Delta^{\top}$$

are equal,

$$\Gamma^{\top}\Gamma = \Delta\Delta^{\top} = \Sigma.$$

Note 3.2 (Kung's algorithm). The combination of the described realization algorithm with the singular value decomposition based rank revealing factorization (Γ,Δ), *i.e.*, unstructured low-rank approximation, is referred to as *Kung's algorithm*. □

79a ⟨$H \mapsto \mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ 79a⟩≡
```
function [sys, hh] = h2ss(h, n, tol, i ,j)
⟨reshape H and define m, p, T 79b⟩
⟨dimension of the Hankel matrix 77c⟩
⟨singular value decomposition of $\mathscr{H}_{i,j}(\sigma H)$ 78b⟩
if ~exist('n', 'var') | isempty(n)
  ⟨order selection 78c⟩
else
  ⟨check n < min(pi − 1, mj) 78a⟩
end
⟨define $\Delta$ and $\Gamma$ 78d⟩
⟨($\Gamma$, $\Delta$) ↦ (A, B, C) 77a⟩, sys = ss(a, b, c, h(:, :, 1), -1);
if nargout > 1, hh = shiftdim(impulse(sys, T), 1); end
```
Defines:
`h2ss`, used in chunks 83, 102e, 103a, 112, 115, and 127c.

Similarly, to the convention (`w`) on page 26 for representing vector and matrix valued trajectories in MATLAB, the impulse response H is stored as an $\mathtt{p} \times \mathtt{m} \times T$ tensor

$$\mathtt{h}(:,\, :,\, \mathtt{t}) = H(t),$$

or, in the case of a single input system, as a $\mathtt{p} \times T$ matrix.

79b ⟨reshape H and define m, p, T 79b⟩≡ (79a 111a)
```
if length(size(h)) == 2
  [p, T] = size(h); if p > T, h = h'; [p, T] = size(h); end
  h = reshape(h, p, 1, T);
end
[p, m, T] = size(h);
```

Note 3.3 (Approximate realization by Kung's algorithm). When H is not realizable by a linear time-invariant system of order less than or equal to $\mathtt{n}_{\max}$, *i.e.*, when $\mathscr{H}_{i,j}(\sigma H)$ is full rank, `h2ss` computes an approximate realization $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ of order $\mathtt{n} \leq \mathtt{n}_{\max}$. The link between the realization problem and Hankel structured low-rank approximation implies that

Kung's algorithm, implemented in the function `h2ss`, is a method for Hankel structured low-rank approximation. The structured low-rank approximation of $\mathscr{H}_{i,j}(\sigma H)$ is $\mathscr{H}_{i,j}(\sigma \widehat{H})$, where $\widehat{H}$ is the impulse response of the approximate realization $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$. □

Note 3.4 (Suboptimality of Kung's algorithm). Used as a method for Hankel structured low-rank approximation, Kung's algorithm is suboptimal. The reason for this is that the factorization

$$\mathscr{H}_{i,j}(\sigma H) \approx \Gamma \Delta,$$

performed by the singular value decomposition is unstructured low-rank approximation and unless the data is exact, Γ and Δ are not extended observability and controllability matrices, respectively. As a result, the shift equations (SE$_1$) and (SE$_2$) do not have solutions and Kung's algorithm computes an approximate solution in the least squares sense. □

Note 3.5 (Unstructured vs structure enforcing methods). The two levels of approximation:

1. approximation of the Hankel matrix, constructed from the data, by unstructured low rank matrix, and
2. computation of an approximate solution of a system of linear equations for the parameter estimate by the ordinary least squares method

are common to the subspace methods. In contrast, methods based on Hankel structured low-rank approximation do not involve approximation on the second stage (model parameter computation). By construction, the approximation computed on the first step is guaranteed to have an exact solution on the second step. □

Note 3.6 (Interpretation of Kung's algorithm as a finite-time balanced model reduction). Kung's algorithm computes a realization in a finite time $\min(i,j)$ balanced bases. In the case of noisy data or data obtained from a high order model, the computed realization is obtain by truncation of the realization, using the user specified state dimension `n` or tolerance `tol`. This justifies Kung's algorithm as a data-driven method for finite-time balanced model reduction. (The term data-driven refers to the fact that a model of the full order system is not used.) The link between Kung's algorithm and model reduction further justifies the choice (i,j) on page 77 for the shape of the Hankel matrix — the choice (i,j) maximizes the horizon for the finite-time balanced realization. □

Computation of the impulse response from general trajectory

In the realization problem the given data is a special trajectory—the impulse response of the model. Therefore, the realization problem is a special exact identification problem. In this section, the general exact identification problem:

$$w_{\text{d}} \xrightarrow{\substack{\text{exact}\\\text{identification}}} \mathscr{B}_{\text{mpum}}(w_{\text{d}})$$

is solved by reducing it to the realization problem:

$$w_{\text{d}} \xrightarrow{\substack{\text{impulse response}\\\text{computation (w2h)}}} H_{\text{mpum}} \xrightarrow{\text{realization (h2ss)}} \mathscr{B}_{\text{mpum}}(w_{\text{d}}). \quad (w_{\text{d}} \mapsto H \mapsto \widehat{\mathscr{B}})$$

First, the impulse response H_{mpum} of the most powerful unfalsified model $\mathscr{B}_{\text{mpum}}(w_{\text{d}})$ is computed from the given general trajectory w_{d}. Then, an input/state/output representation of $\mathscr{B}_{\text{mpum}}(w_{\text{d}})$ is computed from H_{mpum} by a realization algorithm, *e.g.*, Kung's algorithm.

The key observation in finding an algorithm for the computation of the impulse response is that the image of the Hankel matrix $\mathscr{H}_{i,j}(w_{\mathrm{d}})$, with $j > \mathtt{q}i$, constructed from the data w_{d} is the restriction $\mathscr{B}_{\mathrm{mpum}}(w_{\mathrm{d}})|_{[1,i]}$ of the most powerful unfalsified model on the interval $[1,i]$, *i.e.*,

$$\mathscr{B}_{\mathrm{mpum}}(w_{\mathrm{d}})|_{[1,i]} = \operatorname{span}\big(\mathscr{H}_i(w_{\mathrm{d}})\big). \tag{DD}$$

Therefore, any i-samples long trajectory w of $\mathscr{B}_{\mathrm{mpum}}(w_{\mathrm{d}})$ can be constructed as a linear combination of the columns of the Hankel matrix

$$w = \mathscr{H}_i(w_{\mathrm{d}})g$$

for some vector g.

As in the realization problem, in what follows, the default input/output partitioning $w = \operatorname{col}(u,y)$ is assumed. Let e_k be the kth column of the $\mathtt{m} \times \mathtt{m}$ identity matrix and δ be the unit pulse function. The impulse response is a matrix valued trajectory, the columns of which are the $\mathtt{m}$ trajectories corresponding to zero initial conditions and inputs $e_1\delta, \ldots, e_{\mathtt{m}}\delta$. Therefore, the problem of computing the impulse response is reduced to the problem of finding a vector g_k, such that $\mathscr{H}_i(w_{\mathrm{d}})g_k$ is of the form $(e_k\delta, h_k)$, where $h_k(\tau) = 0$, for all $\tau < 0$. The identically zero input/output trajectory for negative time (in the past) implies that the response from time zero on (in the future) is the impulse response.

Let $\mathtt{l}$ be the lag of the most powerful unfalsified model $\mathscr{B}_{\mathrm{mpum}}(w_{\mathrm{d}})$. In order to describe the construction of a vector g_k that achieves the impulse response h_k, define the "past" Hankel matrix

$$\mathbf{H}_{\mathrm{p}} := \mathscr{H}_{\mathtt{l},j}(w_{\mathrm{d}}), \qquad \text{where} \quad j := T - (\mathtt{l} + i)$$

and the "future" input and output Hankel matrices

$$\mathbf{H}_{\mathrm{f},u} := \mathscr{H}_{i,j}(\sigma^{\mathtt{l}} u_{\mathrm{d}}) \qquad \text{and} \qquad \mathbf{H}_{\mathrm{f},y} := \mathscr{H}_{i,j}(\sigma^{\mathtt{l}} y_{\mathrm{d}}).$$

81 ⟨*define* $\mathbf{H}_{\mathrm{p}}$, $\mathbf{H}_{\mathrm{f},u}$, *and* $\mathbf{H}_{\mathrm{f},y}$ 81⟩≡ (82b)
```
j = T - (l + i);
Hp  = blkhank(w, l, j);
Hfu = blkhank(u(:, (l + 1):end), i, j);
Hfy = blkhank(y(:, (l + 1):end), i, j);
```
Uses `blkhank` 25b.

With these definitions, a vector g_k that achieves the impulse response h_k must satisfy the system of linear equations

$$\begin{bmatrix} \mathbf{H}_{\mathrm{p}} \\ \mathbf{H}_{\mathrm{f},u} \end{bmatrix} g_k = \begin{bmatrix} 0_{\mathtt{ql}\times 1} \\ \begin{bmatrix} e_k \\ 0_{(t-1)\mathtt{m}\times 1} \end{bmatrix} \end{bmatrix}. \tag{$*$}$$

By construction, any solution g_k of $(*)$ is such that

$$\mathbf{H}_{\mathrm{f},y} g_k = h_k.$$

Choosing the least norm solution as a particular solution and using matrix notation, the first i samples of the impulse response are given by

$$H = \mathbf{H}_{\mathrm{f},y} \begin{bmatrix} \mathbf{H}_{\mathrm{p}} \\ \mathbf{H}_{\mathrm{f},u} \end{bmatrix}^{+} \begin{bmatrix} 0_{\mathtt{ql}\times \mathtt{m}} \\ \begin{bmatrix} I_{\mathtt{m}} \\ 0_{(i-1)\mathtt{m}\times \mathtt{m}} \end{bmatrix} \end{bmatrix},$$

where A^+ is the pseudo-inverse of A.

82a ⟨*data driven computation of the impulse response* 82a⟩≡ (82b)
```
wini_uf = [zeros(l * q, m); eye(m); zeros((i - 1) * m, m)];
h_ = Hfy * pinv([Hp; Hfu]) * wini_uf;
```

We have the following function for computation of the impulse response of the most powerful unfalsified model from data:

82b ⟨$w \mapsto H$ 82b⟩≡
```
function h = w2h(w, m, n, i)
⟨reshape w and define q, T 26e⟩, p = q - m; l = ceil(n / p);
u = w(1:m, :); y = w((m + 1):q, :);
⟨define Hp, Hf,u, and Hf,y 81⟩
⟨data driven computation of the impulse response 82a⟩
for ii = 1:i
  h(:, :, ii) = h_(((ii - 1) * p + 1):(ii * p), :);
end
```
Defines:
`w2h`, used in chunk 83.

As in the case of the realization problem, when the data is noisy or generated by a high order model (higher than the specified order `n`), `w2h` computes a (suboptimal) approximation.

Using the functions `w2h` and `h2ss`, we obtain a method for exact identification $(w_{\mathrm{d}} \mapsto H \mapsto \widehat{\mathscr{B}})$

82c ⟨*Most powerful unfalsified model in* $\mathscr{L}_{\mathtt{m}}^{\mathtt{q},\mathtt{n}}$ 82c⟩≡ 82d▷
```
function sys = w2h2ss(w, m, n, Th, i, j)
⟨reshape w and define q, T 26e⟩, p = q - m;
```
Defines:
`w2h2ss`, used in chunks 118 and 120.

The optional parameter `Th` specifies the number of samples of the impulse response, to be computed on the first step $w_{\mathrm{d}} \mapsto H$. The default value is the minimum number ($T_{\min}$), defined on page 78.

82d ⟨*Most powerful unfalsified model in* $\mathscr{L}_{\mathtt{m}}^{\mathtt{q},\mathtt{n}}$ 82c⟩+≡ ◁82c 83▷
```
if ~exist('Th') | isempty(Th)
  Th = ceil(n / p) + ceil(n / m) + 1;
end
```

The dimensions i and j of the Hankel matrix $\mathscr{H}_{i,j}(\sigma H)$, to be used at the realization step $w_{\mathrm{d}} \mapsto H$, are also optional input parameters. With exact data, their values are irrelevant as long as the Hankel matrix has the minimum number `n` of rows and columns. However, with noisy data, the values of `Th`, `i`, and `j` affect the approximation. Empirical results suggest that the default choice (i, j) gives best approximation.

83 ⟨*Most powerful unfalsified model in* $\mathscr{L}_{\mathtt{m}}^{\mathtt{q,n}}$ 82c⟩+≡ ◁82d
```
  T = Th; ⟨dimension of the Hankel matrix 77c⟩
  sys = h2ss(w2h(w, m, n, Th), n, [], i, j);
```
Uses `h2ss` 79a and `w2h` 82b.

3.2 Algorithms based on local optimization

Consider the structured low-rank approximation problem

$$\text{minimize} \quad \text{over } \widehat{p} \quad \|p-\widehat{p}\|_W \quad \text{subject to} \quad \operatorname{rank}\big(\mathscr{S}(\widehat{p})\big) \leq r. \tag{SLRA}$$

As discussed in Section 1.4, different methods for solving the problem are obtained by choosing different combinations of

- rank parametrization, and
- optimization method.

In this section, we choose the kernel representation for the rank constraint

$$\operatorname{rank}\big(\mathscr{S}(\widehat{p})\big) \leq r \quad \iff \quad \text{there is } R \in \mathbb{R}^{(m-r)\times m}, \text{ such that}$$
$$R\mathscr{S}(\widehat{p}) = 0 \text{ and } RR^\top = I_{m-r}, \tag{rank$_R$}$$

and the variable projections approach (in combination with standard methods for nonlinear least squares optimization) for solving the resulting parameter optimization problem.

The developed method is applicable for the general affinely structured and weighted low-rank approximation problem (SLRA). The price paid for the generality, however, is lack of efficiency compared to specialized methods exploiting the structure of the data matrix $\mathscr{S}(p)$ and the weight matrix W.

In two special cases—single input single output linear time-invariant system identification and computation of approximate greatest common divisor—efficient methods are described later in the chapter. The notes and references section links the presented material to state-of-the-art methods for structured low-rank approximation. Efficient methods for weighted low-rank approximation problems are developed in Chapter 5.

Representing the constraint of (SLRA) in the kernel form (rank$_R$), leads to the double minimization problem

$$\begin{aligned} &\text{minimize} \quad \text{over } R \quad f(R) \quad \text{subject to} \quad RR^\top = I_{m-r}, \\ &\text{where} \quad f(R) := \min_{\widehat{p}} \|p-\widehat{p}\| \quad \text{subject to} \quad R\mathscr{S}(\widehat{p}) = 0. \end{aligned} \tag{SLRA$_R$}$$

The inner minimization (computation of $f(R)$) is over the correction $\widehat{p}$ and the outer minimization is over the model parameter $R \in \mathbb{R}^{(m-r)\times m}$. The inner minimization problem can be given the interpretation of projecting the columns of $\mathscr{S}(p)$ onto the model $\mathscr{B} := \ker(R)$, for a given matrix R. However, the projection depends on the parameter R, which is the variable in the outer minimization problem.

For affine structures $\mathscr{S}$, the constraint $R\mathscr{S}(\widehat{p}) = 0$ is bilinear in the optimization variables R and $\widehat{p}$. Then, the evaluation of the cost function f for the outer minimization problem is a linear least norm problem. Direct solution has computational complexity $O(n_p^3)$, where n_p is the number of structure parameters. Exploiting the structure of the problem (inherited from $\mathscr{S}$), results in computational methods with cost $O(n_p^2)$ or $O(n_p)$, depending on the type of structure. For a class of structures, which includes block Hankel, block Toeplitz, and block Sylvester ones, efficient $O(n_p)$ cost function evaluation can be done by Cholesky factorization of a block-Toeplitz banded matrix.

A method for affinely structured problems

Structure specification

The general affine structure

$$\mathscr{S}(\widehat{p}) = S_0 + \sum_{k=1}^{n_p} S_k \widehat{p}_k \tag{$\mathscr{S}(\widehat{p})$}$$

is specified by the matrices $S_0, S_1, \dots, S_{n_p} \in \mathbb{R}^{m\times n}$. This data is represented in the code by an $m\times n$ matrix variable `s0`, corresponding to the matrix S_0, and an $mn\times n_p$ matrix variable `bfs`, corresponding to the matrix

$$\mathbf{S} := \begin{bmatrix} \operatorname{vec}(S_1) & \cdots & \operatorname{vec}(S_{n_p}) \end{bmatrix} \in \mathbb{R}^{mn\times n_p}.$$

With this representation, the sum in ($\mathscr{S}(\widehat{p})$) is implemented as a matrix–vector product:

$$\operatorname{vec}\big(\mathscr{S}(\widehat{p})\big) = \operatorname{vec}(S_0) + \mathbf{S}\widehat{p}, \qquad \text{or} \qquad \mathscr{S}(\widehat{p}) = S_0 + \operatorname{vec}^{-1}(\mathbf{S}\widehat{p}). \tag{S}$$

84 ⟨$(S_0, \mathbf{S}, \widehat{p}) \mapsto \widehat{D} = \mathscr{S}(\widehat{p})$ 84⟩≡
```
  dh = s0 + reshape(bfs * ph, m, n);
```

Note 3.7. In many applications the matrices S_k are sparse, so that, for efficiency, they can be stored and manipulated as sparse matrices.

A commonly encountered special case of an affine structure is

$$\big[\mathscr{S}(\widehat{p})\big]_{ij} = \begin{cases} S_{0,ij}, & \text{if } \mathtt{S}_{ij} = 0 \\ \widehat{p}_{\mathtt{S}_{ij}} & \text{otherwise} \end{cases} \qquad \text{for some} \quad \mathtt{S}_{ij} \in \{0,1,\dots,n_p\}^{m\times n}, \tag{S}$$

or, written more compactly,

$$\big[\mathscr{S}(\widehat{p})\big]_{ij} = S_{0,ij} + \widehat{p}_{\mathrm{ext},\mathtt{S}_{ij}}, \qquad \text{where} \quad \widehat{p}_{\mathrm{ext}} := \begin{bmatrix} 0 \\ \widehat{p} \end{bmatrix}.$$

In (S), each element of the structured matrix $\mathscr{S}(p)$ is equal to the corresponding element of the matrix S_0 or to the $\mathtt{S}_{ij}$th element of the parameter vector p. The structure is then specified by the matrices S_0 and S. Although (S) is a special case of the general affine structure ($\mathscr{S}(\widehat{p})$), it covers all linear modeling problems considered in this book and will therefore be used in the implementation of the solution method.

In the implementation of the algorithm, the matrix S corresponds to a variable `tts` and the extended parameter vector p_{ext} corresponds to a variable `pext`. Since in MATLAB indeces are positive integers (zero index is not allowed), in all indexing operations of `pext`, the index is incremented by one. Given the matrices S_0 and S, specifying the structure, and a structure parameter vector $\widehat{p}$, the structured matrix $\mathscr{S}(\widehat{p})$ is constructed by

85a ⟨$(S_0, \mathtt{S}, \widehat{p}) \mapsto \widehat{D} = \mathscr{S}(\widehat{p})$ 85a⟩≡ (87d 99b)
```
phext = [0; ph(:)]; dh = s0 + phext(tts + 1);
```
The matrix dimensions `m`, `n`, and the number of parameters `np` are obtained from S as follows:

85b ⟨$\mathtt{S} \mapsto (m, n, n_p)$ 85b⟩≡ (86c 87e 99a 100b)
```
[m, n] = size(tts); np = max(max(tts));
```
The transition from the specification of (S) to the specification in the general affine case ($\mathscr{S}(\widehat{p})$) is done by

85c ⟨$\mathtt{S} \mapsto \mathbf{S}$ 85c⟩≡ (86c 87e 100b)
```
vec_tts = tts(:); NP = 1:np;
bfs = vec_tts(:, ones(1, np)) == NP(ones(m * n, 1), :);
```
Conversely, for a linear structure of the type (S), defined by $\mathbf{S}$ (and m, n), the matrix S is constructed by

85d ⟨$\mathbf{S} \mapsto \mathtt{S}$ 85d⟩≡
```
tts = reshape(bfs * (1:np)', m, n);
```
In most applications that we consider, the structure $\mathscr{S}$ is linear, so that `s0` is an optional input argument to the solvers with default value the zero matrix.

85e ⟨*default* `s0` 85e⟩≡ (86c 87e 99a 100b)
```
if ~exist('s0', 'var') | isempty(s0), s0 = zeros(m, n); end
```
The default weight matrix W in the approximation criterion is the identity matrix.

85f ⟨*default weight matrix* 85f⟩≡ (86c 87e 100b)
```
if ~exist('w', 'var') | isempty(w), w = eye(np); end
```

Minimization over $\widehat{p}$

In order to solve the optimization problem (SLRA), we change variables

$$\widehat{p} \quad \mapsto \quad \Delta p = p - \widehat{p}.$$

Then, the constraint is written as a system of linear equations with unknown Δp:

$$\begin{aligned} R\mathscr{S}(\widehat{p}) = 0 \quad &\iff \quad R\mathscr{S}(p - \Delta p) = 0 \\ &\iff \quad R\mathscr{S}(p) - R\mathscr{S}(\Delta p) + RS_0 = 0 \\ &\iff \quad \operatorname{vec}\big(R\mathscr{S}(\Delta p)\big) = \operatorname{vec}\big(R\mathscr{S}(p)\big) + \operatorname{vec}(RS_0) \\ &\iff \quad \underbrace{\big[\operatorname{vec}(RS_1) \ \cdots \ \operatorname{vec}(RS_{n_p})\big]}_{G(R)} \Delta p = \underbrace{G(R)p + \operatorname{vec}(RS_0)}_{h(R)} \\ &\iff \quad G(R)\Delta p = h(R). \end{aligned}$$

86a ⟨*form* $G(R)$ *and* $h(R)$ 86a⟩≡ (86c)
```
g = reshape(R * reshape(bfs, m, n * np), size(R, 1) * n, np);
h = g * p + vec(R * s0);
```
The inner minimimization in (SLRA$_R$) with respect to the new variable Δp is a linear least norm problem

$$\text{minimize} \quad \text{over } \Delta p \quad \|\Delta p\|_W \quad \text{subject to} \quad G(R)\Delta p = h(R) \qquad \text{(LNP)}$$

and has the analytic solution

$$\Delta p^*(R) = W^{-1}G^\top(R)\big(G(R)W^{-1}G^\top(R)\big)^{-1}h(R).$$

86b ⟨*solve the least-norm problem* 86b⟩≡ (86c)
```
dp = inv_w * g' * (pinv(g * inv_w * g') * h);
```
Finally, the cost function to be minimized over the parameter R is

$$f(R) = \|\Delta p^*(R)\|_W = \sqrt{\Delta p^{*\top}(R) W \Delta p^*(R)}.$$

The function f corresponds to the data–model misfit function in data modeling problems and will be refered to as the structured low-rank approximation misfit.

86c ⟨*Structured low-rank approximation misfit* 86c⟩≡
```
function [M, ph] = misfit_slra(R, tts, p, w, s0, bfs, inv_w)
⟨S ↦ (m,n,n_p) 85b⟩
⟨default s0 85e⟩, ⟨default weight matrix 85f⟩
if ~exist('bfs') | isempty(bfs), ⟨S ↦ S 85c⟩, end
⟨form G(R) and h(R) 86a⟩
if ~exist('inv_w') | isempty(inv_w), inv_w = inv(w); end
⟨solve the least-norm problem 86b⟩
M = sqrt(dp' * w * dp); ph = p - dp;
```
Defines:
`misfit_slra`, used in chunk 87.

Minimization over R

General purpose constrained optimization methods are used for the outer minimization problem in (SLRA$_R$), *i.e.*, the minimization of f over R, subject to the constraint

$RR^\top = I$. This is a nonconvex optimization problem, so that there is no guarantee that a globally optimal solution is found.

87a ⟨*set optimization solver and options* 87a⟩≡ (87c 90b 193d)
```
prob = optimset();
prob.solver = 'fmincon';
prob.options = optimset('disp', 'off');
```

87b ⟨*call optimization solver* 87b⟩≡ (87c 90b 193d)
```
[x, fval, flag, info] = fmincon(prob); info.M = fval;
```

87c ⟨*nonlinear optimization over R* 87c⟩≡ (87e)
```
⟨set optimization solver and options 87a⟩
prob.x0 = Rini; inv_w = inv(w);
prob.objective = ...
          @(R) misfit_slra(R, tts, p, w, s0, bfs, inv_w);
prob.nonlcon = @(R) deal([], [R * R' - eye(size(R, 1))]);
⟨call optimization solver 87b⟩, R = x;
```
Uses `misfit_slra` 86c.

If not specified, the initial approximation is computed from a heuristic that ignores the structure and replaces the weighted norm by the Frobenius norm, so that the resulting problem can be solved by the singular value decomposition (function `lra`).

87d ⟨*default initial approximation* 87d⟩≡ (87e)
```
if ~exist('Rini') | isempty(Rini)
  ph = p; ⟨(S0,S,p̂) ↦ D̂ = 𝒮(p̂) 85a⟩, Rini = lra(dh, r);
end
```
Uses `lra` 66.

The resulting function is:

87e ⟨*Structured low-rank approximation* 87e⟩≡
```
function [R, ph, info] = slra(tts, p, r, w, s0, Rini)
⟨S ↦ (m,n,n_p) 85b⟩, ⟨S ↦ S 85c⟩
⟨default s0 85e⟩, ⟨default weight matrix 85f⟩
⟨default initial approximation 87d⟩
⟨nonlinear optimization over R 87c⟩
if nargout > 1,
  [M, ph] = misfit_slra(R, tts, p, w, s0, bfs, inv_w);
end
```
Defines:
  `slra`, used in chunks 102e and 110.
Uses `misfit_slra` 86c.

Exercise 3.8. Use `slra` and `r2x` to solve approximately an overdetermined system of linear equations $AX \approx B$ in the least squares sense. Check the accuracy of the answer by using the analytical expression. □

Exercise 3.9. Use `slra` to solve the basic low-rank approximation problem

$$\text{minimize} \quad \text{over } \widehat{D} \quad \|D - \widehat{D}\|_{\text{F}} \quad \text{subject to} \quad \operatorname{rank}(\widehat{D}) \leq \mathtt{m}.$$

(unstructured approximation in the Frobenius norm). Check the accuracy of the answer by the Eckart–Young–Mirsky theorem (`lra`). □

Exercise 3.10. Use `slra` to solve the weighted low-rank approximation problem (unstructured approximation in the weighted norm ($\|\cdot\|_W$), defined on page 62). Check the accuracy of the answer in the special case of two-sided weighted low-rank approximation, using Theorem 2.29. □

Algorithms for linear system identification

Approximate linear system identification problems can be solved as equivalent Hankel structured low-rank approximation problems. Therefore, the function `slra`, implemented in the previous section can be used for linear time-invariant system identification. This approach is developed in Section 4.3.

In this section an alternative approach for approximate system identification that is motivated from a system theoretic view of the problem is used. The Hankel structure in the problem is exploited, which results in efficient computational methods.

Misfit computation

Consider the misfit between the data w_{d} and a model $\mathscr{B}$

$$\operatorname{misfit}(w_{\text{d}}, \mathscr{B}) := \min_{\widehat{w}} \|w_{\text{d}} - \widehat{w}\|_2 \quad \text{subject to} \quad \widehat{w} \in \mathscr{B}. \qquad (\text{misfit } \mathscr{L}_{\mathtt{m},\mathtt{l}})$$

Geometrically, $\operatorname{misfit}(w_{\text{d}}, \mathscr{B})$ is the orthogonal projection of w_{d} on $\mathscr{B}$. Assuming that $\mathscr{B}$ is controllable, $\mathscr{B}$ has a minimal image representation $\operatorname{image}\big(P(\sigma)\big)$. In terms of the parameter P, the constraint $\widehat{w} \in \mathscr{B}$ becomes $\widehat{w} = P(\sigma)\ell$, for some latent variable ℓ. In a matrix form,

$$\widehat{w} = \mathscr{T}_T(P)\ell,$$

where

$$\mathscr{T}_T(P) := \begin{bmatrix} P_0 & P_1 & \cdots & P_{\mathtt{l}} & & & \\ & P_0 & P_1 & \cdots & P_{\mathtt{l}} & & \\ & & \ddots & \ddots & & \ddots & \\ & & & P_0 & P_1 & \cdots & P_{\mathtt{l}} \end{bmatrix} \in \mathbb{R}^{\mathtt{q}T \times (T+\mathtt{l})}. \qquad (\mathscr{T})$$

88 ⟨*Toeplitz matrix constructor* 88⟩≡
```
function TP = blktoep(P, T)
[q, l1] = size(P); l = l1 - 1; TP = zeros(T * q, T + l);
ind = 1 + (0:T - 1) * q * (T + 1);
for i = 1:q
  for j = 1:l1
    TP(ind + (i - 1) + (j - 1) * (T * q)) = P(i, j);
  end
end
```
Defines:
  `blktoep`, used in chunk 89.

The misfit computation problem (misfit $\mathscr{L}_{\mathtt{m},\mathtt{l}}$) is equivalent to the standard linear least squares problem

$$\text{minimize} \quad \text{over } \ell \quad \|w_{\mathrm{d}} - \mathscr{T}_T(P)\ell\|, \qquad (\text{misfit}_P)$$

so that the solution, implemented in the functions `misfit_siso`, is

$$\widehat{w} = \mathscr{T}_T(P)\big(\mathscr{T}_T^\top(P)\mathscr{T}_T(P)\big)^{-1}\mathscr{T}_T^\top(P)w_{\mathrm{d}}.$$

89 ⟨dist($w_{\mathrm{d}}, \mathscr{B}$) 89⟩≡
```
function [M, wh] = misfit_siso(w, P)
try, [M, wh] = misfit_siso_efficient(w, P);
catch
  ⟨reshape w and define q, T 26e⟩
  TP = blktoep(P, T); wh = reshape(TP * (TP \ w(:)), 2, T);
  M  = norm(w - wh, 'fro');
end
```
Defines:
`misfit_siso`, used in chunks 90b, 118d, 120, and 129c.
Uses `blktoep` 88.

First, an efficient implementation (`misfit_siso_efficient`) of the misfit computation function, exploiting the banded Toeplitz structure of the matrix $\mathscr{T}_T(P)$, is attempted. `misfit_siso_efficient` calls a function of the SLICOT library to carry out the computation and requires a mex file, which is platform dependent. If a mex file is not available, the computation is reverted to solution of (misfit$_P$) without exploiting the structure of $\mathscr{T}_T(P)$ (MATLAB backslash operator).

Note 3.11 (Misfit computation by Kalman smoothing). The efficient implementation in `misfit_siso_efficient` is based on structured linear algebra computations (Cholesky factorization of positive definite banded Toeplitz matrix). The computational methods implemented in the SLICOT library use the generalized Schur algorithm and have computational complexity $O(n_p)$

An alternative approach, which also results in $O(n_p)$ methods, is based on the system theoretic interpretation of the problem: equivalence between misfit computation and Kalman smoothing. In this latter approach, the computation is done by a Riccati type recursion.

Misfit minimization

Consider the misfit minimization problem

$$\widehat{\mathscr{B}}^* := \arg\min_{\widehat{\mathscr{B}}} \quad \text{misfit}(w_{\mathrm{d}}, \mathscr{B}) \quad \text{subject to} \quad \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}}. \qquad (\text{SYSID})$$

Using the representation $\mathscr{B} = \text{image}(P)$, (SYSID) is equivalent to

$$\begin{array}{ll} \text{minimize} & \text{over } P \in \mathbb{R}^{\mathtt{q}(\mathtt{l}+1)\times \mathtt{m}} \quad \text{misfit}\big(w_{\mathrm{d}}, \text{image}\,(P(\sigma))\big) \\ \text{subject to} & P^\top P = I_{\mathtt{m}}, \end{array} \qquad (\text{SYSID}_P)$$

which is a constrained nonlinear least squares problem.

90a ⟨*Single input single output system identification* 90a⟩≡
```
function [sysh, wh, info] = ident_siso(w, n, sys)
if ~exist('sys', 'var')
  ⟨suboptimal approximate single input single output system identification 90c⟩
else
  ⟨(TF) ↦ P 90e⟩
end
⟨misfit minimization 90b⟩
```
Defines:
`ident_siso`, used in chunks 91f and 129d.

Optimization Toolbox is used for performing the misfit minimization.

90b ⟨*misfit minimization* 90b⟩≡ (90a)
```
⟨set optimization solver and options 87a⟩
prob.x0 = P;
prob.objective = @(P) misfit_siso(w, P);
prob.nonlcon = @(P) deal([], [P(1, :) * P(1, :)' - 1]);
⟨call optimization solver 87b⟩, P = x;
⟨P ↦ (TF) 90d⟩ sysh = sys;
if nargout > 1, [M, wh] = misfit_siso(w, P); end
```
Uses `misfit_siso` 89.

The initial approximation is computed from a relaxation ignoring the structure constraint:

90c ⟨*suboptimal approximate single input single output system identification* 90c⟩≡ (90a 129c)
```
R = lra(blkhank(w, n + 1), 2 * n + 1); ⟨R ↦ P 90f⟩
```
Uses `blkhank` 25b and `lra` 66.

The solution obtained by the optimization solver is an image representation of a (locally) optimal approximate model $\widehat{\mathscr{B}}^*$. In the function `ident_siso`, the image representation is converted to a transfer function representation as follows:

90d ⟨*P ↦ (TF)* 90d⟩≡ (90b 91b)
```
p = fliplr(P(1, :)); q = fliplr(P(2, :)); sys = tf(q, p, -1);
```

The reverse transformation

90e ⟨*(TF) ↦ P* 90e⟩≡ (90 118d 120)
```
[q, p] = tfdata(tf(sys), 'v'); P = zeros(2, length(p));
P(1, :) = fliplr(p);
P(2, :) = fliplr([q zeros(length(p) - length(q))]);
```

is used when an initial approximation is specified by a transfer function representation. When no initial approximation is supplied, a default one is computed by unstructured low-rank approximation, which produces a kernel representation of the model. Transition from kernel to image representation is done indirectly by passing through a transfer function representation:

90f ⟨*R ↦ P* 90f⟩≡ (90c)
```
⟨R ↦ (TF) 91a⟩ ⟨(TF) ↦ P 90e⟩
```

where

91a ⟨*R ↦ (TF)* 91a⟩≡ (90f)

```
  q = - fliplr(R(1:2:end)); p = fliplr(R(2:2:end));
  sys = tf(q, p, -1);
```

For later use, next, we define also the reverse mapping:

91b ⟨*P ↦ R* 91b⟩≡
⟨*P ↦ (TF)* 90d⟩ ⟨*(TF) ↦ R* 91c⟩

where

91c ⟨*(TF) ↦ R* 91c⟩≡ (91b)

```
  [q, p] = tfdata(tf(sys), 'v'); R = zeros(1, length(p) * 2);
  R(1:2:end) = - fliplr([q zeros(length(p) - length(q))]);
  R(2:2:end) = fliplr(p);
```

Numerical example

The function `ident_siso` is applied on data obtained in the errors-in-variables setup (EIV) on page 71. The true data generating model is a random single input single output linear time-invariant system and the true data w_0 is a random trajectory of that system. In order to make the results reproducible, in all simulations, we first initialize the random number generator:

91d ⟨*initialize the random number generator* 91d⟩≡ (91e 102a 105a 112b 116b 118d 120 123a 127a 129a 145a 164a

```
  randn('seed', 0); rand('seed', 0);
```

91e ⟨*Test* `ident_siso` 91e⟩≡ 91f▷
⟨*initialize the random number generator* 91d⟩

```
  sys0 = drss(n); xini0 = rand(n, 1);
  u0 = rand(T, 1); y0 = lsim(sys0, u0, 1:T, xini0);
  w = [u0 y0] + s * randn(T, 2);
```

Defines:
`test_ident_siso`, used in chunk 91h.

The optimal approximation obtained by `ident_siso`

91f ⟨*Test* `ident_siso` 91e⟩+≡ ◁91e 91g▷

```
  [sysh, wh, info] = ident_siso(w, n); info
```

Uses `ident_siso` 90a.

is verified by comparing it with the approximation obtained by the function `slra` (called by the wrapper function `ident_eiv`, see Section 4.3)

91g ⟨*Test* `ident_siso` 91e⟩+≡ ◁91f

```
  [sysh_, wh_, info_] = ident_eiv(w, 1, n); info_
  norm(sysh - sysh_)
```

Uses `ident_eiv` 118a.

In a specific example

91h ⟨*Compare* `ident_siso` *and* `ident_eiv` 91h⟩≡

```
  n = 2; T = 20; s = 0.1; test_ident_siso
```

Uses `test_ident_siso` 91e.

the norm of the difference between the two computed approximations is of the order of magnitude of the convergence tolerance used by the optimization solvers. This shows that the methods converged to the same locally optimal solution.

Computation of an approximate greatest common divisor

Associated with a polynomial

$$p(z) := p_0 + p_1 z + \cdots + p_n z^n$$

of degree at most n is an $(n+1)$-dimensional coefficients vector

$$p := \operatorname{col}(p_0, p_1, \dots, p_n) \in \mathbb{R}^{n+1}$$

and vice verse a vector $p \in \mathbb{R}^{n+1}$ corresponds to a polynomial p with degree at most n. With some abuse of notation, we denote the polynomial and its coefficients vector with the same letter. The intended meaning is understood from the context.

The coefficients vector of a polynomial, however, is not unique. (Scaling of the coefficients vector by a nonzero number result in the same polynomial.) In order to remove this nonuniqueness, we scale the coefficients, so that the highest power coefficient is equal to one (monic polynomial). In what follows, it is assumed that the coefficients are aways scaled in this way.

The polynomials p and $\widehat{p}$ of degree n are "close" to each other if the distance measure

$$\operatorname{dist}\big(p, \widehat{p}\big) := \|p - \widehat{p}\|_2$$

is "small", *i.e.*, if the norm of the coefficients vector of the error polynomial $\Delta p := p - \widehat{p}$ is small.

Note 3.12. The distance $\operatorname{dist}\big(p, \widehat{p}\big)$, defined above, might not be an appropriate distance measure in applications where the polynomial roots rather than coefficients are of primary interest. Polynomial roots might be sensitive (especially for high order polynomials) to perturbations in the coefficients, so that closeness of coefficients does not necessarily imply closeness of roots. Using the quadratic distance measure in terms of the polynomial coefficients, however, simplifies the solution of the approximate common divisor problem defined next.

Problem 3.13 (Approximate common divisor). Given polynomials p and q, and a natural number `d`, smaller than the degrees of p and q, find polynomials $\widehat{p}$ and $\widehat{q}$ that have a common divisor c of degree `d` and minimize the approximation error

$$\operatorname{dist}\big(\operatorname{col}(p, q), \operatorname{col}(\widehat{p}, \widehat{q})\big).$$

The polynomial c is an optimal (in the specified sense) approximate common divisor of p and q. □

Note 3.14. The object of interest in solving Problem 3.13 is the approximate common divisor c. The approximating polynomials $\widehat{p}$ and $\widehat{q}$ are auxiliary variables introduced for the purpose of defining c.

Note 3.15. Problem 3.13 has the following system theoretic interpretation. Consider the single-input single-output linear time-invariant system $\mathscr{B} = \mathscr{B}_{\text{i/o}}(p,q)$. The system $\mathscr{B}$ is controllable if and only if p and q have no common factor. Therefore, Problem 3.13 finds the nearest uncontrollable system $\widehat{\mathscr{B}} = \mathscr{B}_{\text{i/o}}(\widehat{p},\widehat{q})$ to the given system $\mathscr{B}$. The bigger the approximation error is, the more robust the controllability property of $\mathscr{B}$ is. In particular, with zero approximation error, $\mathscr{B}$ is uncontrollable.

Equivalent optimization problem

By definition, the polynomial c is a common divisor of $\widehat{p}$ and $\widehat{q}$ if there are polynomials u and v, such that

$$\widehat{p} = uc \qquad \text{and} \qquad \widehat{q} = vc. \tag{GCD}$$

With the auxiliary variables u and v, Problem 3.13 becomes the following optimization problem:

$$\begin{array}{lll} \text{minimize} & \text{over } \widehat{p},\, \widehat{q},\, u,\, v, \text{ and } c & \operatorname{dist}\big(\operatorname{col}(p,q), \operatorname{col}(\widehat{p},\widehat{q})\big) \\ \text{subject to} & \widehat{p} = uc, \quad \widehat{q} = vc, \quad \text{and} & \operatorname{degree}(c) = \mathtt{d}. \end{array} \tag{AGCD}$$

Theorem 3.16. *The optimization problem (AGCD) is equivalent to*

$$\text{minimize} \quad \text{over } c_0, \dots, c_{\mathtt{d}-1} \in \mathbb{R} \quad f(c), \tag{AGCD'}$$

where

$$f(c) := \operatorname{trace}\Big(\big[p \;\, q\big]^\top \Big(I - \mathscr{T}_{n+1}(c) \big(\mathscr{T}_{n+1}^\top(c) \mathscr{T}_{n+1}(c)\big)^{-1} \mathscr{T}_{n+1}^\top(c) \Big) \big[p \;\, q\big] \Big),$$

and $\mathscr{T}_{n+1}(c)$ is an upper triangular Toeplitz matrix, defined in ($\mathscr{T}$) on page 88.

The proof is given in Appendix B.

Compared with the original optimization problem (AGCD), in (AGCD'), the constraint and the auxiliary decision variables $\widehat{p}$, $\widehat{q}$, u, and v are eliminated. This achieves significant simplification from a numerical optimization point of view. The equivalent problem (AGCD') is a nonlinear least squares problem and can be solved by standard local optimization methods, see Algorithm 1.

Since

$$f(c) = \operatorname{dist}\big(\operatorname{col}(p,q), \operatorname{col}(\widehat{p},\widehat{q})\big)$$

the value of the cost function $f(c)$ shows the approximation errors in taking c as an approximate common divisor of p and q. Optionally, Algorithm 1 returns a "certificate" $\widehat{p}$ and $\widehat{q}$ for c being an approximate common divisor of p and q with approximation error $f(c)$.

Algorithm 1 Optimal approximate common divisor computation.

```
Input: Polynomials $p$ and $q$ and a positive integer $\mathtt{d}$.
1: Compute an initial approximation $c_{\text{ini}} \in \mathbb{R}^{\mathtt{d}+1}$.
2: Execute a standard optimization algorithm for the minimization (AGCD') with initial approximation $c_{\text{ini}}$.
3: if $\widehat{p}$ and $\widehat{q}$ have to be displayed then
4:     Solve for $u$ and $v$ the linear least squares problem in $u$ and $v$
           $[p \; q] = \mathscr{T}_{n-\mathtt{d}+1}(c) \, [u \; v]$.
5:     Define $\widehat{p} = u \star c$ and $\widehat{q} = v \star c$, where $\star$ denotes discrete convolution.
6: end if
Output: The approximation $c \in \mathbb{R}^{\mathtt{d}+1}$ found by the optimization algorithm upon convergence, the value of the cost function $f(c)$ at the optimal solution, and if computed $\widehat{p}$ and $\widehat{q}$.
```

In order to complete Algorithm 1, next, we specify the computation of the initial approximation c_{ini}. Also, the fact that the analytic expression for $f(c)$ involves the highly structured matrix $\mathscr{T}_{n-\mathtt{d}+1}(c)$ suggests that $f(c)$ (and its derivatives) can be evaluated efficiently.

Efficient cost function evaluation

The most expensive operation in the cost function evaluation is solving the least squares problem

$$\big[p \;\, q\big] = \mathscr{T}_{n-\mathtt{d}+1}(c) \, \big[u \;\, v\big].$$

Since $\mathscr{T}_{n-\mathtt{d}+1}(c)$ is an upper triangular, banded, Toeplitz matrix, this operation can be done efficiently. One approach is to compute efficiently the QR factorization of $\mathscr{T}_{n-\mathtt{d}+1}(c)$, *e.g.*, via the *generalized Schur algorithm*. Another approach is to solve the normal system of equations

$$\mathscr{T}_{n+1}^\top(c) \, \big[p \;\, q\big] = \mathscr{T}_{n-\mathtt{d}+1}^\top(c) \mathscr{T}_{n-\mathtt{d}+1}(c) \, \big[u \;\, v\big],$$

exploiting the fact that $\mathscr{T}_{n-\mathtt{d}+1}^\top(c) \mathscr{T}_{n-\mathtt{d}+1}(c)$ is banded and Toeplitz structured. The first approach is implemented in the function `MB02ID` from the SLICOT library.

Once the least squares problem is solved, the product

$$\mathscr{T}_{n-\mathtt{d}+1}(c) \, \big[u \;\, v\big] = \big[c \star u \quad c \star v\big]$$

is computed efficiently by the *fast Fourier transform*. The resulting algorithm has computational complexity $O(n)$ operations. The first derivative $f'(c)$ can be evaluated also in $O(n)$ operations, so assuming that $\mathtt{d} \ll n$, the overall cost per iteration for Algorithm 1 is $O(n)$.

Initial approximation

Suboptimal initial approximation can be computed by the singular value decomposition of the Sylvester (sub)matrix

$$\mathscr{R}_{\mathtt{d}}(p,q) = \begin{bmatrix}\mathscr{T}^{\top}_{n-\mathtt{d}+1}(p) & \mathscr{T}^{\top}_{n-\mathtt{d}+1}(q)\end{bmatrix} = \begin{bmatrix} p_0 & & & q_0 & & \\ p_1 & p_0 & & q_1 & q_0 & \\ \vdots & p_1 & \ddots & \vdots & q_1 & \ddots \\ p_n & \vdots & \ddots\ p_0 & q_n & \vdots & \ddots\ q_0 \\ & p_n & p_1 & & q_n & q_1 \\ & & \ddots\ \vdots & & & \ddots\ \vdots \\ & & p_n & & & q_n \end{bmatrix} \in \mathbb{R}^{(2n-\mathtt{d}+1)\times(2n-2\mathtt{d}+2)}.$$

Since, the approximate greatest common divisor problem (AGCD) is a structured low-rank approximation problem, ignoring the Sylvester structure constraint results a suboptimal solution method—unstructured low-rank approximation. A suboptimal solution is therefore computable by the singular value decomposition.

The polynomial c is a common divisor of $\widehat{p}$ and $\widehat{q}$ if and only if there are polynomials u and v, such that

$$\widehat{p}v = \widehat{q}u. \tag{$*$}$$

With degree$(c) = \mathtt{d}$, the polynomial equation $(*)$ is equivalent to the system of algebraic equations

$$\mathscr{R}_{\mathtt{d}}(\widehat{p},\widehat{q})\begin{bmatrix} v \\ -u\end{bmatrix} = 0.$$

The degree constraint for c is equivalent to

$$\operatorname{degree}(u) = n - \mathtt{d},$$

or equivalently $u_{n-\mathtt{d}+1} \neq 0$. Since u is defined up to a scaling factor, we impose the normalization $u_{n-\mathtt{d}+1} = 1$. This shows that problem (AGCD) is equivalent to

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{p},\widehat{q} \in \mathbb{R}^{n+1} \text{ and } u,v \in \mathbb{R}^{n-\mathtt{d}+1} \quad \left\| \begin{bmatrix} p & q\end{bmatrix} - \begin{bmatrix}\widehat{p} & \widehat{q}\end{bmatrix}\right\|_{\mathrm{F}} \\ &\text{subject to} \quad \mathscr{R}_{\mathtt{d}}(\widehat{p},\widehat{q})\begin{bmatrix} v \\ -u\end{bmatrix} = 0 \quad \text{and} \quad u_{n-\mathtt{d}+1} = 1. \end{aligned} \tag{AGCD''}$$

The approximate common factor c is not explicitly computed in (AGCD”). Once the optimal u and v are known, however, c can be found from (GCD). (By construction these equations have unique solution). Alternatively, without using the auxiliary variables $\widehat{p}$ and $\widehat{q}$, c can be computed from the least squares problem

$$\begin{bmatrix} p \\ q\end{bmatrix} = \begin{bmatrix} u \\ v\end{bmatrix} c,$$

or in linear algebra notation

$$\begin{bmatrix} p \\ q\end{bmatrix} = \begin{bmatrix} \mathscr{T}^{\top}_{\mathtt{d}+1}(u) \\ \mathscr{T}^{\top}_{\mathtt{d}+1}(v)\end{bmatrix} c. \tag{3.1}$$

Problem (AGCD”) is a structured low-rank approximation problem: it aims to find a Sylvester rank deficient matrix $\mathscr{R}_{\mathtt{d}}(\widehat{p},\widehat{q})$ as close as possible to a given matrix $\mathscr{R}_{\mathtt{d}}(p,q)$ with the same structure. If p and q have no common divisor of degree $\mathtt{d}$, $\mathscr{R}_{\mathtt{d}}(p,q)$ is full rank so that an approximation is needed.

The (unstructured) low-rank approximation problem

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{D} \text{ and } r \quad \left\| \mathscr{R}_{\mathtt{d}}(p,q) - \widehat{D}\right\|^2_{\mathrm{F}} \\ &\text{subject to} \quad \widehat{D}r = 0 \quad \text{and} \quad r^{\top}r = 1 \end{aligned} \tag{LRA$_r$}$$

has an analytic solution in terms of the singular value decomposition of $\mathscr{R}_{\mathtt{d}}(p,q)$. The vector $r \in \mathbb{R}^{2(n-\mathtt{d}+1)}$ corresponding to the optimal solution of (LRA$_r$) is equal to the right singular vector of $\mathscr{R}_{\mathtt{d}}(p,q)$ corresponding to the smallest singular value. The vector $\operatorname{col}(v,-u)$ composed of the coefficients of the approximate divisors v and $-u$ is up to a scaling factor (that enforces the normalization constraint $u_{n-\mathtt{d}+1} = 1$) equal to r. This gives Algorithm 2 as a method for computing a suboptimal initial approximation.

Algorithm 2 Suboptimal approximate common divisor computation.

```
Input: Polynomials $p$ and $q$ and an integer $\mathtt{d}$.
 1: Solve the unstructured low-rank approximation problem (LRA$_r$).
 2: Let $\operatorname{col}(v,-u) := r$, where $u,v \in \mathbb{R}^{n-\mathtt{d}+1}$.
 3: Solve the least squares problem (3.1).
Output: The solution $c$ of the least squares problem.
```

Numerical examples

Implementation of the method for computation of approximate common divisor, described in this section, is available from the book’s web page. We verify the results obtained by Algorithm 1 on examples from (Zhi and Yang, 2004) and (Karmarkar and Lakshman, 1998). Up to the number of digits shown the results match the ones reported in the literature.

Example 4.1 from (Zhi and Yang, 2004)

The given polynomials are

$$p(z) = (4+2z+z^2)(5+2z)+0.05+0.03z+0.04z^2$$
$$q(z) = (4+2z+z^2)(5+\ z)+0.04+0.02z+0.01z^2$$

and an approximate common divisor c of degree $d=2$ is sought. Algorithm 1 converges in 4 iteration steps with the following answer

$$c(z) = 3.9830+1.9998z+1.0000z^2.$$

To this approximate common divisor correspond approximating polynomials

$$\widehat{p}(z) = 20.0500+18.0332z+9.0337z^2+2.0001z^3$$
$$\widehat{q}(z) = 20.0392+14.0178z+7.0176z^2+0.9933z^3$$

and the approximation error is

$$f(c) = \operatorname{dist}^2\big(p,\widehat{p}\big)+\operatorname{dist}^2\big(q,\widehat{q}\big) = 1.5831\times 10^{-4}.$$

Example 4.2, case 1, from (Zhi and Yang, 2004) (originally given in (Karmarkar and Lakshman, 1998))

The given polynomials are

$$p(z) = (1-z)(5-z) = 5-6z+z^2$$
$$q(z) = (1.1-z)(5.2-z) = 5.72-6.3z+z^2$$

and an approximate common divisor c of degree $\mathtt{d}=1$ (a common root) is sought. Algorithm 1 converges in 6 iteration steps with the following answer

$$c(z) = -5.0989+1.0000z.$$

The corresponding approximating polynomials are

$$\widehat{p}(z) = 4.9994-6.0029z+0.9850z^2$$
$$\widehat{q}(z) = 5.7206-6.2971z+1.0150z^2$$

and the approximation error is $f(c) = 4.6630\times 10^{-4}$.

3.3 Data modeling using the nuclear norm heuristic

The nuclear norm heuristic leads to a semidefinite optimization problem, which can be solved by existing algorithms with provable convergence properties and readily available high quality software packages. Apart from theoretical justification and easy implementation in practice, formulating the problem as a semidefinite program has the advantage of flexibility. For example, adding regularization and affine inequality constraints in the data modeling problem still leads to semidefinite optimization problems that can be solved by the same algorithms and software as the original problem.

A disadvantage of using the nuclear norm heuristic is the fact that the number of optimization variables in the semidefinite optimization problem depends quadratically on the number of data points in the data modeling problem. This makes methods based on the nuclear norm heuristic impractical for problems with more than a few hundreds of data points. Such problems are "small size" data modeling problem.

Nuclear norm heuristics for structured low-rank approximation

Regularized nuclear norm minimization

The nuclear norm of a matrix is the sum of the matrix's singular values

$$\|M\|_* = \text{sum of the singular values of } M. \tag{NN}$$

Recall the mapping $\mathscr{S}$, see ($\mathscr{S}(\widehat{p})$), on page 84, from a structure parameter space $\mathbb{R}^{n_p}$ to the set of matrices $\mathbb{R}^{m\times n}$. Regularized nuclear norm minimization

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{p} \quad \|\mathscr{S}(\widehat{p})\|_* + \gamma\|p-\widehat{p}\| \\ \text{subject to} & G\widehat{p}\le h \end{array} \tag{NNM}$$

is a convex optimization problem and can be solved globally and efficiently. Using the fact

$$\|\widehat{D}\|_* < \mu \quad \iff \quad \frac{1}{2}\big(\operatorname{trace}(U)+\operatorname{trace}(V)\big) < \mu \quad \text{and} \quad \begin{bmatrix} U & \widehat{D}^\top \\ \widehat{D} & V \end{bmatrix} \succeq 0,$$

we obtain an equivalent problem

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{p}, U, V, \text{ and } \nu \quad \frac{1}{2}\big(\operatorname{trace}(U)+\operatorname{trace}(V)\big)+\gamma\nu \\ \text{subject to} & \begin{bmatrix} U & \mathscr{S}(\widehat{p})^\top \\ \mathscr{S}(\widehat{p}) & V \end{bmatrix} \succeq 0, \\ & \|p-\widehat{p}\| < \nu, \quad \text{and} \quad G\widehat{p}\le h, \end{array} \tag{NNM'}$$

which can further be reduced to a semidefinite programming problem and solved by standard methods.

Structured low-rank approximation

Consider the affine structured low-rank approximation problem (SLRA). Due to the rank constraint, this problem is non-convex. Replacing the rank constraint by a constraint on the nuclear norm of the affine structured matrix, however, results in a convex relaxation of (SLRA)

$$\text{minimize} \quad \text{over } \widehat{p} \quad \|p-\widehat{p}\| \quad \text{subject to} \quad \|\mathscr{S}(\widehat{p})\|_* \leq \mu. \tag{RLRA}$$

The motivation for this heuristic of solving (SLRA) is that approximation with an appropriately chosen bound on the nuclear norm tends to give solutions $\mathscr{S}(\widehat{p})$ of low (but nonzero) rank. Moreover, the nuclear norm is the tightest relaxation of the rank function, in the same way ℓ_1-norm is the tightest relaxation of the function mapping a vector to the number of its nonzero entries.

Problem (RLRA) can also be written in the equivalent unconstrained form

$$\text{minimize} \quad \text{over } \widehat{p} \quad \|\mathscr{S}(\widehat{p})\|_* + \gamma\|p-\widehat{p}\|. \tag{RLRA'}$$

Here γ is a regularization parameter that is related to the parameter μ in (RLRA). The latter formulation of the relaxed affine structured low-rank approximation problem is a regularized nuclear norm minimization problem (NNM').

Literate programs

Regularized nuclear norm minimization

The CVX package is used in order to automatically translate problem (NNM') into a standard convex optimization problem and solve it by existing optimization solvers.

99a ⟨*Regularized nuclear norm minimization* 99a⟩≡ 99b▷
```
function [ph, info] = nucnrm(tts, p, gamma, nrm, w, s0, g, h)
⟨S ↦ (m,n,n_p) 85b⟩, ⟨default s0 85e⟩
```
Defines:
`nucnrm`, used in chunks 100c and 105.

The code consists of definition of the optimization variables:

99b ⟨*Regularized nuclear norm minimization* 99a⟩+≡ ◁99a 100a▷
```
cvx_begin sdp; cvx_quiet(true);
  variable U(n, n) symmetric;
  variable V(m, m) symmetric;
  variables ph(np) nu;
  ⟨(S_0, S, p̂) ↦ D̂ = 𝒮(p̂) 85a⟩
```

and direct rewriting of the cost function and constraints of (NNM') in CVX syntax:

100a ⟨*Regularized nuclear norm minimization* 99a⟩+≡ ◁99b
```
    minimize( trace(U) / 2 + trace(V) / 2 + gamma * nu );
    subject to
      [U dh'; dh V] > 0;
      norm(w * (p - ph), nrm) < nu;
      if (nargin > 6) & ~isempty(g), g * ph < h; end
  cvx_end
```
The `w` argument specifies the norm ($\|\cdot\|_w$) and is equal to 1, 2, `inf`, or (in the case of a weighted 2-norm) a $n_p \times n_p$ positive semidefinite matrix. The `info` output variable is a structure with fields `optval` (the optimal value) and `status` (a string indicating the convergence status).

Structured low-rank approximation

The following function finds suboptimal solution of the structured low-rank approximation problem by solving the relaxation problem (RLRA'). Affine structures of the type (S) are considered.

100b ⟨*Structured low-rank approximation using the nuclear norm* 100b⟩≡ 100d▷
```
  function [ph, gamma] = slra_nn(tts, p, r, gamma, nrm, w, s0)
  ⟨S ↦ (m,n,n_p) 85b⟩, ⟨S ↦ S 85c⟩, ⟨default s0 85e⟩, ⟨default weight matrix 85f⟩
  if ~exist('gamma', 'var'), gamma = []; end % default gamma
  if ~exist('nrm', 'var'),   nrm = 2;    end % default norm
```
Defines:
`slra_nn`, used in chunks 102d, 103a, 127b, and 129b.

If a parameter γ is supplied, the convex relaxation (RLRA') is completely specified and can be solved by a call to `nucnrm`.

100c ⟨*solve the convex relaxation (RLRA') for given γ parameter* 100c⟩≡ (100d 101a)
```
  ph = nucnrm(tts, p, gamma, nrm, w, s0);
```
Uses `nucnrm` 99a.

Large values of γ lead to solutions $\widehat{p}$ with small approximation error $\|p-\widehat{p}\|_W$, but potentially high rank. Vice verse, small values of γ lead to solutions $\widehat{p}$ with low rank, but potentially high approximation error $\|p-\widehat{p}\|_W$. If not given as an input argument, a value of γ which gives an approximation matrix $\mathscr{S}(\widehat{p})$ with numerical rank r can be found by bisection on an a priori given interval $[\gamma_{\min}, \gamma_{\max}]$. The interval can be supplied via the input argument `gamma`, in which case it is a vector $[\gamma_{\min}, \gamma_{\max}]$.

100d ⟨*Structured low-rank approximation using the nuclear norm* 100b⟩+≡ ◁100b
```
  if ~isempty(gamma) & isscalar(gamma)
    ⟨solve the convex relaxation (RLRA') for given γ parameter 100c⟩
  else
    if ~isempty(gamma)
      gamma_min = gamma(1); gamma_max = gamma(2);
    else
      gamma_min = 0; gamma_max = 100;
    end
    ⟨parameters of the bisection algorithm 101b⟩
    ⟨bisection on γ 101a⟩
  end
```

On each iteration of the bisection algorithm, the convex relaxation (RLRA') is solved for γ equal to the mid point $(\gamma_{\min} + \gamma_{\max})/2$ of the interval and the numerical rank of the approximation $\mathscr{S}(\widehat{p})$ is checked by computing the singular values of the approximation. If the numerical rank is higher than r, $\gamma_{\max}$ is redefined to the mid point, so that the search continuous on smaller values of γ (which have the potential of decreasing the rank). Otherwise, $\gamma_{\max}$ is redefined to the mid point, so that the search continuous on higher values of γ (which have the potential of increasing the rank). The search continuous till the interval $[\gamma_{\min}, \gamma_{\max}]$ is sufficiently small or a maximum number of iterations is exceeded.

101a ⟨*bisection on* γ 101a⟩≡ (100d)

```
  iter = 0;
  while ((gamma_max - gamma_min) / gamma_max > rel_gamma_tol) ...
        & (iter < maxiter)
    gamma = (gamma_min + gamma_max) / 2;
    ⟨solve the convex relaxation (RLRA') for given γ parameter 100c⟩
    sv = svd(ph(tts));
    if (sv(r + 1) / sv(1) > rel_rank_tol) ...
      & (sv(1) > abs_rank_tol)
      gamma_max = gamma;
    else
      gamma_min = gamma;
    end
    iter = iter + 1;
  end
```

The rank test and the interval width test involve a priori set tolerances.

101b ⟨*parameters of the bisection algorithm* 101b⟩≡ (100d)

```
  rel_rank_tol  = 1e-6; abs_rank_tol = 1e-6;
  rel_gamma_tol = 1e-5; maxiter      = 20;
```

Examples

Unstructured and Hankel structured problems

The function `slra_nn` for affine structured low-rank approximation by the nuclear norm heuristic is tested on randomly generated Hankel structured and unstructured examples. A rank deficient "true" data matrix is constructed, where the rank r_0 is a simulation parameter. In the case of a Hankel structure, the "true" structure parameter vector p_0 is generated as the impulse response (skipping the first sample) of a discrete-time random linear time-invariant system of order r_0. This ensures that the "true" Hankel structured data matrix $\mathscr{S}(p_0)$ has the desired rank r_0.

102a ⟨*Test* `slra_nn` 102a⟩≡ 102b▷

```
  ⟨initialize the random number generator 91d⟩
  if strcmp(structure, 'hankel')
    np = m + n - 1; tts = hankel(1:m, m:np);
    p0 = impulse(drss(r0), np + 1); p0 = p0(2:end);
```

Defines:
`test_slra_nn`, used in chunk 103.

In the unstructured case, the data matrix is generated by multiplication of random $m \times r_0$ and $r_0 \times n$ factors of a rank revealing factorization of the data matrix $\mathscr{S}(p_0)$.

102b ⟨*Test* `slra_nn` 102a⟩+≡ ◁102a 102c▷

```
  else % unstructured
    np = m * n; tts = reshape(1:np, m, n);
    p0 = rand(m, r0) * rand(r0, n); p0 = p0(:);
  end
```

The data parameter p, passed to the low-rank approximation function, is a noisy version of the true data parameter p_0, where the additive noise's standard deviation is a simulation parameter.

102c ⟨*Test* `slra_nn` 102a⟩+≡ ◁102b 102d▷

```
  e = randn(np, 1); p = p0 + nl * e / norm(e) * norm(p0);
```

The results obtained by `slra_nn`

102d ⟨*Test* `slra_nn` 102a⟩+≡ ◁102c 102e▷

```
  [ph, gamma] = slra_nn(tts, p, r0);
```

Uses `slra_nn` 100b.

are compared with the ones of alternative methods by checking the singular values of $\mathscr{S}(\widehat{p})$, indicating the numerical rank, and the fitting error $\|p - \widehat{p}\|$.

In the case of a Hankel structure, the alternative methods, being used, is Kung's method (implemented in the function `h2ss`) and the method based on local optimization (implemented in the function `slra`).

102e ⟨*Test* `slra_nn` 102a⟩+≡ ◁102d 102f▷

```
  if strcmp(structure, 'hankel')
    sysh = h2ss([0; p], r0);
    ph2 = impulse(sysh, np + 1); ph2 = ph2(2:end);
    tts_ = hankel(1:(r0 + 1), (r0 + 1):np);
    [Rh, ph3] = slra(tts_, p, r0);
    sv = [svd(p(tts)) svd(ph(tts)) svd(ph2(tts)) svd(ph3(tts))]
    cost = [norm(p - p) norm(p - ph) ...
            norm(p - ph2) norm(p - ph3)]
```

Uses `h2ss` 79a and `slra` 87e.

In the unstructured case, the alternative method is basic low-rank approximation (`lra`), which gives globally optimal result in this setup.

102f ⟨*Test* `slra_nn` 102a⟩+≡ ◁102e

```
  else % unstructured
    [Rh, Ph, dh] = lra(p(tts)', r0); dh = dh';
    sv = [svd(p(tts)) svd(ph(tts)) svd(dh)]
    cost = [norm(p - p) norm(p - ph) norm(p - dh(:))]
  end
  ⟨trade-off curve 103a⟩
```

Uses `lra` 66.

Finally, the numerical rank vs fitting error trade-off curves are computed and plotted for the methods based on nuclear norm minimization and unstructured low-rank approximation.

103a ⟨*trade-off curve* 103a⟩≡ (102f)

```
E = []; E_ = [];
for rr = 1:min(m,n) - 1
  ph = slra_nn(tts, p, rr); E  = [E  norm(p - ph)];
  if strcmp(structure, 'hankel')
    sysh = h2ss([0;p], rr);
    ph = impulse(sysh, np + 1); ph = ph(2:end);
  else % unstructured
    if m > n, [Rh, Ph, dh] = lra(p(tts)', rr); dh = dh';
    else      [Rh, Ph, dh] = lra(p(tts), rr);  end
    ph = dh(:);
  end
  E_ = [E_ norm(p - ph)];
end
plot(E , 1:min(m,n)-1, 'bx', 'markersize', 8), hold on
plot(E_, 1:min(m,n)-1, 'ro', 'markersize', 8)
legend('slra_nn','lra')
plot(E , 1:min(m,n)-1, 'b-', 'linewidth', 2, 'markersize', 8)
plot(E_, 1:min(m,n)-1, 'r-.', 'linewidth', 2, 'markersize', 8)
print_fig(structure)
```

Uses `h2ss` 79a, `lra` 66, `print_fig` 25a, and `slra_nn` 100b.

The first test example is a 5×5, unstructured matrix, whose true value has rank 3. Note that in this case the method `lra`, which is based on the singular value decomposition gives an optimal approximation.

103b ⟨*Test* `slra_nn` *on unstructured problem* 103b⟩≡

```
m = 5; n = 5; r0 = 3; nl = 1; structure = 'unstructured';
test_slra_nn
```

Uses `test_slra_nn` 102a.

The output of `test_slra_nn` is given in Table 3.1, left. It shows that the numerical rank (with tolerance 10^{-5}) of both approximations is equal to the specified rank but the approximation error achieved by the nuclear norm heuristic is about two times the approximation error of the optimal approximation. The trade-off curve is shown in Figure 3.1, left plot.

The second test example is a 5×5, Hankel structured matrix, whose true value has rank 3. In this case the singular value decomposition-based method `h2ss` and the local optimization based method `slra` are also heuristics for solving the Hankel structured low-rank approximation problem and give, respectively, suboptimal and locally optimal results.

103c ⟨*Test* `slra_nn` *on Hankel structured problem* 103c⟩≡

```
m = 5; n = 5; r0 = 3; nl = 0.05; structure = 'hankel';
test_slra_nn
```

Uses `test_slra_nn` 102a.

The output of the `test_slra_nn` is given in Table 3.1, right. It again shows that the approximations have numerical rank matching the specification but the nuclear

Table 3.1 Output of `test_slra_nn` in unstructured problem.

```
sv =

    4.8486    3.7087    4.8486
    2.1489    1.0090    2.1489
    1.5281    0.3882    1.5281
    1.1354    0.0000    0.0000
    0.5185    0.0000    0.0000


cost =

         0    2.3359    1.2482
```

norm heuristic gives more than two times larger approximation error. The corresponding trade-off curve is shown in Figure 3.1, right plot.

Table 3.2 Output of `test_slra_nn` in Hankel structured problem.

```
sv =

    0.8606    0.8352    0.8667    0.8642
    0.1347    0.1270    0.1376    0.1376
    0.0185    0.0011    0.0131    0.0118
    0.0153    0.0000    0.0000    0.0000
    0.0037    0.0000    0.0000    0.0000


cost =

         0    0.0246    0.0130    0.0127
```

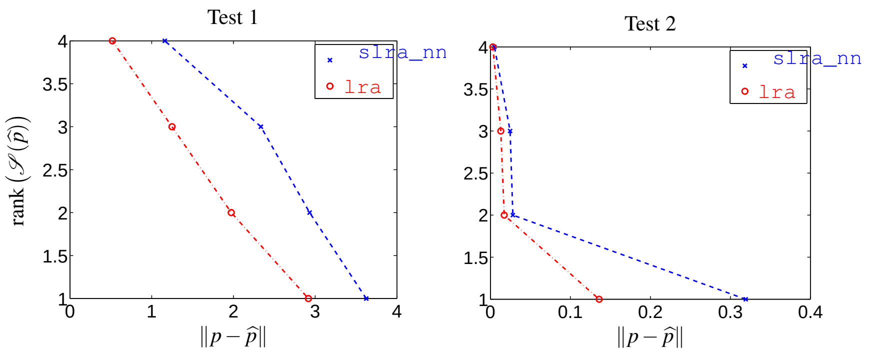

Fig. 3.1 Rank vs approximation error trade-off curve.

Missing data estimation

A random rank deficient "true" data matrix is constructed, where the matrix dimensions $m \times n$ and its rank r_0 are simulation parameters.

105a ⟨*Test missing data* 105a⟩≡ 105b▷
```
  ⟨initialize the random number generator 91d⟩
  p0 = rand(m, r0) * rand(r0, n); p0 = p0(:);
```
Defines:
`test_missing_data`, used in chunk 106b.

The true matrix is unstructured:

105b ⟨*Test missing data* 105a⟩+≡ ◁105a 105c▷
```
  np = m * n; tts = reshape(1:np, m, n);
```
and is perturbed by a sparse matrix with sparsity level `od`, where `od` is a simulation parameter. The perturbation has constant values `nl` (a simulation parameter) in order to simulate outliers.

105c ⟨*Test missing data* 105a⟩+≡ ◁105b 105d▷
```
  pt = zeros(np, 1); no = round(od * np);
  I  = randperm(np); I = I(1:no);
  pt(I) = nl * ones(no, 1); p = p0 + pt;
```
Under certain conditions, derived in (Candés et al, 2009), the problem of recovering the true values from the perturbed data can be solved *exactly* by the regularized nuclear norm heuristic with 1-norm regularization and regularization parameter

$$\gamma = \sqrt{\frac{1}{\min(m,n)}}.$$

105d ⟨*Test missing data* 105a⟩+≡ ◁105c 105e▷
```
  ph1 = nucnrm(tts, p, 1 / sqrt(max(m, n)), 1, eye(np));
```
Uses `nucnrm` 99a.

In addition, the method can deal with missing data at known locations by setting the corresponding entries of the weight vector w to zero. In order to test this feature, we simulate the first element of the data matrix as missing and recover it by the approximation problem

105e ⟨*Test missing data* 105a⟩+≡ ◁105d 105f▷
```
  p(1) = 0;
  ph2 = nucnrm(tts, p, 1 / sqrt(max(m, n)), ...
                1, diag([0; ones(np - 1, 1)]));
```
Uses `nucnrm` 99a.

We check the approximation errors $\|p_0 - \widehat{p}\|_2$, were p_0 is the true value of the data parameter and $\widehat{p}$ is its approximation, obtained by the nuclear norm heuristic method. For comparison, we print also the perturbation size $\|p_0 - p\|_2$.

105f ⟨*Test missing data* 105a⟩+≡ ◁105e 106a▷
```
  [norm(p0 - ph1)  norm(p0 - ph2) norm(p0 - p)]
```

Finally, we check the error of the recovered missing value.

106a ⟨*Test missing data* 105a⟩+≡ ◁105f
```
  [abs(p0(1) - ph1(1)) abs(p0(1) - ph2(1))]
```
The result of a particular test

106b ⟨*Test* `slra_nn` *on small problem with missing data* 106b⟩≡
```
  m = 50; n = 100; r0 = 5; nl = 0.4; od = 0.15; test_missing_data
```
Uses `test_missing_data` 105a.

is

```
ans =

    0.0000    0.0000   10.9969


ans =

   1.0e-09 *

    0.4362    0.5492
```
showing that the method indeed recovers the missing data exactly.

3.4 Notes and references

Efficient software for structured low-rank approximation

The SLICOT library includes high quality FORTRAN implementation of algorithms for Cholesky factorization of positive definite Toeplitz banded matrices. The library is used in a software package (Markovsky and Van Huffel, 2005; Markovsky et al, 2005) for solving structured low-rank approximation problems, based on the variable projections approach (Golub and Pereyra, 2003) and Levenberg–Marquardt's algorithm, implemented in MINPACK. This algorithm is globally convergent with a superlinear convergence rate.

Approximate greatest common divisor

An alternative method for solving structured low-rank approximation problems, called structured total least norm, has been modified for Sylvester structured matrices and applied to computation of approximate common divisor in (Zhi and Yang, 2004). The structured total least norm approach is different from the approach present in this chapter because it solves directly problem (AGCD) and does not use the elimination step leading to the equivalent problem (AGCD').

Nuclear norm heuristic

The nuclear norm relaxation for solving rank minimization problems (RM) was proposed in (Fazel, 2002). It is a generalization of the ℓ_1-norm heuristic from sparse vector approximation problems to low rank matrix approximation problems. The CVX package is developed and maintained by Grant and Boyd (????), see also (Grant and Boyd, 2008). A Python version is also available (Dahl and Vandenberghe, 2010).

The computational engines of `CVX` are SDPT3 and SeDuMi. These solvers can deal with a few tens of parameters ($n_p < 100$). An efficient interior point method for solving (NNM), which can deal with up to 500 parameters, is presented in (Liu and Vandenberghe, 2009). The method is implemented in Python.

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Chapter 4
Applications in system, control, and signal processing

Summary: In this chapter, applications of structured low-rank approximation for

1. approximate realization,
2. model reduction,
3. linear prediction (also known as output only identification and sum-of-damped exponentials modeling),
4. harmonic retrieval,
5. errors-in-variables system identification,
6. output error system identification,
7. finite impulse response system identification (or, equivalently, deconvolution),
8. distance to uncontrollability, and
9. pole placement by a low-order controller,

are reviewed. The types of structure occurring in these applications are affine: (block) Hankel, Toeplitz, and Sylvester.

4.1 Introduction

Structured low-rank approximation is defined as deterministic data approximation.

Problem SLRA (Structured low-rank approximation). Given a structure specification

$$\mathscr{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m\times n}, \qquad \text{with } m \le n,$$

a parameter vector $p \in \mathbb{R}^{n_p}$, a vector norm $\|\cdot\|$, and an integer r, $0 < r < \min(m,n)$,

$$\text{minimize} \quad \text{over } \widehat{p} \quad \|p - \widehat{p}\| \quad \text{subject to} \quad \operatorname{rank}\big(\mathscr{S}(\widehat{p})\big) \le r. \tag{SLRA}$$

□

Equivalently, the problem can be posed as (maximum likelihood) parameter estimation in the errors-in-variables setting:

$$p = p_0 + \widetilde{p}, \qquad \text{where} \quad \operatorname{rank}\big(\mathscr{S}(p_0)\big) \le r \quad \text{and} \quad \widetilde{p} \sim \mathrm{N}(0, \sigma^2 V).$$

The statistical setting gives a recipe for choosing the norm ($\|\cdot\| = \|\cdot\|_{V^{-1}}$) and a "quality certificate" for the approximation method (SLRA): the method works "well" (consistency) and is optimal in a statistical sense (minimal asymptotic error covariance) under certain specified conditions.

The assumptions underlying the statistical setting are that the data p is generated by a true model that is in the considered model class with additive noise $\widetilde{p}$ that is a stochastic process satisfying certain additional assumptions. Model-data mismatch, however is often due to a restrictive linear time-invariant model class being used and not (only) due to measurement noise. This implies that the approximation aspect of the method is often more important than the stochastic estimation one. The problems reviewed in this chapter are stated as deterministic approximation problems although they can be given also the interpretation of defining maximum likelihood estimators under appropriate stochastic assumptions.

All problems are special cases of Problem SLRA for certain specified choices of the norm $\|\cdot\|$, structure $\mathscr{S}$, and rank r. In all problems the structure is affine, so that the algorithm and corresponding function `slra`, developed in Chapter 3, for solving affine structured low-rank approximation problems can be used for solving the problems in this chapter.

110 ⟨*solve Problem SLRA* 110⟩≡ (111a 115 118a 119a 122a)
```
  [R, ph, info] = slra(tts, par, r, [], s0);
```
Uses `slra` 87e.

4.2 Model reduction

Approximate realization

Define the 2-norm $\|\Delta H\|_2$ of a matrix-valued signal $\Delta H \in (\mathbb{R}^{\mathtt{p}\times\mathtt{m}})^{T+1}$ as

$$\|\Delta H\|_2 := \sqrt{\sum_{t=0}^{T} \|\Delta H(t)\|_{\mathrm{F}}^2},$$

and let σ be the shift operator

$$\sigma(H)(t) = H(t+1).$$

Acting on a finite time series $\big(H(0), H(1), \ldots, H(T)\big)$, σ removes the first sample $H(0)$.

Problem 4.1 (Approximate realization). Given $H_d \in (\mathbb{R}^{p\times m})^T$ and a complexity specification $\mathtt{l}$, find an optimal approximate model for H_d of a bounded complexity $(\mathtt{m},\mathtt{l})$, such that

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{H} \text{ and } \widehat{\mathscr{B}} \quad \|H_d - \widehat{H}\|_2 \\ &\text{subject to} \quad \widehat{H} \text{ is the impulse response of } \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{l}}. \end{aligned} \qquad \square$$

111a ⟨*2-norm optimal approximate realization* 111a⟩≡
```
function [sysh, hh, info] = h2ss_opt(h, l)
⟨reshape H and define m, p, T 79b⟩
⟨approximate realization structure 111b⟩
⟨solve Problem SLRA 110⟩
⟨p̂ ↦ Ĥ 111c⟩, ⟨Ĥ ↦ B̂ 112a⟩
```
Defines:
`h2ss_opt`, used in chunks 112–14.

Problem 4.1 is equivalent to Problem SLRA, with

- norm $\|\cdot\| = \|\cdot\|_2$,
- Hankel structured data matrix $\mathscr{S}(p) = \mathscr{H}_{\mathtt{l}+1}(\sigma H_d)$, and
- rank reduction by the number of outputs $\mathtt{p}$.

111b ⟨*approximate realization structure* 111b⟩≡ (111a)
```
par = vec(h(:, :, 2:end)); s0 = []; r = l * p;
tts = blkhank(reshape(1:length(par), p, m, T - 1), l + 1);
```
Uses `blkhank` 25b.

The statement follows from the equivalence

$$\widehat{H} \text{ is the impulse response of } \widehat{\mathscr{B}} \in \mathscr{L}_{\mathtt{m},\mathtt{l}} \quad \Longleftrightarrow \quad \operatorname{rank}\big(\mathscr{H}_{\mathtt{l}+1}(\sigma\widehat{H})\big) \leq \mathtt{pl}.$$

The optimal approximate model $\widehat{\mathscr{B}}^*$ does not depend on the shape of the Hankel matrix as long as the Hankel matrix dimensions are sufficiently large: at least $\mathtt{p}(\mathtt{l}+1)$ rows and at least $\mathtt{m}(\mathtt{l}+1)$ columns. However, solving the low-rank approximation problem for a data matrix $\mathscr{H}_{\mathtt{l}'+1}(\sigma H_d)$, where $\mathtt{l}' > \mathtt{l}$, one needs to achieve rank reduction by $\mathtt{p}(\mathtt{l}'-\mathtt{l}+1)$ instead of by $\mathtt{p}$. Larger rank reduction leads to more difficult computational problems. On one hand, the cost per iteration gets higher and on another hand, the search space gets higher dimensional, which makes the optimization algorithm more susceptible to local minima.

The mapping $\widehat{p} \mapsto \widehat{H}$ from the solution $\widehat{p}$ of the structured low-rank approximation problem to the optimal approximation $\widehat{H}$ of the noisy impulse response H is reshaping the vector $\widehat{p}$ as a $\mathtt{m}\times\mathtt{p}\times T$ tensor `hh`, representing the sequence $\widehat{H}(1),\dots,\widehat{H}(T-1)$ and setting $\widehat{H}(0) = H(0)$ (since $\widehat{D} = H(0)$).

111c ⟨$\widehat{p} \mapsto \widehat{H}$ 111c⟩≡ (111a)
```
hh = zeros(p, m, T); hh(:, :, 1) = h(:, :, 1);
hh(:, :, 2:end) = reshape(ph(:), p, m, T - 1);
```

The mapping $\widehat{H} \mapsto \widehat{\mathscr{B}}$ is system realization, *i.e.*, the 2-norm (locally) optimal realization $\widehat{\mathscr{B}}^*$ is obtained by exact realization of the approximation $\widehat{H}$, computed by the structured low-rank approximation method.

112a ⟨$\widehat{H} \mapsto \widehat{\mathscr{B}}$ 112a⟩≡ (111a)
```
sysh = h2ss(hh, l * p);
```
Uses `h2ss` 79a.

By construction, the approximation $\widehat{H}$ of H has an exact realization in the model class $\mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{l}}$.

Note 4.2. In the numerical solution of the structured low-rank approximation problem, the kernel representation (rank_R) on page 83 of the rank constraint is used. The parameter R, computed by the solver, gives a kernel representation of the optimal approximate model $\widehat{\mathscr{B}}^*$. The kernel representation can subsequently be converted to a state space representation. This gives an alternative way of implementing the function `h2ss_opt` to the one using system realization ($\widehat{H} \mapsto \widehat{\mathscr{B}}$). The same note applies to the other problems, reviewed in the chapter. □

Example

The following script verifies that the local optimization based method `h2ss_opt` improves the suboptimal approximation computed by Kung's method `h2ss`. The data is a noisy impulse response of a random stable linear time-invariant system. The number of inputs `m` and outputs `p`, the order `n` of the system, the number of data points `T`, and the noise standard deviation `s` are simulation parameters.

112b ⟨*Test* `h2ss_opt` 112b⟩≡ 112c▷
```
⟨initialize the random number generator 91d⟩
n = p * l; sys0 = drss(n, p, m);
h0 = reshape(shiftdim(impulse(sys0, T), 1), p, m, T);
h = h0 + s * randn(size(h0));
```
Defines:
`test_h2ss_opt`, used in chunk 112d.

The solutions, obtained by the unstructured and Hankel structured low-rank approximation methods, are computed and the relative approximation errors are printed.

112c ⟨*Test* `h2ss_opt` 112b⟩+≡ ◁112b
```
[sysh, hh] = h2ss(h, n); norm(h(:) - hh(:)) / norm(h(:))
[sysh_, hh_, info] = h2ss_opt(h, l);
norm(h(:) - hh_(:)) / norm(h(:))
```
Uses `h2ss` 79a and `h2ss_opt` 111a.

The optimization based method improves the suboptimal results of the singular value decomposition based method at the price of extra computation, a process refered to as *iterative refinement* of the solution.

112d ⟨*Compare* `h2ss` *and* `h2ss_opt` 112d⟩≡
```
m = 2; p = 3; l = 1; T = 25; s = 0.2; test_h2ss_opt
```
Uses `test_h2ss_opt` 112b.

$\rightsquigarrow$ 0.6231 for `h2ss` and 0.5796 for `h2ss_opt`

Model reduction

The finite time-T H$_2$ norm $\|\Delta\mathscr{B}\|_{2,T}$ of a linear time-invariant system $\Delta\mathscr{B}$ is defined as the 2-norm of the sequence of its first T Markov parameters, *i.e.*, if ΔH is the impulse response of $\Delta\mathscr{B}$, $\|\Delta\mathscr{B}\|_{2,T} := \|\Delta H\|_2$.

Problem 4.3 (Finite time H$_2$ model reduction). Given a linear time-invariant system $\mathscr{B}_\mathrm{d} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}}$ and a complexity specification $\mathtt{l}_\mathrm{red} < \mathtt{l}$, find an optimal approximation of $\mathscr{B}_\mathrm{d}$ with bounded complexity $(\mathtt{m}, \mathtt{l}_\mathrm{red})$, such that

$$\text{minimize} \quad \text{over } \widehat{\mathscr{B}} \quad \|\mathscr{B}_\mathrm{d} - \widehat{\mathscr{B}}\|_{2,T} \quad \text{subject to} \quad \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}_\mathrm{red}}. \qquad \square$$

Problem 4.3 is equivalent to Problem SLRA with

- norm $\|\cdot\| = \|\cdot\|_2$,
- Hankel structured data matrix $\mathscr{S}(p) = \mathscr{H}_{\mathtt{l}+1}(\sigma H_\mathrm{d})$, where H_d is the impulse response of $\mathscr{B}_\mathrm{d}$, and
- rank reduction by the number of outputs $\mathtt{p} := \mathtt{q} - \mathtt{m}$,

which shows that finite time H$_2$ model reduction is equivalent to the approximate realization problem with H_d being the impulse response of $\mathscr{B}_\mathrm{d}$. In practice, $\mathscr{B}_\mathrm{d}$ need not be linear time-invariant system since in the model reduction problem only the knowledge of its impulse response H_d is used.

113 ⟨*Finite time H$_2$ model reduction* 113⟩≡
```
function [sysh, hh, info] = mod_red(sys, T, lred)
[sysh, hh, info] = h2ss_opt(shiftdim(impulse(sys, T), 1), lred);
```
Defines:
`mod_red`, used in chunk 127d.
Uses `h2ss_opt` 111a.

Exercise 4.4. Compare the results of `mod_red` with the ones obtained by using unstructured low-rank approximation (finite-time balanced model reduction) on simulation examples. □

Output only identification

Excluding the cases of multiple poles, the model class of autonomous linear time-invariant systems $\mathscr{L}^{\mathtt{p}}_{0,\mathtt{l}}$ is equivalent to the *sum-of-damped exponentials model* class, *i.e.*, signals y that can be represented in the form

$$y(t) = \sum_{k=1}^{\mathtt{l}} \alpha_k e^{\beta_k t} e^{\mathbf{i}(\omega_k t + \phi_k)}, \qquad (\mathbf{i} = \sqrt{-1}).$$

The parameters $\{\alpha_k, \beta_k, \omega_k, \phi_k\}_{j=1}^{\mathtt{l}}$ of the sum-of-damped exponentials model have the following meaning: α_k are amplitudes, β_k damping factors, ω_k frequencies, and ϕ_k initial phases.

Problem 4.5 (Output only identification). Given a signal $y_\mathrm{d} \in (\mathbb{R}^{\mathtt{p}})^T$ and a complexity specification $\mathtt{l}$, find an optimal approximate model for y_d of bounded complexity $(0, \mathtt{l})$, such that

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{y} \quad \|y_\mathrm{d} - \widehat{y}\|_2 \\ &\text{subject to} && \widehat{y} \in \widehat{\mathscr{B}}|_{[1,T]} \text{ and } \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{p}}_{0,\mathtt{l}}. \end{aligned} \qquad \square$$

Problem 4.5 is equivalent to Problem SLRA with

- norm $\|\cdot\| = \|\cdot\|_2$,
- Hankel structured data matrix $\mathscr{S}(p) = \mathscr{H}_{\mathtt{l}+1}(y_\mathrm{d})$, and
- rank reduction by the number of outputs $\mathtt{p}$,

which shows that output only identification is equivalent to approximate realization and is, therefore, also equivalent to finite time H$_2$ model reduction. In the signal processing literature, the problem is known as *linear prediction*.

114a ⟨*Output only identification* 114a⟩≡
```
function [sysh, yh, xinih, info] = ident_aut(y, l)
[sysh, yh, info] = h2ss_opt(y, l);
```
⟨*impulse response realization ↦ autonomous system realization* 114b⟩
Defines:
`ident_aut`, used in chunk 211c.
Uses `h2ss_opt` 111a.

Let $\mathscr{B}_{\mathrm{i/s/o}}(A,b,C,d)$ be a realization of y. Then the response of the autonomous system $\mathscr{B}_\mathrm{ss}(A,C)$ to initial condition $x(0) = b$ is y. This gives a link between impulse response realization and autonomous system realization:

114b ⟨*impulse response realization ↦ autonomous system realization* 114b⟩≡ (114a 115)
```
xinih = sysh.b; sysh = ss(sysh.a, [], sysh.c, [], -1);
```

Exercise 4.6. Compare the results of `ident_aut` with the ones obtained by using unstructured low-rank approximation on simulation examples. □

Harmonic retrieval

The aim of the harmonic retrieval problem is to approximate the data by a sum of sinusoids. From a system theoretic point of view, harmonic retrieval aims to approximate the data by a marginally stable linear time-invariant autonomous system[1].

Problem 4.7 (Harmonic retrieval). Given a signal $y_\mathrm{d} \in (\mathbb{R}^{\mathtt{p}})^T$ and a complexity specification $\mathtt{l}$, find an optimal approximate model for y_d that is in the model class $\mathscr{L}^{\mathtt{p}}_{0,\mathtt{l}}$ and is marginally stable, *i.e.*,

[1] A linear time-invariant autonomous system is marginally stable if all its trajectories, except for the $y = 0$ trajectory, are bounded and do not converge to zero.

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{y} \quad \|y_\mathrm{d} - \widehat{y}\|_2 \\ &\text{subject to} \quad \widehat{y} \in \widehat{\mathscr{B}}|_{[1,T]},\ \widehat{\mathscr{B}} \in \mathscr{L}_{0,\mathtt{l}}^{\mathtt{p}}, \text{ and } \widehat{\mathscr{B}} \text{ is marginally stable.} \quad \square \end{aligned}$$

Due to the stability constraint, Problem 4.7 is not a special case of problem SLRA. In the univariate case $\mathtt{p} = 1$, however, a necessary condition for an autonomous model $\mathscr{B}$ to be marginally stable is that a kernel representation $\ker(R)$ of $\mathscr{B}$ is either palindromic,

$$R(z) := \sum_{i=0}^{\mathtt{l}} z^i R_i \text{ is palindromic} \quad :\iff \quad R_{\ell-i} = R_i, \text{ for } i = 0,1,\ldots,\mathtt{l}$$

or antipalindromic,

$$R(z) \text{ is antipalindromic} \quad :\iff \quad R_{\ell-i} = -R_i, \text{ for } i = 0,1,\ldots,\mathtt{l}.$$

The antipalindromic case is nongeneric in the space of the marginally stable systems, so as relaxation of the stability constraint, we can use the constraint that the kernel representation is palindromic.

Problem 4.8 (Harmonic retrieval, relaxed version, scalar case). Given a signal $y_\mathrm{d} \in (\mathbb{R})^T$ and a complexity specification $\mathtt{l}$, find an optimal approximate model for y_d that is in the model class $\mathscr{L}_{0,\mathtt{l}}^1$ and has a palindromic kernel representation, such that

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{y} \quad \|y_\mathrm{d} - \widehat{y}\|_2 \\ &\text{subject to} \quad \widehat{y} \in \widehat{\mathscr{B}}|_{[1,T]},\ \widehat{\mathscr{B}} \in \mathscr{L}_{0,\mathtt{l}}^1 \text{ and } \ker(\widehat{R}) = \widehat{\mathscr{B}}, \text{with } R \text{ palindromic.} \quad \square \end{aligned}$$

115 ⟨*Harmonic retrieval* 115⟩≡
```
function [sysh, yh, xinih, info] = harmonic_retrieval(y, l)
⟨harmonic retrieval structure 116a⟩
⟨solve Problem SLRA 110⟩, yh = ph; sysh  = h2ss(yh, n);
⟨impulse response realization ↦ autonomous system realization 114b⟩
```
Defines:
`harmonic_retrieval`, used in chunk 116b.
Uses `h2ss` 79a.

The constraint "R palindromic" can be expressed as a structural constraint on the data matrix, which reduces the relaxed harmonic retrieval problem to the structured low-rank approximation problem. Problem 4.8 is equivalent to Problem SLRA with

- norm $\|\cdot\| = \|\cdot\|_2$,
- structured data matrix composed of a Hankel matrix next to a Toeplitz matrix:

$$\mathscr{S}(p) = \begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(y) & \updownarrow\mathscr{H}_{\mathtt{l}+1}(y) \end{bmatrix},$$

where

$$\updownarrow\mathscr{H}_{\mathtt{l}+1}(y) := \begin{bmatrix} y_{\mathtt{l}+1} & y_{\mathtt{l}+2} & \cdots & y_T \\ \vdots & \vdots & & \vdots \\ y_2 & y_3 & \cdots & y_{T-\mathtt{l}+1} \\ y_1 & y_2 & \cdots & y_{T-\mathtt{l}} \end{bmatrix},$$

and
- rank reduction by one.

116a ⟨*harmonic retrieval structure* 116a⟩≡ (115)
```
par = y(:); np = length(par); n = l * 1; r = n; s0 = [];
tts = [blkhank(1:np, n + 1) flipud(blkhank(1:np, n + 1))];
```
Uses `blkhank` 25b.

The statement follows from the equivalence

$$\widehat{y} \in \widehat{\mathscr{B}}|_{[1,T]},\ \widehat{\mathscr{B}} \in \mathscr{L}_{0,\mathtt{l}}^1 \text{ and } \ker(\widehat{R}) = \widehat{\mathscr{B}} \text{ is palindromic}$$
$$\iff \quad \operatorname{rank}\left(\begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{y}) & \updownarrow\mathscr{H}_{\mathtt{l}+1}(\widehat{y}) \end{bmatrix}\right) \leq \mathtt{l}.$$

In order to show it, let $\ker(R)$, with $R(z) = \sum_{i=0}^{\mathtt{l}} z^i R_i$ full row rank, be a kernel representation of $\mathscr{B} \in \mathscr{L}_{0,\mathtt{l}}^1$. Then $\widehat{y} \in \widehat{\mathscr{B}}|_{[1,T]}$ is equivalent to

$$\begin{bmatrix} R_0 & R_1 & \cdots & R_{\mathtt{l}} \end{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{y}) = 0.$$

If, in addition, R is palindromic, then

$$\begin{bmatrix} R_{\mathtt{l}} & \cdots & R_1 & R_0 \end{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{y}) = 0 \quad \iff \quad \begin{bmatrix} R_0 & R_1 & \cdots & R_{\mathtt{l}} \end{bmatrix} \updownarrow\mathscr{H}_{\mathtt{l}+1}(\widehat{y}) = 0.$$

We have that

$$\begin{bmatrix} R_0 & R_1 & \cdots & R_{\mathtt{l}} \end{bmatrix} \begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{y}) & \updownarrow\mathscr{H}_{\mathtt{l}+1}(\widehat{y}) \end{bmatrix} = 0. \qquad (*)$$

which is equivalent to

$$\operatorname{rank}\left(\begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{y}) & \updownarrow\mathscr{H}_{\mathtt{l}+1}(\widehat{y}) \end{bmatrix}\right) \leq \mathtt{l}.$$

Conversely, $(*)$ implies $\widehat{y} \in \widehat{\mathscr{B}}|_{[1,T]}$ and R palindromic.

Example

The data is generated as a sum of random sinusoids with additive noise. The number `hn` of sinusoids, the number of samples `T`, and the noise standard deviation `s` are simulation parameters.

116b ⟨*Test* `harmonic_retrieval` 116b⟩≡
```
⟨initialize the random number generator 91d⟩
t  = 1:T; f = 1 * pi * rand(hn, 1); phi = 2 * pi * rand(hn, 1);
y0 = sum(sin(f * t + phi(:, ones(1, T))));
yt = randn(size(y0)); y = y0 + s * norm(y0) * yt / norm(yt);
[sysh, yh, xinih, info] = harmonic_retrieval(y, hn * 2);
```

```
  plot(t, y0, 'k-', t, y, 'k:', t, vec(yh), 'b-'),
  ax = axis; axis([1 T ax(3:4)])
  print_fig('test_harmonic_retrieval')
```
Defines:
`test_harmonic_retrieval`, used in chunk 117.
Uses `harmonic_retrieval` 115 and `print_fig` 25a.

Figure 4.1 shows the true signal, the noisy signal, and the estimate obtained with `harmonic_retrieval` in the following simulation example:

117 ⟨*Example of harmonic retrieval* 117⟩≡
```
  clear all, T = 50; hn = 2; s = 0.015; test_harmonic_retrieval
```
Uses `test_harmonic_retrieval` 116b.

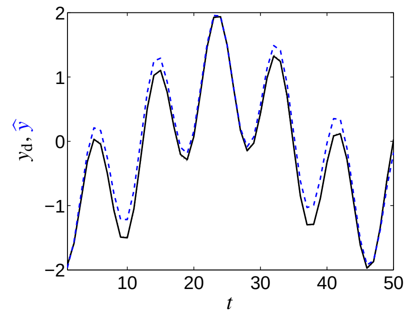

Fig. 4.1 Results of `harmonic_retrieval`: solid line — true system's trajectory y_0, dotted dotted — noisy data y_d, dashed line — best approximation $\widehat{y}$.

4.3 System identification

Errors-in-variables identification

In errors-in-variables data modeling problems, the observed variables are a priori known (or assumed) to be noisy. This prior knowledge is used to correct the data, so that the corrected data is consistent with a model in the model class. The resulting problem is equivalent of the misfit minimization problem (see, Problem 2.33), considered in Chapter 2.

Problem 4.9 (Errors-in-variables identification). Given T samples, $\mathtt{q}$ variables, vector signal $w_d \in (\mathbb{R}^{\mathtt{q}})^T$, a signal norm $\|\cdot\|$, and a model complexity $(\mathtt{m}, \mathtt{l})$,

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{w} \quad \|w_d - \widehat{w}\| \\ &\text{subject to} \quad \widehat{w} \in \widehat{\mathscr{B}}|_{[1,T]} \text{ and } \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}}. \end{aligned} \qquad \square$$

118a ⟨*Errors-in-variables identification* 118a⟩≡
```
  function [sysh, wh, info] = ident_eiv(w, m, l)
```
  ⟨*reshape w and define* q*, T* 26e⟩
  ⟨*errors-in-variables identification structure* 118b⟩
  ⟨*solve Problem SLRA* 110⟩`, wh = reshape(ph(:), q, T);`
  ⟨*exact identification:* $\widehat{w} \mapsto \widehat{\mathscr{B}}$ 118c⟩

Defines:
`ident_eiv`, used in chunks 91g and 118d.

Problem 4.9 is equivalent to Problem SLRA with

- Hankel structured data matrix $\mathscr{S}(p) = \mathscr{H}_{\mathtt{l}+1}(w_d)$ and
- rank reduction with the number of outputs $\mathtt{p}$

118b ⟨*errors-in-variables identification structure* 118b⟩≡ (118a)
```
  par = w(:); np = length(par); n = l * 1;
  p = q - m; r = m * (l + 1) + n;
  tts = blkhank(reshape(1:np, q, T), l + 1); s0 = [];
```
Uses `blkhank` 25b.

The identified system is recovered from the optimal approximating trajectory $\widehat{w}$ by exact identification.

118c ⟨*exact identification:* $\widehat{w} \mapsto \widehat{\mathscr{B}}$ 118c⟩≡ (118a 119a)
```
  sysh = w2h2ss(wh, m, n);
```
Uses `w2h2ss` 82c.

Example

In this example, the approximate model computed by the function `ident_eiv` is compared with the model obtained by the function `w2h2ss`. Although `w2h2ss` is an exact identification method, it can be used as a heuristic for approximate identification. The data is generated in the errors-in-variables setup (see, (EIV) on page 71). The true system is a random single input single output system.

118d ⟨*Test* `ident_eiv` 118d⟩≡
  ⟨*initialize the random number generator* 91d⟩
```
  m = 1; p = 1; n = p * l; sys0 = drss(n, p, m);
  xini0 = rand(n, 1); u0 = rand(T, m);
  y0 = lsim(sys0, u0, 1:T, xini0);
  w = [u0'; y0'] + s * randn(m + p, T);
```
  `sys = w2h2ss(w, m, n);` ⟨*(TF)* ↦ *P* 90e⟩ `misfit_siso(w, P)`
```
  [sysh, wh, info] = ident_eiv(w, m, l); info.M
```
Defines:
`test_ident_eiv`, used in chunk 118e.
Uses `ident_eiv` 118a, `misfit_siso` 89, and `w2h2ss` 82c.

In a particular example

118e ⟨*Compare* `w2h2ss` *and* `ident_eiv` 118e⟩≡
```
  l = 4; T = 30; s = 0.1; test_ident_eiv
```
Uses `test_ident_eiv` 118d.

the obtained results are misfit 1.2113 for `w2h2ss` and 0.2701 for `ident_eiv`.

Output error identification

In the errors-in-variables setting, using an input-output partitioning of the variables, both the input and the output are noisy. In some applications, however, the input is not measured; it is designed by the user. Then, it is natural to assume that the input is noise free. This leads to the output error identification problem.

Problem 4.10 (Output error identification). Given a signal

$$w_d = \big(w_d(1), \dots, w_d(T)\big), \qquad w_d(t) \in \mathbb{R}^{\mathtt{q}},$$

with an input/output partitioning $w = (u, y)$, $\dim(u) = \mathtt{m}$, and a complexity specification $\mathtt{l}$, find an optimal approximate model for w_d of a bounded complexity $(\mathtt{m}, \mathtt{l})$, such that

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{y} \quad \|y_d - \widehat{y}\|_2 \\ \text{subject to} & (u_d, \widehat{y}) \in \widehat{\mathscr{B}}|_{[1,T]} \text{ and } \widehat{\mathscr{B}} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}}. \end{array} \qquad \square$$

119a ⟨*Output error identification* 119a⟩≡
```
  function [sysh, wh, info] = ident_oe(w, m, l)
  ⟨reshape w and define q, T 26e⟩
  ⟨output error identification structure 119b⟩
  ⟨solve Problem SLRA 110⟩, wh = [w(1:m, :); reshape(ph(:), p, T)];
  ⟨exact identification: ŵ ↦ B̂ 118c⟩
```
Defines:
`ident_oe`, used in chunks 120 and 208b.

Output error identification is a limiting case of the errors-in-variables identification problem when the noise variance tends to zero. Alternatively, output error identification is a special case in the prediction error setting when the noise term is not modeled.

As shown next, Problem 4.10 is equivalent to Problem SLRA with

- norm $\|\cdot\| = \|\cdot\|_2$,
- data matrix
$$\mathscr{S}(p) = \begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(u_d) \\ \mathscr{H}_{\mathtt{l}+1}(y_d) \end{bmatrix}$$
composed of a fixed block and a Hankel structured block, and
- rank reduction by the number of outputs $\mathtt{p}$.

119b ⟨*output error identification structure* 119b⟩≡ (119a)
```
  par = vec(w((m + 1):end, :)); np = length(par); p = q - m;
  j = T - l; n = l * p; r = m * (l + 1) + n;
  s0  = [blkhank(w(1:m, :), l + 1); zeros((l + 1) * p, j)];
  tts = [zeros((l + 1) * m, j); blkhank(reshape(1:np, p, T), l + 1)];
```
Uses `blkhank` 25b.

The statement is based on the equivalence

$$(u_d, \widehat{y})|_{[1,T-1]} \in \widehat{\mathscr{B}}|_{[1,T-1]} \text{ and } \widehat{\mathscr{B}} \in \mathscr{L}_{\mathtt{m},\mathtt{l}}$$
$$\iff \quad \operatorname{rank}\left(\begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(u_d) \\ \mathscr{H}_{\mathtt{l}+1}(\widehat{y}) \end{bmatrix}\right) \leq \mathtt{m}(\mathtt{l}+1) + \mathtt{p}\mathtt{l},$$

which is a corollary of the following lemma.

Lemma 4.11. *The signal w is a trajectory of a linear time-invariant system of complexity bounded by* $(\mathtt{m}, \mathtt{l})$, i.e.,

$$w|_{[1,T-1]} \in \mathscr{B}|_{[1,T-1]} \quad \textit{and} \quad \mathscr{B} \in \mathscr{L}^{\mathtt{q}}_{\mathtt{m},\mathtt{l}} \tag{$*$}$$

if and only if

$$\operatorname{rank}\big(\mathscr{H}_{\mathtt{l}+1}(w)\big) \leq \mathtt{m}(\mathtt{l}+1) + (\mathtt{q} - \mathtt{m})\mathtt{l}. \tag{$**$}$$

Proof. ($\Longrightarrow$) Assume that ($*$) holds and let $\ker(R)$, with

$$R(z) = \sum_{i=0}^{\mathtt{l}} z^i R_i \in \mathbb{R}^{g \times \mathtt{q}}[z]$$

full row rank, be a kernel representation of $\mathscr{B}$. The assumption $\mathscr{B} \in \mathscr{L}_{\mathtt{m},\mathtt{l}}$ implies that $g \geq \mathtt{p} := \mathtt{q} - \mathtt{m}$. From $w \in \mathscr{B}|_{[1,T]}$, we have that

$$\begin{bmatrix} R_0 & R_1 & \cdots & R_{\mathtt{l}} \end{bmatrix} \mathscr{H}_{\mathtt{l}+1}(w) = 0, \tag{$***$}$$

which implies that ($**$) holds.

($\Longleftarrow$) Assume that ($**$) holds. Then, there is a full row rank matrix

$$R := \begin{bmatrix} R_0 & R_1 & \cdots & R_{\mathtt{l}} \end{bmatrix} \in \mathbb{R}^{\mathtt{p} \times \mathtt{q}(\mathtt{l}+1)},$$

such that ($***$). Define the polynomial matrix $R(z) = \sum_{i=0}^{\mathtt{l}} z^i R_i$. Then the system $\mathscr{B}$ induced by $R(z)$ via the kernel representation $\ker\big(R(\sigma)\big)$ is such that ($*$) holds. $\square$

Example

This example is analogous to the example of the errors-in-variables identification method. The approximate model obtained with the function `w2h2ss` is compared with the approximate model obtained with `ident_oe`. In this case, the data is generated in the output error setting, *i.e.*, the input is exact and the output is noisy. In this simulation setup we expect that the optimization based method `ident_oe` improves the result obtained with the subspace based method `w2h2ss`.

120 ⟨*Test* `ident_oe` 120⟩≡
```
  ⟨initialize the random number generator 91d⟩
  m = 1; p = 1; n = l * p; sys0 = drss(n, p, m);
  xini0 = rand(n, 1); u0 = rand(T, m); y0 = lsim(sys0, u0, 1:T, xini0);
  w = [u0'; y0'] + s * [zeros(m, T); randn(p, T)];
  sys = w2h2ss(w, m, n); ⟨(TF) ↦ P 90e⟩ misfit_siso(w, P)
  [sysh, wh, info] = ident_oe(w, m, l); info.M
```

Defines:
`test_ident_oe`, used in chunk 121a.
Uses `ident_oe` 119a, `misfit_siso` 89, and `w2h2ss` 82c.

In the following simulation example

121a ⟨*Example of output error identification* 121a⟩≡
```
  l = 4; T = 30; s = 0.1; test_ident_oe
```
Uses `test_ident_oe` 120.

`w2h2ss` achieves misfit 1.0175 and `ident_oe` achieves misfit 0.2331.

Finite impulse response system identification

Let $\text{FIR}_{\mathtt{m},\mathtt{l}}$ be the model class of finite impulse response linear time-invariant systems with $\mathtt{m}$ inputs and lag at most $\mathtt{l}$, *i.e.*,

$$\text{FIR}_{\mathtt{m},\mathtt{l}} := \{\,\mathscr{B} \in \mathscr{L}_{\mathtt{m},\mathtt{l}} \mid \mathscr{B} \text{ has finite impulse response and } \mathtt{m} \text{ inputs}\,\}.$$

Identification of a finite impulse response model in the output error setting leads to the ordinary linear least squares problem

$$\begin{bmatrix}\widehat{H}(0) & \widehat{H}(1) & \cdots & \widehat{H}(\mathtt{l})\end{bmatrix} \mathscr{H}_{\mathtt{l}+1}(u_{\mathrm{d}}) = \begin{bmatrix}y_{\mathrm{d}}(1) & \cdots & y_{\mathrm{d}}(T-\mathtt{l})\end{bmatrix}.$$

121b ⟨*Output error finite impulse response identification* 121b⟩≡
```
  function [hh, wh] = ident_fit_oe(w, m, l)
  ⟨reshape w and define q, T 26e⟩
  ⟨Finite impulse response identification structure 122b⟩
  D = par(tts);
  hh_ = D(((m * (l + 1)) + 1):end, :) / D(1:(m * (l + 1)), :);
  hh = reshape(hh_, p, m, l + 1); hh = hh(:, :, end:-1:1);
  uh = w(1:m, :); yh = [hh_ * D(1:(m * (l + 1)), :) zeros(p, l)];
  wh = [uh; yh];
```
Defines:
`ident_fir_oe`, used in chunk 123b.

Next, we define the finite impulse response identification problem in the errors-in-variables setting.

Problem 4.12 (Errors-in-variables finite impulse response identification). Given a signal

$$w_{\mathrm{d}} = \big(w_{\mathrm{d}}(1),\dots,w_{\mathrm{d}}(T)\big), \qquad w_{\mathrm{d}}(t) \in \mathbb{R}^{\mathtt{q}},$$

with an input/output partition $w=(u,y)$, with $\dim(u)=\mathtt{m}$, and a complexity specification $\mathtt{l}$, find an optimal approximate finite impulse response model for w_{d} of bounded complexity $(\mathtt{m},\mathtt{l})$, such that

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{w} \quad \|w_{\mathrm{d}}-\widehat{w}\|_2 \\ &\text{subject to} && \widehat{w} \in \widehat{\mathscr{B}}|_{[1,T]} \text{ and } \widehat{\mathscr{B}} \in \text{FIR}_{\mathtt{m},\mathtt{l}}. \end{aligned} \qquad \square$$

122a ⟨*Errors-in-variables finite impulse response identification* 122a⟩≡
```
  function [hh, wh, info] = ident_fir_eiv(w, m, l)
  ⟨reshape w and define q, T 26e⟩
  ⟨Finite impulse response identification structure 122b⟩
  ⟨solve Problem SLRA 110⟩, hh = rio2x(R)';
  hh = reshape(hh, p, m, l + 1);
  hh = hh(:, :, end:-1:1);
  uh = reshape(ph(1:(T * m)), m, T);
  yh = reshape(ph(((T * m) + 1):end), p, T - l);
  wh = [uh; [yh zeros(p, l)]];
```
Defines:
`ident_fir_eiv`, used in chunk 123b.
Uses `rio2x` 43b.

Problem 4.12 is equivalent to Problem SLRA with

- norm $\|\cdot\| = \|\cdot\|_2$,
- data matrix
$$\mathscr{S}(p) = \begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(u_{\mathrm{d}}) \\ \begin{bmatrix} y_{\mathrm{d}}(1) & \cdots & y_{\mathrm{d}}(T-\mathtt{l}) \end{bmatrix} \end{bmatrix},$$
composed of a fixed block and a Hankel structured block, and
- rank reduction by the number of outputs $\mathtt{p}$.

122b ⟨*Finite impulse response identification structure* 122b⟩≡ (121b 122a)
```
  p = q - m; r = (l + 1) * m;
  par = vec([w(1:m, :), w((m + 1):end, 1:(T - l))]); s0 = [];
  tts = [blkhank((1:(T * m)), l + 1);
         reshape(T * m + (1:((T - l) * p)), p, T - l)];
```
Uses `blkhank` 25b.

The statement follows from the equivalence

$$\widehat{w}|_{1,T-1} \in \mathscr{B}|_{[1,T-\mathtt{l}]} \text{ and } \widehat{\mathscr{B}} \in \text{FIR}_{\mathtt{m},\mathtt{l}}$$
$$\iff \quad \operatorname{rank}\left(\begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{u}) \\ \begin{bmatrix}\widehat{y}(1) & \cdots & \widehat{y}(T-\mathtt{l})\end{bmatrix}\end{bmatrix}\right) \le \mathtt{m}(\mathtt{l}+1).$$

In order to show it, let

$$H = \big(H(0), H(1), \dots, H(\mathtt{l}), 0, 0, \dots\big).$$

be the impulse response of $\widehat{\mathscr{B}} \in \text{FIR}_{\mathtt{m},\mathtt{l}}$. The signal $\widehat{w} = (\widehat{u},\widehat{y})$ is a trajectory of $\mathscr{B}$ if and only if

$$\begin{bmatrix}H(\mathtt{l}) & \cdots & H(1) & H(0)\end{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{u}) = \begin{bmatrix}\widehat{y}(1) & \cdots & \widehat{y}(T-\mathtt{l})\end{bmatrix}.$$

Equivalently, $\widehat{w} = (\widehat{u},\widehat{y})$ is a trajectory of $\mathscr{B}$ if and only if

$$\begin{bmatrix}H(\mathtt{l}) & \cdots & H(1) & H(0) & -I_{\mathtt{p}}\end{bmatrix} \begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{u}) \\ \begin{bmatrix}\widehat{y}(1) & \cdots & \widehat{y}(T-\mathtt{l})\end{bmatrix}\end{bmatrix} = 0,$$

or,

$$\operatorname{rank}\left(\begin{bmatrix} \mathscr{H}_{\mathtt{l}+1}(\widehat{u}) \\ [\widehat{y}(1) \cdots \widehat{y}(T-\mathtt{l})] \end{bmatrix}\right) \leq \mathtt{m}(\mathtt{l}+1).$$

For exact data, *i.e.*, assuming that

$$y_{\mathrm{d}}(t) = (H \star u_{\mathrm{d}})(t) := \sum_{\tau=0}^{\mathtt{l}} H(\tau) u_{\mathrm{d}}(t-\tau)$$

the finite impulse response identification problem is equivalent to the deconvolution problem: Given the signals u_{d} and $y_{\mathrm{d}} := H \star u_{\mathrm{d}}$, find the signal H. For noisy data, the finite impulse response identification problem can be viewed as an *approximate deconvolution problem*. The approximation is in the sense of finding the nearest signals $\widehat{u}$ and $\widehat{y}$ to the given ones u_{d} and y_{d}, such that $\widehat{y} := \widehat{H} \star \widehat{u}$, for a signal $\widehat{H}$ with a given length $\mathtt{l}$.

Example

Random data from a moving average finite impulse response system is generated in the errors-in-variables setup. The number of inputs and outputs, the system lag, number of observed data points, and the noise standard deviation are simulation parameters.

123a ⟨*Test* `ident_fir` 123a⟩≡ 123b▷

```
  ⟨initialize the random number generator 91d⟩,
  h0 = ones(m, p, l + 1); u0 = rand(m, T); t = 1:(l + 1);
  y0 = conv(h0(:), u0); y0 = y0(end - T + 1:end);
  w0 = [u0; y0]; w = w0 + s * randn(m + p, T);
```

Defines:
`test_ident_fir`, used in chunk 123c.

The output error and errors-invariables finite impulse response identification methods `ident_fir_oe` and `ident_fir_eiv` are applied on the data and the relative fitting errors $\|w_{\mathrm{d}} - \widehat{w}\| / \|w_{\mathrm{d}}\|$ are computed.

123b ⟨*Test* `ident_fir` 123a⟩+≡ ◁123a

```
  [hh_oe, wh_oe] = ident_fir_oe(w, m, l);
  e_oe = norm(w(:) - wh_oe(:)) / norm(w(:))
  [hh_eiv, wh_eiv, info] = ident_fir_eiv(w, m, l);
  e_eiv = norm(w(:) - wh_eiv(:)) / norm(w(:))
```

Uses `ident_fir_eiv` 122a and `ident_fir_oe` 121b.

The obtained result in the following example

123c ⟨*Example of finite impulse response identification* 123c⟩≡

```
  m = 1; p = 1; l = 10; T = 50; s = 0.5; test_ident_fir
```

Uses `test_ident_fir` 123a.

are: relative error 0.2594 for `ident_fir_oe` and 0.2391 for `ident_fir_eiv`.

4.4 Analysis and synthesis

Distance to uncontrollability

Checking controllability of a linear time-invariant system $\mathscr{B}$ is a rank test problem. However, the matrices which rank deficiency indicates lack of controllability for $\mathscr{B}$ are *structured* and, depending on the representation of $\mathscr{B}$, might be nonlinear transformations of the system parameters. Computing the numerical rank of a structured matrix by the singular value decomposition no longer gives a guarantee that there is a nearby matrix with the specified rank that has the same structure as the given matrix. For checking controllability, this implies that the system might be declared close to uncontrollable, but that there is no nearby system that is uncontrollable. In other words, the standard singular value decomposition test might be pessimistic.

Let $\overline{\mathscr{L}_{\mathrm{ctrb}}}$ be the set of uncontrollable linear time-invariant systems and let $\operatorname{dist}(\mathscr{B}, \widehat{\mathscr{B}})$ be a measure for the distance from $\mathscr{B}$ to $\widehat{\mathscr{B}}$. Consider for simplicity the single input single output case and let $\mathscr{B}_{\mathrm{i/o}}(P,Q)$, be an input/output representation of $\mathscr{B}$. Moreover, without loss of generality, assume that P is monic. With this normalization the parameters P,Q are unique and, therefore, the distance measure

$$\operatorname{dist}(\mathscr{B}, \widehat{\mathscr{B}}) := \sqrt{\|P-\widehat{P}\|_2^2 + \|Q-\widehat{Q}\|_2^2} \qquad \text{(dist)}$$

is a property of the pair of systems $(\mathscr{B}, \widehat{\mathscr{B}})$.

In terms of the parameters $\widehat{P}$ and $\widehat{Q}$, the constraint $\widehat{\mathscr{B}} \in \overline{\mathscr{L}_{\mathrm{ctrb}}}$ is equivalent to rank deficiency of the Sylvester matrix $\mathscr{R}(\widehat{P},\widehat{Q})$ (see ($\mathscr{R}$) on page 11). With respect to the distance measure (dist), the problem of computing the distance from $\mathscr{B}$ to uncontrollability is equivalent to a Sylvester structured low-rank approximation problem

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{P} \text{ and } \widehat{Q} \quad \|P-\widehat{P}\|_2^2 + \|Q-\widehat{Q}\|_2^2 \\ &\text{subject to} && \operatorname{rank}\big(\mathscr{R}(\widehat{P},\widehat{Q})\big) \leq \operatorname{degree}(P) + \operatorname{degree}(Q) - 1, \end{aligned}$$

for which numerical algorithms are developed in Section 3.2. The implementation details are left as an exercise for the reader (see Note 3.15 and Problem P.20).

Pole placement by a low-order controller

Consider the single input single output feedback system shown in Figure 4.2. The polynomials P and Q, define the transfer function Q/P of the plant and are given. They are assumed to be relatively prime and the transfer function Q/P is assumed to satisfy the constraint

$$\deg(Q) \leq \deg(P) =: \mathtt{l}_P,$$

which ensures that the plant is a causal linear time-invariant system. The polynomials Y and X parameterize the controller $\mathscr{B}_{\mathrm{i/o}}(X,Y)$ and are unknowns. The design constraints are that the controller should be causal and have order bounded by a specified integer $\mathtt{l}_X$. These specifications translate to the following constraints on the polynomials Y and X

$$\deg(Y) \leq \deg(X) =: \mathtt{l}_X < \mathtt{l}_P. \tag{deg}$$

The pole placement problem is to determine X and Y, so that the poles of the closed-loop system are as close as possible in some specified sense to desired locations, given by the roots of a polynomial F, where $\deg(F) = \mathtt{l}_X + \mathtt{l}_P$. We consider a modification of the pole placement problem that aims to assign exactly the poles of a plant that is as close to the given plant as possible.

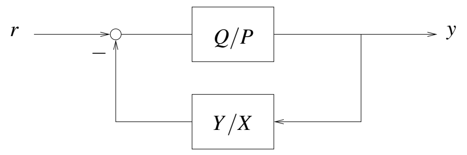

Fig. 4.2 Feedback control system.

In what follows, we use the correspondence between $\mathtt{l}_P + 1$ dimensional vectors and $\mathtt{l}_P$th degree polynomials

$$\operatorname{col}(P_0, P_1, \dots, P_{\mathtt{l}_P}) \in \mathbb{R}^{\mathtt{l}_P+1} \quad \leftrightarrow \quad P(z) = P_0 + P_1 z + \cdots + P_{\mathtt{l}_P} z^{\mathtt{l}_P} \in \mathbb{R}[z],$$

and (with some abuse of notation) refer to P as both a vector and a polynomial.

Problem 4.13 (Pole placement by low-order controller). Given

1. the transfer function Q/P of a plant,
2. a polynomial F, whose roots are the desired poles of the closed-loop system, and
3. a bound $\mathtt{l}_X < \deg(P)$ on the order of the controller,

find the transfer function Y/X of the controller, such that

1. the degree constraint (deg) is satisfied and
2. the controller assigns the poles of a system whose transfer function $\widehat{Q}/\widehat{P}$ is as close as possible to the transfer function Q/P in the sense that

$$\left\| \operatorname{col}(P,Q) - \operatorname{col}(\widehat{P},\widehat{Q}) \right\|_2$$

is minimized. □

Next, we write down explicitly the considered optimization problem, which shows its equivalence to a structured low-rank approximation problem. The closed-loop transfer function is

$$\frac{QX}{PX+QY},$$

so that a solution to the pole placement problem is given by a solution to the Diophantine equation

$$PX + QY = F$$

The Diophantine equation can be written as a Sylvester structured system of equations

$$\underbrace{\begin{bmatrix} P_0 & & & Q_0 & & \\ P_1 & \ddots & & Q_1 & \ddots & \\ \vdots & \ddots & P_0 & \vdots & \ddots & Q_0 \\ P_{\mathtt{l}_P} & & P_1 & Q_{\mathtt{l}_P} & & Q_1 \\ & \ddots & \vdots & & \ddots & \vdots \\ & & P_{\mathtt{l}_P} & & & Q_{\mathtt{l}_P} \end{bmatrix}}_{\mathscr{R}_{\mathtt{l}_X+1}(P,Q)} \begin{bmatrix} X_0 \\ \vdots \\ X_{\mathtt{l}_X} \\ Y_0 \\ \vdots \\ Y_{\mathtt{l}_X} \end{bmatrix} = \underbrace{\begin{bmatrix} F_0 \\ \vdots \\ F_{\mathtt{l}_P} \\ F_{\mathtt{l}_P+1} \\ \vdots \\ F_{\mathtt{l}_P+\mathtt{l}_X} \end{bmatrix}}_{F},$$

which is an overdetermined system of equations due to the degree constraint (deg). Therefore Problem 4.13 can be written as

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{P}, \widehat{Q} \in \mathbb{R}^{\mathtt{l}_P+1} \text{ and } X, Y \in \mathbb{R}^{\mathtt{l}_X+1} \quad \left\| \begin{bmatrix} P \\ Q \end{bmatrix} - \begin{bmatrix} \widehat{P} \\ \widehat{Q} \end{bmatrix} \right\|_2 \\ &\text{subject to} \quad \mathscr{R}_{\mathtt{l}_X+1}(\widehat{P},\widehat{Q}) \begin{bmatrix} X \\ Y \end{bmatrix} = F. \end{aligned}$$

Problem 4.13 is equivalent to Problem SLRA with

- norm $\|\cdot\| = \|\cdot\|_2$,
- data matrix

$$\mathscr{S}(p) = \begin{bmatrix} \begin{bmatrix} F_0 \; F_1 \; \cdots \; F_{\mathtt{l}_P+\mathtt{l}_X} \end{bmatrix} \\ \mathscr{R}^{\top}_{\mathtt{l}_X+1}(P,Q) \end{bmatrix},$$

  composed of a fixed block and a Sylvester structured block, and
- rank reduction by one.

Indeed

$$\mathscr{R}_{\mathtt{l}_X+1}(\widehat{P},\widehat{Q}) \begin{bmatrix} X \\ Y \end{bmatrix} = F \quad \iff \quad \operatorname{rank}\left(\mathscr{S}(\widehat{p})\right) \leq 2\mathtt{l}_X + 1.$$

Exercise 4.14. Implement the method for pole placement by low-order controller, outlined in this section, using the function `slra`. Test it on simulation examples and compare the results with the ones obtained with the MATLAB function `place`.

4.5 Simulation examples

Model reduction

In this section, we compare the nuclear norm heuristic based methods, developed in Section 3.3, for structured low-rank approximation with classical methods for Hankel structured low-rank approximation, such as Kung's method and local optimization based methods, on single input single output model reduction problems. The order `n` of the system $\mathscr{B}_d$, the bound $\mathtt{n}_{\text{red}}$ for the order of the reduced system $\widehat{\mathscr{B}}$, and the approximation horizon T are simulation parameters. The system $\mathscr{B}$ with the specified order `n` is selected as a random stable single input single output system.

127a ⟨*Test model reduction* 127a⟩≡ 127b▷

```
⟨initialize the random number generator 91d⟩
sys = c2d(rss(n), 1);
h   = impulse(sys, T); sh = h(2:(T + 1));
```

Defines:
`test_mod_red`, used in chunk 128.

The nuclear norm approximation is computed by the function `slra_nn`.

127b ⟨*Test model reduction* 127a⟩+≡ ◁127a 127c▷

```
tts = blkhank(1:T, lred + 1); hh1 = [h(1); slra_nn(tts, sh, lred)];
```

Uses `blkhank` 25b and `slra_nn` 100b.

Kung's method is a singular value decomposition-based heuristic and is implemented in the function `h2ss`.

127c ⟨*Test model reduction* 127a⟩+≡ ◁127b 127d▷

```
[sysh2, hh2] = h2ss(h, r); hh2 = hh2(:);
```

Uses `h2ss` 79a.

Model reduction, based on local optimization, is done by solving Hankel structured low-rank approximation problem, using the function `mod_red`.

127d ⟨*Test model reduction* 127a⟩+≡ ◁127c 127e▷

```
[sysh3, hh3] = mod_red(sys, T, r); hh3 = hh3(:);
```

Uses `mod_red` 113.

We compare the results by checking the (numerical) rank of $\mathscr{H}_{n_{\text{red}}+1}(\sigma\widehat{H})$ and the approximation error $\|H-\widehat{H}\|_2$.

127e ⟨*Test model reduction* 127a⟩+≡ ◁127d 127f▷

```
sh = h(2:end); shh1 = hh1(2:end); shh2 = hh2(2:end); shh3 = hh3(2:end);
sv = [svd(sh(tts)) svd(shh1(tts)) svd(shh2(tts)) svd(shh3(tts))]
cost = [norm(h - h) norm(h - hh1) norm(h - hh2) norm(h - hh3)]
```

The Markov parameters of the high order system and the low order approximations are plotted for visual inspection of the quality of the approximations.

127f ⟨*Test model reduction* 127a⟩+≡ ◁127e

```
plot(h, ':k', 'linewidth', 4), hold on,
plot(hh1, 'b-'), plot(hh2, 'r-.'), plot(hh3, 'r-')
legend('high order sys.', 'nucnrm', 'kung', 'slra')
```

The results of an approximation of a 50th order system by a 4th order system with time horizon 25 time steps

128 ⟨*Test structured low-rank approximation methods on a model reduction problem* 128⟩≡

```
l = 50; lred = 4; T = 25; test_mod_red, print_fig('test_mod_red')
```

Uses `print_fig` 25a and `test_mod_red` 127a.

are

```
sv =

    0.8590    0.5660    0.8559    0.8523
    0.6235    0.3071    0.6138    0.6188
    0.5030    0.1009    0.4545    0.4963
    0.1808    0.0190    0.1462    0.1684
    0.1074    0.0000    0.0000    0.0000


cost =

         0    0.3570    0.0904    0.0814
```

and Figure 4.3. The nuclear norm approximation gives worse results than the singular value decomposition based heuristic, which in turn can be further improved by the local optimization heuristic.

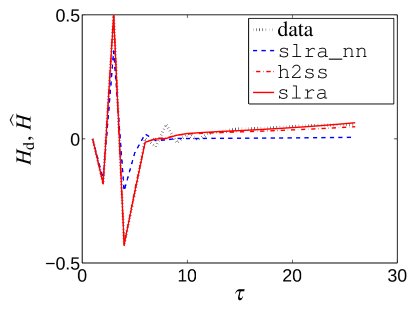

Fig. 4.3 Impulse responses of the high order system (dotted line) and the low-order approximations obtained by the nuclear norm heuristic (dashed line), Kung's method (dashed dotted line), and a local optimization based method (solid line).

System identification

Next we compare the nuclear norm heuristic with an alternative heuristic method, based on the singular value decomposition, and a method based on local optimization, on single input single output system identification problems. The data is generated according to the errors-in-variables model (EIV). A trajectory w_0 of a linear time-invariant system $\mathscr{B}_0$ of order $\mathtt{n}_0$ is corrupted by noise, where the noise $\widetilde{w}$ is zero mean, white, Gaussian with covariance σ^2, *i.e.*,

$$w_\mathrm{d} = w_0 + \widetilde{w}.$$

The system $\mathscr{B}_0$, referred to as the "true system", is generated as a random stable single input single output system. The trajectory w_0 is then generated as a random trajectory of $\mathscr{B}_0$. The order $\mathtt{n}_0$, the trajectory length T, and the noise standard deviation σ are simulation parameters. The approximation order is set equal to the order of the true system.

129a ⟨*Test system identification* 129a⟩≡ 129b▷

⟨*initialize the random number generator* 91d⟩
```
sys0 = drss(n0); u0 = randn(T, 1); xini0 = randn(n0, 1);
y0   = lsim(sys0, u0, 1:T, xini0); w0 = [u0'; y0'];
w    = w0 + nl * randn(size(w0)); n = n0;
```
Defines:
`test_sysid`, used in chunk 129g.

The nuclear norm approximation is computed by

129b ⟨*Test system identification* 129a⟩+≡ ◁129a 129c▷
```
tts = blkhank(reshape(1:(2 * T), 2, T), n + 1);
wh1 = slra_nn(tts, w(:), 2 * n + 1);
```
Uses `blkhank` 25b and `slra_nn` 100b.

Next we apply an identification method obtained by solving suboptimally the Hankel structured low-rank approximation problem ignoring the structure:

129c ⟨*Test system identification* 129a⟩+≡ ◁129b 129d▷

⟨*suboptimal approximate single input single output system identification* 90c⟩
```
[M2, wh2] = misfit_siso(w, P);
```
Uses `misfit_siso` 89.

Finally, we apply the optimization based method `ident_siso`

129d ⟨*Test system identification* 129a⟩+≡ ◁129c 129e▷
```
[sysh3, wh3, info] = ident_siso(w, n); M3 = info.M;
```
Uses `ident_siso` 90a.

The results are compared by checking the rank constraint, the approximation error,

129e ⟨*Test system identification* 129a⟩+≡ ◁129d 129f▷
```
sv   = [svd(wh1(tts)) svd(wh2(tts)) svd(wh3(tts))]
cost = [norm(w(:) - wh1) norm(w(:) - wh2(:)) norm(w(:) - wh3(:))]
```
and plotting the approximations on top of the data.

129f ⟨*Test system identification* 129a⟩+≡ ◁129e
```
plot(w(2, :), 'k'), hold on, plot(wh1(2:2:end), 'r')
plot(wh2(2, :), 'b-'), plot(wh3(2, :), 'c-.')
legend('data', 'nucnrm', 'lra', 'slra')
```
The results of

129g ⟨*Test structured low-rank approximation methods on system identification* 129g⟩≡
```
n0 = 2; T = 25; nl = 0.2; test_sysid, print_fig('test_sysid')
```
Uses `print_fig` 25a and `test_sysid` 129a.

are

```
sv =

    3.3862    4.6877    4.7428
    2.8827    4.2789    4.2817
    2.8019    4.1504    4.1427
    0.6283    1.2102    1.3054
    0.0000    0.3575    0.4813
    0.0000    0.0000    0.0000

cost =

    1.6780    0.8629    0.6676
```

They are consistent with previous experiments: the nuclear norm approximation gives worse results than the singular value decomposition based heuristic, which in turn can be further improved by the local optimization heuristic.

4.6 Notes and references

System theory

Survey on applications of structured low-rank approximation is given in De Moor (1993) and (Markovsky, 2008). Approximate realization is a special identification problem (the input is a pulse and the initial conditions are zeros). Nevertheless the exact version of this problem is a well studied problem. The classical references are the Ho-Kalman's realization algorithm (Ho and Kalman, 1966), see also (Kalman et al, 1969, Chapter 10). Approximate realization methods, based on the singular value decomposition, are proposed in (Kung, 1978; Zeiger and McEwen, 1974).

Comprehensive treatment of model reduction methods is given in (Antoulas, 2005). The balanced model reduction method is proposed by Moore (1981) and error bounds are derived by Glover (1984). Proper orthogonal decomposition is a popular method for nonlinear model reduction. This method is unstructured low-rank approximation of a matrix composed of "snapshots" of the state vector of the system. The method is data-driven in the sense that the method operates on data of the full order system and a model of that system is not derived.

Errors-in-variables system identification methods are developed in (Aoki and Yue, 1970; Lemmerling and De Moor, 2001; Markovsky et al, 2005; Pintelon et al, 1998; Roorda, 1995; Roorda and Heij, 1995). Their consistency properties are studied in (Kukush et al, 2005; Pintelon and Schoukens, 2001). A survey paper on errors-in-variables system identification is (Söderström, 2007). Most of the work on the subject is presented in the classical input/output setting, *i.e.*, the proposed methods are defined in terms of transfer function, matrix fraction description, or input/state/output representations. The salient feature of the errors-in-variables problems, however, is that all variables are treated on an equal footing as noise corrupted.

Therefore, the input/output partitioning implied by the classical model representations is irrelevant in the errors-in-variables problem.

Signal processing

Linear prediction methods based on optimization techniques are developed in (Bresler and Macovski, 1986; Cadzow, 1988). Cadzow (1988) proposed a method for Hankel structured low-rank approximation that alternates between unstructured low-rank approximation and structure approximation. This method however does not converge to a locally optimal solution. See (De Moor, 1994) for a counter example. Application of structured low-rank approximation methods for audio processing is described in (Lemmerling et al, 2003). The so called shape from moments problem (Golub et al, 1999; Gustafsson et al, 2000; Milanfar et al, 1995) is equivalent to Hankel structured low-rank approximation (Schuermans et al, 2006).

Computer vision

An overview of the application of low-rank approximation (total least squares) in motion analysis is given in (Mühlich and Mester, 1998). Image deblurring applications are presented in (Fu and Barlow, 2004; Mastronardi et al, 2004; Pruessner and O'Leary, 2003). The image deblurring problem is solved by regularized structured low-rank approximation methods in (Mastronardi et al, 2005; Ng et al, 2000, 2002; Younan and Fan, 1998).

Analysis problems

The distance to uncontrollability with respect to the distance measure dist is naturally defined as

$$\min_{\widehat{\mathscr{B}} \in \mathscr{L}_{\text{ctrb}}} \operatorname{dist}(\mathscr{B}, \widehat{\mathscr{B}}).$$

The distance to uncontrollability proposed in (Paige, 1981, Section X) matches the definition given in this book by taking as distance measure

$$\operatorname{dist}(\mathscr{B}, \widehat{\mathscr{B}}) = \left\| \begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} \right\|_2^2, \qquad (*)$$

where A, B and $\widehat{A}, \widehat{B}$ are parameters of input/state/output representations

$$\mathscr{B} = \mathscr{B}_{\text{i/s/o}}(A, B, C, D) \qquad \text{and} \qquad \widehat{\mathscr{B}} = \mathscr{B}_{\text{i/s/o}}(\widehat{A}, \widehat{B}, \widehat{C}, \widehat{D}),$$

respectively. Computing distance to uncontrollability with respect to $(*)$ received significant attention in the literature, but has a drawback: *$(*)$ depends on the choice of the state space basis.* In other words, $(*)$ is representation dependent and, therefore, not a genuine property of the pair of systems $(\mathscr{B}, \widehat{\mathscr{B}})$.

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Part II
Miscellaneous generalizations

Chapter 5
Missing data, centering, and constraints

Summary: Linear model identification from data with missing values is posed in Section 5.1 as a weighted low-rank approximation problem with weights related to the missing values equal to zero. Alternating projections and variable projections methods for solving the resulting problem are outlined and implemented. The methods are evaluated on synthetic data and real data from the MovieLens data sets.

low-rank approximation is a data modeling tool. Data centering, on the other hand, is a common preprocessing step. The combination of low-rank approximation with data centering is studied in Section 5.2. In the case of approximation in the Frobenius norm (uniform weighting) and no constraints apart from the rank constraint, the common preprocessing practice of mean subtraction leads to optimal results. Preprocessing by mean subtraction, however, is not the only way to optimally preprocess the data. In the case of approximation by a weighted norm and/or structure constraints on the approximation, preprocessing by mean subtraction leads, in general, to suboptimal results. We show, how classical solution methods for weighted and structured low-rank approximation can be modified for doing optimal preprocessing at the same time as low-rank approximation.

The problem of solving approximately in the least squares sense an overdetermined system of linear equations with complex valued coefficients, where the elements of the solution vector are constrained to have the same phase is reduced in Section 5.3 to a generalized low rank matrix approximation.

An approximate rank revealing factorization problem with structure constraints on the normalized factors is considered. Examples of structure, motivated by an application of the problem in microarray data analysis, are sparsity, nonnegativity, periodicity, and smoothness. An alternating projections algorithm is developed. Although the algorithm is motivated by a specific application in microarray data analysis, the approach is applicable to other types of structure.

5.1 Weighted low-rank approximation with missing data

Modeling problems with missing data occur in

- factor analysis of data from questioners due to questions left unanswered,
- computer vision due to occlusions,
- signal processing due to irregular measurements in time/space, and
- control due to malfunction of measurement devices.

In this section, we present a method for linear static modeling with missing data. The problem is posed as an element-wise weighted low-rank approximation problem with nonnegative weights, *i.e.*,

$$\text{minimize} \quad \text{over } \widehat{D} \quad \|D - \widehat{D}\|_\Sigma \quad \text{subject to} \quad \operatorname{rank}(\widehat{D}) \leq \mathtt{m}, \qquad \text{(EWLRA)}$$

where

$$\|\Delta D\|_\Sigma := \|\Sigma \odot \Delta D\|_\mathrm{F} = \sqrt{\sum_{i=1}^{\mathtt{q}} \sum_{j=1}^{N} \sigma_{ij} e_{ij}}, \qquad \Sigma \in \mathbb{R}^{\mathtt{q} \times N} \text{ and } \Sigma \geq 0$$

is a seminorm. (The σ_{ij}'s are weights; not noise standard deviations.) In the extreme case of a zero weight, *e.g.*, $\sigma_{ij} = 0$, the corresponding element d_{ij} of D is not taken into account in the approximation and therefore it is treated as a missing value. In this case, the approximation problem is called a singular problem. The algorithms, described in Chapter 3, for the regular weighted low-rank approximation problem fail in the singular case. In this section, the methods are extended to solve singular problems and therefore account for missing data.

Exercise 5.1 (Missing rows and columns). Show that in the case of missing rows and/or columns of the data matrix, the singular low-rank approximation problem reduces to a smaller dimensional regular problem. □

Using the image representation, we have

$$\operatorname{rank}(\widehat{D}) \leq \mathtt{m} \quad \iff \quad \text{there are } P \in \mathbb{R}^{\mathtt{q} \times \mathtt{m}} \text{ and } L \in \mathbb{R}^{\mathtt{m} \times N}, \quad \text{such that } \widehat{D} = PL, \qquad \text{(RRF)}$$

which turns problem (EWLRA) into the following parameter optimization problem

$$\text{minimize} \quad \text{over } P \in \mathbb{R}^{\mathtt{q} \times \mathtt{m}} \text{ and } L \in \mathbb{R}^{\mathtt{m} \times N} \quad \|D - PL\|_\Sigma. \qquad (\text{EWLRA}_P)$$

Unfortunately the problem is nonconvex and there are no efficient methods to solve it. We present local optimization methods based on the alternating projections and variable projection approaches. These methods are initialized by a suboptimal solution of (EWLRA$_P$), computed by a direct method.

Algorithms

Direct method

The initial approximation for the iterative optimization methods is obtained by solving unweighted low-rank approximation problem where all missing elements (encoded as `NaN`'s) are filled in by zeros.

139a ⟨*low-rank approximation with missing data* 139a⟩≡
```
function [p, l] = lra_md(d, m)
d(isnan(d)) = 0; [q, N] = size(d);
if nargout == 1, ⟨data compression 139c⟩, end
⟨matrix approximation 139b⟩
```
Defines:
`lra_md`, used in chunks 142b and 146b.

The problem is solved using the singular value decomposition, however, in view of the large scale of the data the function `svds` which computes selected singular values and corresponding singular vectors is used instead of the function `svd`.

139b ⟨*matrix approximation* 139b⟩≡ (139a)
```
[u, s, v] = svds(d, m); p = u(:, 1:m); l = p' * d;
```
The model $\widehat{\mathscr{B}} = \operatorname{image}(P)$ depends only on the left singular vectors of the data matrix D. Therefore, $\widehat{\mathscr{B}}$ is an optimal model for the data DQ, where Q is any orthogonal matrix. Let

$$D^\top = Q\begin{bmatrix} R_1 \\ 0 \end{bmatrix}, \qquad \text{where} \quad R_1 \text{ is upper triangular} \tag{QR}$$

be the QR factorization of $D^\top$. For $N \gg \mathtt{q}$, computing the QR factorization and the singular value decomposition of R_1 is a more efficient alternative for finding an image representation of the optimal subspace than computing the singular value decomposition of D.

139c ⟨*data compression* 139c⟩≡ (139a)
```
d = triu(qr(d'))'; d = d(1:q, :);
```
(After these assignments, the variable `d` is equal to R_1.)

Alternating projections

The alternating projections method exploits the fact that problem (EWLRA$_P$) is a linear least squares problem in either P or L. This suggests a method of alternatively minimizing over P with L fixed to the value computed on the previous iteration step and minimizing over L with P fixed to the value computed on the previous iteration step. A summary of the alternating projections method is given in Algorithm 3. MATLAB-like notation is used for indexing a matrix. For a $\mathtt{q} \times N$ matrix D and subsets $\mathscr{I}$ and $\mathscr{J}$ of the sets of, respectively, row and column indexes, $D_{\mathscr{I},\mathscr{J}}$ denotes

the submatrix of D with elements whose indexes are in $\mathscr{I}$ and $\mathscr{J}$. Either of $\mathscr{I}$ and $\mathscr{J}$ can be replaced by ":" in which case all rows/columns are indexed.

On each iteration step of the alternating projections algorithm, the cost function value is guaranteed to be non-increasing and is typically decreasing. It can be shown that the iteration converges and that the local convergence rate is linear.

The quantity $e^{(k)}$, computed on step 9 of the algorithm is the squared approximation error

$$e^{(k)} = \|D - \widehat{D}^{(k)}\|_\Sigma^2$$

on the kth iteration step. Convergence of the iteration is judged on the basis of the relative decrease of the error $e^{(k)}$ after an update step. This corresponds to choosing a tolerance on the relative decrease of the cost function value. More expensive alternatives are to check the convergence of the approximation $\widehat{D}^{(k)}$ or the size of the gradient of the cost function with respect to the model parameters.

Variable projections

In the second solution method, (EWLRA$_P$) is viewed as a double minimization problem

$$\text{minimize} \quad \text{over } P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}} \quad \underbrace{\min_{L\in\mathbb{R}^{\mathtt{m}\times N}} \|D - PL\|_\Sigma^2}_{f(P)}. \tag{EWLRA$'_P$}$$

The inner minimization is a weighted least squares problem and therefore can be solved in closed form. Using MATLAB set indexing notation, the solution is

$$f(P) = \sum_{j=1}^N D_{\mathscr{J},j}^\top \operatorname{diag}(\Sigma_{\mathscr{J},j}^2) P_{\mathscr{J},:} \big(P_{\mathscr{J},:}^\top \operatorname{diag}(\Sigma_{\mathscr{J},j}^2) P_{\mathscr{J},:}\big)^{-1} P_{\mathscr{J},:}^\top \operatorname{diag}(\Sigma_{\mathscr{J},j}^2) D_{\mathscr{J},j}, \tag{5.1}$$

where $\mathscr{J}$ is the set of indexes of the non-missing elements in the jth column of D.

Exercise 5.2. Derive the expression (5.1) for the function f in (EWLRA$'_P$). □

The outer minimization is a nonlinear least squares problem and can be solved by general purpose local optimization methods. The inner minimization is a weighted projection on the subspace spanned by the columns of P. Consequently, $f(P)$ has the geometric interpretation of the sum of squared distances from the data points to the subspace. Since the parameter P is modified by the outer minimization, the projections are on a varying subspace.

Note 5.3 (Gradient and Hessian of f). In the implementation of the method, we are using finite difference numerical computation of the gradient and Hessian of f. (These approximations are computed by the optimization method.) More efficient alternative, however, is to supply to the method analytical expressions for the gradient and the Hessian.

Algorithm 3 Alternating projections algorithm for weighted low-rank approximation with missing data.

```
Input: Data matrix $D \in \mathbb{R}^{q \times N}$, rank constraint m, elementwise nonnegative weight matrix $\Sigma \in \mathbb{R}^{q \times N}$, and relative convergence tolerance $\varepsilon$.
 1: Initial approximation: compute the Frobenius norm low-rank approximation of $D$ with missing
    elements filled in with zeros
        $P^{(0)} := \texttt{lra\_md}(D, \mathtt{m}).$
 2: Let $k := 0$.
 3: repeat
 4:   Let $e^{(k)} := 0$.
 5:   for $j = 1, \dots, N$ do
 6:     Let $\mathscr{J}$ be the set of indexes of the non-missing elements in $D_{:,j}$.
 7:     Define
          $c := \operatorname{diag}(\Sigma_{\mathscr{J},j}) D_{\mathscr{J},j} = \Sigma_{\mathscr{J},j} \odot D_{\mathscr{J},j}$
          $P := \operatorname{diag}(\Sigma_{\mathscr{J},j}) P^{(k)}_{\mathscr{J},:} = (\Sigma_{\mathscr{J},j} \mathbf{1}_{\mathtt{m}}^\top) \odot P^{(k)}_{\mathscr{J},:}$
 8:     Compute
          $\ell_j^{(k)} := \left(P^\top P\right)^{-1} P^\top c.$
 9:     Let
          $e^{(k)} := e^{(k)} + \|c - P\ell_j^{(k)}\|^2.$
10:   end for
11:   Define
          $L^{(k)} = \begin{bmatrix} \ell_1^{(k)} & \cdots & \ell_N^{(k)} \end{bmatrix}.$
12:   Let $e^{(k+1)} := 0$.
13:   for $i = 1, \dots, \mathtt{q}$ do
14:     Let $\mathscr{I}$ be the set of indexes of the non-missing elements in the $i$th row $D_{i,:}$.
15:     Define
          $r := D_{i,\mathscr{I}} \operatorname{diag}(\Sigma_{i,\mathscr{I}}) = D_{i,\mathscr{I}} \odot \Sigma_{i,\mathscr{I}}$
          $L := L^{(k)}_{:,\mathscr{I}} \operatorname{diag}(\Sigma_{i,\mathscr{I}}) = L^{(k)}_{:,\mathscr{I}} \odot (\mathbf{1}_{\mathtt{m}} \Sigma_{i,\mathscr{I}}).$
16:     Compute
          $p_i^{(k+1)} := r L^\top \left(L L^\top\right)^{-1}.$
17:     Let
          $e^{(k+1)} := e^{(k+1)} + \|r - p_i^{(k+1)} L\|^2.$
18:   end for
19:   Define
          $P^{(k+1)} = \begin{bmatrix} p_1^{(k+1)} \\ \vdots \\ p_{\mathtt{q}}^{(k+1)} \end{bmatrix}.$
20:   $k = k + 1$.
21: until $|e^{(k)} - e^{(k-1)}| / e^{(k)} < \varepsilon$.
Output: Locally optimal solution $\widehat{D} = \widehat{D}^{(k)} := P^{(k)} L^{(k)}$ of (EWLRA$_P$).
```

Implementation

Both the alternating projections and the variable projections methods for solving weighted low-rank approximation problems with missing data are callable through the function `wlra`.

142a ⟨*Weighted low-rank approximation* 142a⟩≡
```
function [p, l, info] = wlra(d, m, s, opt)
tic, ⟨default parameters opt 142b⟩
switch lower(opt.Method)
case {'altpro', 'ap'}
  ⟨alternating projections method 143a⟩
case {'varpro', 'vp'}
  ⟨variable projections method 144b⟩
otherwise
  error('Unknown method %s', opt.Method)
end
info.time = toc;
```
Defines:
`wlra`, used in chunks 146b and 232.

The output parameter `info` gives the

- approximation error $\|D - \widehat{D}\|_\Sigma^2$ (`info.err`),
- number of iterations (`info.iter`), and
- execution time (`info.time`) for computing the local approximation $\widehat{D}$.

The optional parameter `opt` specifies the

- method (`opt.Method`) and, in the case of the variable projections method, algorithm (`opt.alg`) to be used,
- initial approximation (`opt.P`),
- convergence tolerance ε (`opt.TolFun`),
- an upper bound on the number of iterations (`opt.MaxIter`), and
- level of printed information (`opt.Display`).

The initial approximation `opt.P` is a $\mathtt{q} \times \mathtt{m}$ matrix, such that the columns of $P^{(0)}$ form a basis for the span of the columns of $\widehat{D}^{(0)}$, where $\widehat{D}^{(0)}$ is the initial approximation of D, see step 1 in Algorithm 3. If it is not provided via the parameter `opt`, the default initial approximation is chosen to be the unweighted low-rank approximation of the data matrix with all missing elements filled in with zeros.

Note 5.4 (Large scale, sparse data). In an application of (EWLRA) to building recommender systems, the data matrix D is large but only a small fraction of the elements are given. Such problems can be handled efficiently, encoding D and Σ as sparse matrices. The convention in this case is that missing elements are zeros.

142b ⟨*default parameters* opt 142b⟩≡ (142a)
```
if ~exist('opt.MaxIter'), opt.MaxIter = 100;         end
if ~exist('opt.TolFun'),  opt.TolFun  = 1e-5;        end
if ~exist('opt.Display'), opt.Display = 'off';       end
if ~exist('opt.Method'),  opt.Method  = 'ap';        end
```

```
  if ~exist('opt.alg'),      opt.alg     = 'lsqnonlin'; end
  if ~exist('opt.P'), p = lra_md(d, m); else p = opt.P, end
```

Uses `lra_md` 139a.

Alternating projections

The iteration loop for the alternating projections algorithm is:

143a ⟨*alternating projections method* 143a⟩≡ (142a)

```
  [q, N] = size(d); sd = norm(s .* d, 'fro') ^ 2;
  cont = 1; k = 0;
  while (cont)
    ⟨compute L, given P 143b⟩
    ⟨compute P, given L 143c⟩
    ⟨check exit condition 143d⟩
    ⟨print progress information 144a⟩
  end
  info.err = el; info.iter = k;
```

The main computational steps on each iteration of the algorithm are the two weighted least squares problems.

143b ⟨*compute L, given P* 143b⟩≡ (143 144)

```
  dd = []; % vec(D - DH)
  for j = 1:N
    J   = find(s(:, j));
    sJj = full(s(J, j));
    c   = sJj .* full(d(J, j));
    P   = sJj(:, ones(1, m)) .* p(J, :); % = diag(sJj) * p(J, :)
    l(:, j) = P \ c; dd = [dd; c - P * l(:, j)];
  end
  ep = norm(dd) ^ 2;
```

143c ⟨*compute P, given L* 143c⟩≡ (143a)

```
  dd = []; % vec(D - DH)
  for i = 1:q
    I   = find(s(i, :));
    sIi = full(s(i, I));
    r   = sIi .* full(d(i, I));
    L   = sIi(ones(m, 1), :) .* l(:, I); % = l(:, I) * diag(sIi)
    p(i, :) = r / L; dd = [dd, r - p(i, :) * L];
  end
  el = norm(dd) ^ 2;
```

The convergence is checked by the size of the relative decrease in the approximation error $e^{(k)}$ after one update step.

143d ⟨*check exit condition* 143d⟩≡ (143a)

```
  k = k + 1; re = abs(el - ep) / el;
  cont = (k < opt.MaxIter) & (re > opt.TolFun) & (el > eps);
```

If the optional parameter `opt.Display` is set to `'iter'`, `wlra` prints on each iteration step the relative approximation error.

144a ⟨*print progress information* 144a⟩≡ (143a)

```
  switch lower(opt.Display)
    case 'iter',
      fprintf('%2d : relative error = %18.8f\n', k, el / sd)
  end
```

Variable projections

Optimization Toolbox is used for performing the outer minimization in (EWLRA$'_P$), *i.e.*, the nonlinear minimization over the P parameter. The parameter `opt.alg` specifies the algorithm to be used. The available options are

- `fminunc` — a quasi-Newton type algorithm, and
- `lsqnonlin` — a nonlinear least squares algorithm.

Both algorithm allow for numerical approximation of the gradient and Hessian through finite difference computations. In version of the code shown next, the numerical approximation is used.

144b ⟨*variable projections method* 144b⟩≡ (142a)

```
  switch lower(opt.alg)
    case {'fminunc'}
      [p, err, f, info] = fminunc(@(p)mwlra(p, d, s), p, opt);
    case {'lsqnonlin'}
      [p, rn, r, f, info] = ...
                    lsqnonlin(@(p)mwlra2(p, d, s), p, [], []);
    otherwise
      error('Unknown algorithm %s.', opt.alg)
  end
  [info.err, l] = mwlra(p, d, s); % obtain the L parameter
```

Uses `mwlra` 144c and `mwlra2` 144d.

The inner minimization in (EWLRA$'_P$) has an analytic solution (5.1). The implementation of (5.1) is the chunk of code for computing the L parameter, given the P parameter, already used in the alternating projections algorithm.

144c ⟨dist($\mathscr{D}$,$\mathscr{B}$) *(weighted low-rank approximation)* 144c⟩≡

```
  function [ep, l] = mwlra(p, d, s)
  N = size(d, 2); m = size(p, 2); ⟨compute L, given P 143b⟩
```

Defines:
`mwlra`, used in chunk 144b.

In the case of using a nonlinear least squares type algorithm, the cost function is not the sum of squares of the errors but the correction matrix ΔD (`dd`).

144d ⟨*Weighted low-rank approximation correction matrix* 144d⟩≡

```
  function dd = mwlra2(p, d, s)
  N = size(d, 2); m = size(p, 2); ⟨compute L, given P 143b⟩
```

Defines:
`mwlra2`, used in chunk 144b.

Test on simulated data

A “true” random rank-m matrix D_0 is selected by generating randomly its factors P_0 and L_0 in a rank revealing factorization

$$D_0 = P_0 L_0, \qquad \text{where } P_0 \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}} \text{ and } L_0 \in \mathbb{R}^{\mathtt{m}\times N}.$$

145a ⟨*Test missing data 2* 145a⟩≡ 145b▷
```
  ⟨initialize the random number generator 91d⟩
  p0 = rand(q, m); l0 = rand(m, N);
```
Defines:
  `test_missing_data2`, used in chunks 147 and 148.

The location of the given elements is chosen randomly row by row. The number of given elements is such that the sparsity of the resulting matrix, defined as the ratio of the number of missing elements to the total number qN of elements, matches the specification `r`.

The number of given elements of the data matrix is

145b ⟨*Test missing data 2* 145a⟩+≡ ◁145a 145c▷
```
  ne  = round((1 - r) * q * N);
```

Then the number of given elements of the data matrix per row is

145c ⟨*Test missing data 2* 145a⟩+≡ ◁145b 145d▷
```
  ner = round(ne / q);
```

The variables `I` and `J` contain the row and column indeces of the given elements. They are randomly chosen.

145d ⟨*Test missing data 2* 145a⟩+≡ ◁145c 145e▷
```
  I = []; J = [];
  for i = 1:q
    I = [I i*ones(1, ner)]; rp = randperm(N); J = [J rp(1:ner)];
  end
  ne = length(I);
```

By construction there are `ner` given elements in each row of the data matrix, however, there may be columns with a few (or even zero) given elements. Columns with less than m given elements can not be recovered from the given observations, even when the data is noise-free. Therefore, we remove such columns from the data matrix.

145e ⟨*Test missing data 2* 145a⟩+≡ ◁145d 146a▷
```
  tmp = (1:N)';
  J_del = find(sum(J(ones(N, 1),:) ...
                   == tmp(:, ones(1, ne)), 2) < m);
  l0(:, J_del) = [];
  tmp = sparse(I, J, ones(ne, 1), q, N); tmp(:, J_del) = [];
  [I, J] = find(tmp); N = size(l0, 2);
```

Next, a noisy data matrix with missing elements is constructed by adding to the true values of the given data elements independent, identically, distributed, zero

mean, Gaussian noise, with a specified standard deviation `s`. The weight matrix Σ is binary: $\sigma_{ij} = 1$ if d_{ij} is given and $\sigma_{ij} = 1$ if d_{ij} is missing.

146a ⟨*Test missing data 2* 145a⟩+≡ ◁145e 146b▷
```
  d0 = p0 * l0;
  Ie = I + q * (J - 1);
  d  = zeros(q * N, 1);
  d(Ie) = d0(Ie) + sigma * randn(size(d0(Ie)));
  d  = reshape(d, q, N);
  s  = zeros(q, N); s(Ie) = 1;
```

The methods implemented in `lra` and `wlra` are applied on the noisy data matrix D with missing elements and the results are validated against the complete true matrix D_0.

146b ⟨*Test missing data 2* 145a⟩+≡ ◁146a 146c▷
```
  tic, [p0, l0] = lra_md(d, m); t0 = toc;
  err0 = norm(s .* (d - p0 * l0), 'fro') ^ 2;
  e0   = norm(d0 - p0 * l0, 'fro') ^ 2;
  [ph1, lh1, info1] = wlra(d, m, s);
  e1   = norm(d0 - ph1 * lh1, 'fro') ^ 2;
  opt.Method = 'vp'; opt.alg = 'fminunc';
  [ph2, lh2, info2] = wlra(d, m, s, opt);
  e2 = norm(d0 - ph2 * lh2, 'fro') ^ 2;
  opt.Method = 'vp'; opt.alg = 'lsqnonlin';
  [ph3, lh3, info3] = wlra(d, m, s, opt);
  e3 = norm(d0 - ph3 * lh3, 'fro') ^ 2;
```
Uses `lra_md` 139a and `wlra` 142a.

For comparison, we use also a method for low rank matrix completion, called *singular value thresholding* (Cai et al, 2009).. Although the singular value thresholding method is initially designed for the of exact case, it can cope with noisy data as well, *i.e.*, solve low-rank approximation problems with missing data. The method is based on convex relaxation of the rank constraint and does not require an initial approximation.

146c ⟨*Test missing data 2* 145a⟩+≡ ◁146b 147a▷
```
  tau = 5 * sqrt(q * N); delta = 1.2 / (ne / q / N);
  try
    tic, [U, S, V] = SVT([q N], Ie, d(Ie), tau, delta);
    t4 = toc;
    dh4 = U(:, 1:m) * S(1:m, 1:m) * V(:, 1:m)';
  catch
    dh4 = NaN; t4 = NaN; % SVT not installed
  end
  err4 = norm(s .* (d - dh4), 'fro') ^ 2;
  e4   = norm(d0 - dh4, 'fro') ^ 2;
```

The final result shows the

- relative approximation error $\|D - \widehat{D}\|_\Sigma^2 / \|D\|_\Sigma^2$,
- estimation error $\|D_0 - \widehat{D}\|_\text{F}^2 / \|D_0\|_\text{F}^2$, and
- computation time

for the five methods.

147a ⟨*Test missing data 2* 145a⟩+≡ ◁146c
```
nd = norm(s .* d, 'fro')^2; nd0 = norm(d0, 'fro') ^ 2;
format long
res = [err0/nd info1.err/nd  info2.err/nd  info3.err/nd err4/nd;
       e0/nd0  e1/nd0        e2/nd0        e3/nd0       e4/nd0;
       t0      info1.time    info2.time    info3.time   t4]
```

First, we call the test script with exact (noise-free) data.

147b ⟨*Missing data experiment 1: small sparsity, exact data* 147b⟩≡
```
q = 10; N = 100; m = 2; r = 0.1; sigma = 0;
test_missing_data2
```
Uses `test_missing_data2` 145a.

The experiment corresponds to a matrix completion problem (Candés and Recht, 2009). The results, summarized in Tables 5.1, show that all methods, except for `lra_md`, complete correctly (up to numerical errors) the missing elements. As proved by Candés and Recht (2009), exact matrix completion is indeed possible in the case of Experiment 1.

Table 5.1 Results for Experiment 1. (SVT — singular value thresholding, VP — variable projections)

	`lra_md`	`ap`	VP + `fminunc`	VP + `lsqnonlin`	SVT
$\\|D-\widehat{D}\\|_\Sigma^2/\\|D\\|_\Sigma^2$	0.02	0	0	0	0
$\\|D_0-\widehat{D}\\|_F^2/\\|D\\|_F^2$	0.03	0	0	0	0
Execution time (sec)	0.04	0.18	0.17	0.18	1.86

The second experiment is with noisy data.

147c ⟨*Missing data experiment 2: small sparsity, noisy data* 147c⟩≡
```
q = 10; N = 100; m = 2; r = 0.1; sigma = 0.1;
test_missing_data2
```
Uses `test_missing_data2` 145a.

The results, shown in Tables 5.2, indicate that the methods implemented in `wlra` converge to the same (locally) optimal solution. The alternating projections method, however, is about 100 times faster than the variable projections methods, using the Optimization Toolbox functions `fminunc` and `lsqnonlin`, and about 10 times faster than the singular value thresholding method. The solution produces by the singular value thresholding method is suboptimal but close to being (locally) optimal.

Table 5.2 Results for Experiment 2.

	`lra`	`ap`	VP + `fminunc`	VP + `lsqnonlin`	SVT
$\\|D-\widehat{D}\\|_\Sigma^2/\\|D\\|_\Sigma^2$	0.049	0.0257	0.0257	0.0257	0.025
$\\|D_0-\widehat{D}\\|_F^2/\\|D\\|_F^2$	0.042	0.007	0.007	0.007	0.007
Execution time (sec)	0.04	0.11	0.11	0.11	1.51

In the third experiment we keep the noise standard deviation the same as in Experiment 2 but increase the sparsity.

148 ⟨*Missing data experiment 3: bigger sparsity, noisy data* 148⟩≡
```
q = 10; N = 100; m = 2; r = 0.4; sigma = 0.1;
test_missing_data2
```
Uses `test_missing_data2` 145a.

The results, shown in Tables 5.3, again indicate that the methods implemented in `wlra` converge to the same (locally) optimal solutions. In this case, the singular value thresholding method is further away from being (locally) optimal, but is still much better than the solution of `lra_md` — 1% vs 25% relative prediction error.

Table 5.3 Results for Experiment 3

	`lra_md`	`ap`	VP + `fminunc`	VP + `lsqnonlin`	SVT
$\\|D-\widehat{D}\\|_\Sigma^2/\\|D\\|_\Sigma^2$	0.17	0.02	0.02	0.02	0.02
$\\|D_0-\widehat{D}\\|_F^2/\\|D\\|_F^2$	0.27	0.018	0.018	0.018	0.17
Execution time (sec)	0.04	0.21	0.21	0.21	1.87

The three methods based on local optimization (`ap`, VP + `fminunc`, VP + `lsqnonlin`) need not compute the same solution even when started from the same initial approximation. The reason for this is that the methods only guarantee convergence to a locally optimal solution, however, the problem is non convex and may have multiple local minima. Moreover, the trajectories of the three methods in the parameter space are different because the update rules of the methods are different.

The computation times for the three methods are different. The number of floating point operations per iteration can be estimated theoretically which gives an indication which of the methods may be the faster per iteration. Note, however, that the number of iterations, needed for convergence, is not easily predictable, unless the methods are started "close" to a locally optimal solution. The alternating projections methods is most efficient per iteration but needs most iteration steps. In the current implementation of the methods, the alternating projections method is still the winner of the the three methods for large scale data sets because for q more than a few hundreds optimization methods are too computationally demanding. This situation may be improved by analytically computing the gradient and Hessian.

Test on the MovieLens data

The MovieLens data sets were collected and published by the GroupLens Research Project at the University of Minnesota in 1998. Currently, they are recognized as a benchmark for predicting missing data in recommender systems. The "100K data set" consists of 100000 ratings of $\mathtt{q} = 943$ users' on $N = 1682$ movies and demographic information for the users. (The ratings are encoded by integers in the range from 1 to 5.) Here, we use only the ratings, which constitute a $\mathtt{q} \times N$ matrix with missing elements. The task of a recommender system is to fill in the missing elements.

Assuming that the true complete data matrix is rank deficient, building a recommender system is a problem of low-rank approximation with missing elements. The assumption that the true data matrix is low rank is reasonable in practice because user ratings are influences by a few factors. Thus, we can identify typical users (related to different combinations of factors) and reconstruct the ratings of any user as a linear combination of the ratings of the typical users. As long as the typical users are fewer than the number of users, the data matrix is low rank. In reality, the number of factors is not small but there are a few dominant ones, so that the true data matrix is approximately low rank.

It turns out that two factors allow us to reconstruct the missing elements with 7.1% average error. The reconstruction results are validated by cross validation with 80% identification data and 20% validation data. Five such partitionings of the data are given on the MovieLens web site. The matrix

$$\Sigma_{\text{idt}}^{(k)} \in \{0,1\}^{\mathtt{q}\times N}$$

indicates the positions of the given elements in the kth partition:

- $\Sigma_{\text{idt},ij}^{(k)} = 1$ means that the element D_{ij} is used for identification and
- $\Sigma_{\text{idt},ij}^{(k)} = 0$ means that D_{ij} is missing.

Similarly, $\Sigma_{\text{val}}^{(k)}$ indicates the validation elements in the kth partition.

Table 5.4 shows the mean relative identification and validation errors

$$e_{\text{idt}} := \frac{1}{5}\sum_{k=1}^{5} \|D - \widehat{D}^{(k)}\|^2_{\Sigma_{\text{idt}}^{(k)}} / \|D\|^2_{\Sigma_{\text{idt}}^{(k)}}$$

and

$$e_{\text{val}} := \frac{1}{5}\sum_{k=1}^{5} \|D - \widehat{D}^{(k)}\|^2_{\Sigma_{\text{val}}^{(k)}} / \|D\|^2_{\Sigma_{\text{val}}^{(k)}},$$

where $\widehat{D}^{(k)}$ is the reconstructed matrix in the kth partitioning of the data. The singular value thresholding method issues a message "Divergence!", which explains the poor results obtained by this method.

Table 5.4 Results on the MovieLens data.

	`lra_md`	`ap`	SVT
Mean identification error e_{idt}	0.100	0.060	0.298
Mean prediction error e_{val}	0.104	0.071	0.307
Mean execution time (sec)	1.4	156	651

5.2 Affine data modeling

Problem formulation

Closely related to the linear model is the affine one. The observations

$$\mathscr{D} = \{d_1, \dots, d_N\}$$

satisfy an *affine static model* $\mathscr{B}$ if $\mathscr{D} \subset \mathscr{B}$, where $\mathscr{B}$ is an affine set, *i.e.*, $\mathscr{B} = c + \mathscr{B}'$, with $\mathscr{B}' \subset \mathbb{R}^{\mathtt{q}}$ a linear model and $c \in \mathbb{R}^{\mathtt{q}}$ an offset vector. Obviously, the affine model class contains as a special case the linear model class. The parameter c, however, allows us to account for a constant offset in the data. Consider, for example, the data

$$\mathscr{D} = \{ \left[\begin{smallmatrix}1\\1\end{smallmatrix}\right], \left[\begin{smallmatrix}1\\-1\end{smallmatrix}\right] \},$$

which satisfies the affine model

$$\mathscr{B} = \left[\begin{smallmatrix}1\\0\end{smallmatrix}\right] + \{ d \mid \left[\begin{matrix}1 & 0\end{matrix}\right] d = 0 \}$$

but is not fitted by a linear model of dimension one.

Subtracting the offset c from the data vector d, reduces the affine modeling problem with known offset parameter to an equivalent linear modeling problem. In a realistic data modeling setup, however, the offset parameter is unknown and has to be identified together with the linear model $\mathscr{B}'$. An often used heuristic for solving this problem is to replace the offset c by the mean

$$\mathbf{E}(D) := \frac{1}{N} D \mathbf{1}_N = (d_1 + \cdots + d_N)/N \in \mathbb{R}^{\mathtt{q}},$$

where

$$D = \left[d_1 \ \cdots d_N\right]$$

is the data matrix and $\mathbf{1}_N$ is the vector in $\mathbb{R}^N$ with all elements equal to one. This leads to the following two-stage procedure for identification of affine models:

1. *pre-processing step:* subtract the mean from the data points,
2. *linear identification step:* identify a linear model for the centered data.

When the aim is to derive an optimal in some specified sense approximate affine model, the two-stage procedure may lead to suboptimal results. Indeed, even if the data centering and linear identification steps are individually optimal with respect to the desired optimality criterion, their composition need not be optimal for the affine modeling problem, *i.e.*, simultaneous subspace fitting and centering.

It is not clear a priori whether the two-stage procedure is optimal when combined with other data modeling approaches. It turns out that, in the case of low-rank approximation in the Frobenius norm with no additional constraints, the two-stage procedure is optimal. It follows from the analysis that a solution is not unique. Also, counter examples show that in the more general cases of weighted and Hankel structured low-rank approximation problems, the two-stage procedure is suboptimal. Methods based on the alternating projections and variable projections algorithms are developed in these cases.

Matrix centering

The matrix centering operation is subtraction of the mean $\mathbf{E}(D)$ from all columns of the data matrix D:

$$\mathbf{C}(D) := D - \mathbf{E}(D)\mathbf{1}_N^\top = D(I - \frac{1}{N}\mathbf{1}_N\mathbf{1}_N^\top).$$

The following proposition justifies the name "matrix centering" for $\mathbf{C}(\cdot)$.

Proposition 5.5 (Matrix centering) *The matrix* $\mathbf{C}(D)$ *is column centered,* i.e.*, its mean is zero:*

$$\mathbf{E}\big(\mathbf{C}(D)\big) = 0.$$

The proof is left as an exercise, see Problem P.21.

Next we give an interpretation of the mean computation as a simple optimal modeling problem.

Proposition 5.6 (Mean computation as an optimal modeling) $\mathbf{E}(D)$ *is solution of the following optimization problem:*

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D} \text{ and } c \quad \|D - \widehat{D}\|_\text{F} \\ \text{subject to} & \widehat{D} = c\mathbf{1}_N^\top. \end{array} \qquad \square$$

The proof is left as an exercise, see Problem P.22.

Note 5.7 (Intercept). Data fitting with an intercept is a special case of centering when all but one of the row means are set to zero, *i.e.*, centering of one row. Intercept is appropriate when an input/output partition of the variables is imposed and there is a single output that has an offset.

Unweighted low-rank approximation with centering

In this section, we consider the low-rank approximation problem in the Frobenius norm with centering:

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D} \text{ and } c \quad \|D - c\mathbf{1}_N^\top - \widehat{D}\|_\text{F} \\ \text{subject to} & \operatorname{rank}(\widehat{D}) \le \mathtt{m}. \end{array} \tag{LRA$_c$}$$

The following theorem shows that the two-stage procedure yields a solution to (LRA$_c$).

Theorem 5.8 (Optimality of the two-stage procedure). *A solution to (LRA$_c$) is the mean of D,* $c^* = \mathbf{E}(D)$*, and an optimal in a Frobenius norm rank-*$\mathtt{m}$ *approximation* $\widehat{D}^*$ *of the centered data matrix* $\mathbf{C}(D)$*.*

Proof. Using a kernel representation of the rank constraint

$$\operatorname{rank}(\widehat{D}) \le \mathtt{m} \quad \iff \quad \text{there is full rank matrix } R \in \mathbb{R}^{(\mathtt{q}-\mathtt{m})\times\mathtt{q}}, \text{ such that } R\widehat{D} = 0,$$

we have the following equivalent problem to (LRA$_c$)

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D},\, c, \text{ and } R \in \mathbb{R}^{(\mathtt{q}-\mathtt{m})\times\mathtt{q}} \quad \|D - c\mathbf{1}_N^\top - \widehat{D}\|_\text{F}^2 \\ \text{subject to} & R\widehat{D} = 0 \quad \text{and} \quad RR^\top = I_{\mathtt{q}-\mathtt{m}}. \end{array} \tag{LRA$_{c,R}$}$$

The Lagrangian of (LRA$_{c,R}$) is

$$L(\widehat{D}, c, R, \Lambda, \Xi) := \sum_{i=1}^{\mathtt{q}} \sum_{j=1}^{N} (d_{ij} - c_i - \widehat{d}_{ij})^2 + 2\operatorname{trace}(R\widehat{D}\Lambda) + \operatorname{trace}\big(\Xi(I - RR^\top)\big).$$

Setting the partial derivatives of L to zero, we obtain the necessary optimality conditions

$$\partial L/\partial \widehat{D} = 0 \quad \Longrightarrow \quad D - c\mathbf{1}_N^\top - \widehat{D} = R^\top \Lambda^\top, \tag{L1}$$

$$\partial L/\partial c = 0 \quad \Longrightarrow \quad Nc = (D - \widehat{D})\mathbf{1}_N, \tag{L2}$$

$$\partial L/\partial R = 0 \quad \Longrightarrow \quad \widehat{D}\Lambda = R^\top \Xi, \tag{L3}$$

$$\partial L/\partial \Lambda = 0 \quad \Longrightarrow \quad R\widehat{D} = 0, \tag{L4}$$

$$\partial L/\partial \Xi = 0 \quad \Longrightarrow \quad RR^\top = I. \tag{L5}$$

The theorem follows from the system of equations (L1–L5). Next we list the derivation steps.

From (L3), (L4), and (L5), it follows that $\Xi = 0$ and from (L1), we obtain

$$D - \widehat{D} = c\mathbf{1}_N^\top + R^\top \Lambda^\top.$$

Substituting the last identity in (L2), we have

$$\begin{aligned} Nc = (c\mathbf{1}_N^\top + R^\top \Lambda^\top)\mathbf{1}_N = Nc + R^\top \Lambda^\top \mathbf{1}_N \quad &\Longrightarrow \quad R^\top \Lambda^\top \mathbf{1}_N = 0 \\ &\Longrightarrow \quad \Lambda^\top \mathbf{1}_N = 0. \end{aligned}$$

Multiplying (L1) from the left by R and using (L4) and (L5), we have

$$R(D - c\mathbf{1}_N^\top) = \Lambda^\top. \tag{$*$}$$

Now, multiplication of the last identity from the right by $\mathbf{1}_N$ and use of $\Lambda^\top \mathbf{1}_N = 0$, shows that c is the row mean of the data matrix D,

$$R(D\mathbf{1}_N - Nc) = 0 \quad \Longrightarrow \quad c = \frac{1}{N} D\mathbf{1}_N.$$

Next, we show that $\widehat{D}$ is an optimal in a Frobenius norm rank-$\mathtt{m}$ approximation of $D - c\mathbf{1}_N^\top$. Multiplying (L1) from the right by Λ and using $\widehat{D}\Lambda = 0$, we have

$$(D - c\mathbf{1}_N^\top)\Lambda = R^\top \Lambda^\top \Lambda. \tag{$**$}$$

Defining

$$\Sigma := \sqrt{\Lambda^\top \Lambda} \quad \text{and} \quad V := \Lambda \Sigma^{-1},$$

$(*)$ and $(**)$ become

$$\begin{aligned} R(D - c\mathbf{1}_N^\top) &= \Sigma V^\top, \qquad & V^\top V &= I \\ (D - c\mathbf{1}_N^\top)V &= R^\top \Sigma, \qquad & RR^\top &= I. \end{aligned}$$

The above equations show that the rows of R and the columns of V span, respectively, left and right $\mathtt{m}$-dimensional singular subspaces of the centered data matrix $D - c\mathbf{1}_N^\top$. The optimization criterion is minimization of

$$\|D - \widehat{D} - c\mathbf{1}_N^\top\|_{\text{F}} = \|R^\top \Lambda^\top\|_{\text{F}} = \sqrt{\operatorname{trace}(\Lambda\Lambda^\top)} = \operatorname{trace}(\Sigma).$$

Therefore, a minimum is achieved when the rows of R and the columns of V span the, respectively left and right $\mathtt{m}$-dimensional singular subspaces of the centered data matrix $D - c\mathbf{1}_N^\top$, corresponding to the $\mathtt{m}$ smallest singular values. The solution is unique if and only if the $\mathtt{m}$th singular value is strictly bigger than the $(\mathtt{m}+1)$st singular value. Therefore, $\widehat{D}$ is a Frobenius norm optimal rank-$\mathtt{m}$ approximation of the centered data matrix $D - c\mathbf{1}_N^\top$, where $c = D\mathbf{1}_N/N$. □

Theorem 5.9 (Nonuniqueness). *Let*

$$\widehat{D} = PL, \qquad \textit{where} \quad P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}} \textit{ and } L \in \mathbb{R}^{\mathtt{m}\times N}$$

be a rank revealing factorization of an optimal in a Frobenius norm rank-$\mathtt{m}$ approximation of the centered data matrix $\mathbf{C}(D)$. The solutions of (LRA$_c$) are of the form

$$\begin{aligned} c^*(z) &= \mathbf{E}(D) + Pz \\ \widehat{D}^*(z) &= P(L - z\mathbf{1}_N^\top) \end{aligned} \qquad \textit{for} \quad z \in \mathbb{R}^{\mathtt{m}}.$$

Proof.

$$\begin{aligned} c\mathbf{1}_N^\top + \widehat{D} &= c\mathbf{1}_N^\top + PL \\ &= c\mathbf{1}_N^\top + Pz\mathbf{1}_N^\top + PL - Pz\mathbf{1}_N^\top \\ &= \underbrace{(c + Pz)}_{c'}\mathbf{1}_N^\top + P\underbrace{(L - z\mathbf{1}_N^\top)}_{L'} = c'\mathbf{1}_N^\top + \widehat{D}' \end{aligned}$$

Therefore, if $(c, \widehat{D})$ is a solution, then $(c', \widehat{D}')$ is also a solution. From Theorem 5.8, it follows that $c = \mathbf{E}(D)$, $\widehat{D} = PL$ is a solution. □

The same type of nonuniqueness appears in weighted and structured low-rank approximation problems with centering. This can cause problems in the optimization algorithms and implies that solutions produced by different methods can not be compared directly.

Weighted low-rank approximation with centering

Consider the weighted low-rank approximation problem with centering:

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{D} \text{ and } c \quad \|D - \widehat{D} - c\mathbf{1}^\top\|_W \\ &\text{subject to} && \operatorname{rank}(\widehat{D}) \leq \mathtt{m}, \end{aligned} \tag{WLRA$_c$}$$

where W is a symmetric positive definite matrix and $\|\cdot\|_W$ is the weighted norm, defined in ($\|\cdot\|_W$). The two-stage procedure of computing the mean in a preprocessing step and then the weighted low-rank approximation of the centered data matrix, in general, yields a suboptimal solution to (WLRA$_c$). We present two algorithms for finding a locally optimal solution to (WLRA$_c$). The first one is an alternating projections type method and the second one is a variable projections type method. First, however, we present a special case of (WLRA$_c$) with analytic solution that is more general than the case $W = \alpha I$, with $\alpha \neq 0$.

Two-sided weighted low-rank approximation

Theorem 5.10 (Reduction to an unweighted problem). *A solution to (WLRA$_c$), in the case*

$$W = W_{\text{r}} \otimes W_{\text{l}}, \qquad \textit{where} \quad W_{\text{l}} \in \mathbb{R}^{\mathtt{q}\times\mathtt{q}} \textit{ and } W_{\text{r}} \in \mathbb{R}^{N\times N} \tag{$W_{\text{r}} \otimes W_{\text{l}}$}$$

with $W_{\text{r}}\mathbf{1}_N = \lambda\mathbf{1}_N$, for some λ, is

$$c^* = \sqrt{W_{\text{l}}^{-1}}\, c_{\text{m}}^* / \sqrt{\lambda}, \qquad \widehat{D}^* = \sqrt{W_{\text{l}}^{-1}}\, \widehat{D}_{\text{m}}^* \sqrt{W_{\text{r}}^{-1}},$$

where $(c_{\text{m}}^*, \widehat{D}_{\text{m}}^*)$ is a solution to the unweighted low-rank approximation problem with centering

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{D}_{\text{m}} \text{ and } c_{\text{m}} \quad \|D_{\text{m}} - c_{\text{m}}\mathbf{1}_N^\top - \widehat{D}_{\text{m}}\|_{\text{F}} \\ &\text{subject to} && \operatorname{rank}(\widehat{D}_{\text{m}}) \leq \mathtt{m}. \end{aligned}$$

for the modified data matrix $D_{\text{m}} := \sqrt{W_{\text{l}}} D \sqrt{W_{\text{r}}}$.

Proof. Using the property $W_r \mathbf{1}_N = \lambda \mathbf{1}_N$ of W_r, we have

$$\begin{aligned}\|D - \widehat{D} - c\mathbf{1}^\top\|_W &= \|\sqrt{W_l}(D - \widehat{D} - c\mathbf{1}^\top)\sqrt{W_r}\|_F \\ &= \|D_m - \widehat{D}_m - c_m\mathbf{1}^\top\|_F\end{aligned}$$

where

$$D_m = \sqrt{W_l} D \sqrt{W_r}, \qquad \widehat{D}_m = \sqrt{W_l}\widehat{D}\sqrt{W_r}, \quad \text{and} \quad c_m = \sqrt{W_l} c \sqrt{\lambda}.$$

Therefore, the considered problem is equivalent to the low-rank approximation problem (LRA$_c$) for the modified data matrix D_m. □

Alternating projections algorithm

Using the image representation of the rank constraint

$$\operatorname{rank}(\widehat{D}) \leq \mathtt{m} \quad \iff \quad \widehat{D} = PL, \quad \text{where } P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}} \text{ and } L \in \mathbb{R}^{\mathtt{m}\times N},$$

we obtain the following problem equivalent to (WLRA$_c$)

$$\text{minimize} \quad \text{over } P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}, L \in \mathbb{R}^{\mathtt{m}\times N}, \text{ and } c \in \mathbb{R}^{\mathtt{q}} \quad \|D - PL - c\mathbf{1}_N^\top\|_W. \tag{WLRA$_{c,P}$}$$

The method is motivated by the fact that (WLRA$_{c,P}$) is linear in c and P as well as in c and L. Indeed,

$$\begin{aligned}\|D - c\mathbf{1}_N^\top - PL\|_W &= \left\| \operatorname{vec}(D) - \begin{bmatrix} I_N \otimes P & \mathbf{1}_N \otimes I_{\mathtt{q}} \end{bmatrix} \begin{bmatrix} \operatorname{vec}(L) \\ c \end{bmatrix} \right\|_W \\ &= \left\| \operatorname{vec}(D) - \begin{bmatrix} L^\top \otimes I_{\mathtt{q}} & \mathbf{1}_N \otimes I_{\mathtt{q}} \end{bmatrix} \begin{bmatrix} \operatorname{vec}(P) \\ c \end{bmatrix} \right\|_W.\end{aligned}$$

This suggests an iterative algorithm alternating between minimization over c and P with a fixed L and over c and L with a fixed P, see Algorithm 4. Each iteration step is a weighted least squares problem, which can be solved globally and efficiently. The algorithm starts from an initial approximation $c^{(0)}$, $P^{(0)}$, $L^{(0)}$ and on each iteration step updates the parameters with the newly computed values from the last least squares problem. Since on each iteration the cost function value is guaranteed to be non increasing and the cost function is bounded from below, the sequence of cost function values, generated by the algorithm converges. Moreover, it can be shown that the sequence of parameter approximations $c^{(k)}$, $P^{(k)}$, $L^{(k)}$ converges to a locally optimal solution of (WLRA$_{c,P}$).

Example 5.11. Implementation of the methods for weighted and structured low-rank approximation with centering, presented in this section, are available from the book's web page. Figure 5.1 shows the sequence of the cost function values for a randomly generated weighted rank-1 approximation problem with $\mathtt{q} = 3$ variables

and $N = 6$ data points. The mean of the data matrix and the approximation of the mean, produced by the Algorithm 4 are, respectively

$$c^{(0)} = \begin{bmatrix} 0.5017 \\ 0.7068 \\ 0.3659 \end{bmatrix} \qquad \text{and} \qquad \widehat{c} = \begin{bmatrix} 0.4365 \\ 0.6738 \\ 0.2964 \end{bmatrix}.$$

The weighted rank-1 approximation of the matrix $D - c^{(0)}\mathbf{1}_N^\top$ has approximation error 0.1484, while the weighted rank-1 approximation of the matrix $D - \widehat{c}\mathbf{1}_N^\top$ has approximation error 0.1477. This proves the suboptimality of the two-stage procedure—data centering, followed by weighted low-rank approximation.

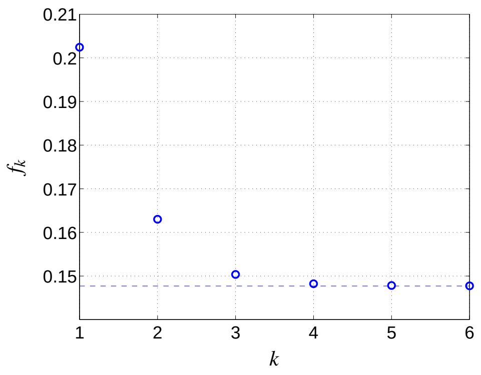

Fig. 5.1 Sequence of cost function values, produced by Algorithm 4.

Variable projections algorithm

The variable projections approach is based on the observation that (WLRA$_{c,P}$) is a double minimization problem

$$\text{minimize} \quad \text{over } P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}} \quad f(P)$$

where the inner minimization is a weighted least squares problem

$$f(P) := \min_{L \in \mathbb{R}^{\mathtt{m}\times N},\ c \in \mathbb{R}^{\mathtt{q}}} \|D - PL - c\mathbf{1}_N^\top\|_W$$

and therefore can be solved analytically. This reduces the original problem to a nonlinear least squares problem over P only. We have that

$$f(P) = \sqrt{\operatorname{vec}^\top(D) W \mathbf{P} \left(\mathbf{P}^\top W \mathbf{P}\right)^{-1} \mathbf{P}^\top W \operatorname{vec}(D)},$$

Algorithm 4 Alternating projections algorithm for weighted low-rank approximation with centering.

```
Input: data matrix $D \in \mathbb{R}^{\mathtt{q}\times N}$, rank constraint $\mathtt{m}$, positive definite weight matrix $W \in \mathbb{R}^{N\mathtt{q}\times N\mathtt{q}}$, and
    relative convergence tolerance $\varepsilon$.
1: Initial approximation: compute the mean $c^{(0)} := \mathbf{E}(D)$ and the rank-$\mathtt{m}$ approximation $\widehat{D}^{(0)}$ of
    the centered matrix $D - c^{(0)}\mathbf{1}_N^\top$. Let $P^{(0)} \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}$ and $L^{(0)} \in \mathbb{R}^{\mathtt{m}\times N}$ are full rank matrices, such
    that $\widehat{D}^{(0)} = P^{(0)}L^{(0)}$.
2: $k := 0$.
3: repeat
4:    Let $\mathbf{P} := \begin{bmatrix} I_N \otimes P^{(k)} & \mathbf{1}_N \otimes I_\mathtt{q} \end{bmatrix}$ and
          $\begin{bmatrix} \operatorname{vec}(L^{(k+1)}) \\ \widehat{c}^{(k+1)} \end{bmatrix} := \left(\mathbf{P}^\top W \mathbf{P}\right)^{-1} \mathbf{P}^\top W \operatorname{vec}(D)$.
5:    Let $\mathbf{L} := \begin{bmatrix} L^{(k+1)\top} \otimes I_\mathtt{q} & \mathbf{1}_N \otimes I_\mathtt{q} \end{bmatrix}$ and
          $\begin{bmatrix} \operatorname{vec}(P^{(k+1)}) \\ \widehat{c}^{(k+1)} \end{bmatrix} := \left(\mathbf{L}^\top W \mathbf{L}\right)^{-1} \mathbf{L}^\top W \operatorname{vec}(D)$.
6:    Let $\widehat{D}^{(k+1)} := P^{(k+1)}L^{(k+1)}$.
7:    $k = k+1$.
8: until $\|\widehat{D}^{(k)} - \widehat{D}^{(k-1)}\|_W / \|\widehat{D}^{(k)}\|_W < \varepsilon$.
Output: Locally optimal solution $\widehat{c} := \widehat{c}^{(k)}$ and $\widehat{D}^* = \widehat{D}^{(k)}$ of (WLRA$_{c,P}$).
```

where

$$\mathbf{P} := \begin{bmatrix} I_N \otimes P & \mathbf{1}_N \otimes I_\mathtt{q} \end{bmatrix}.$$

For the outer minimization any standard unconstrained nonlinear (least squares) algorithm is used.

Example 5.12. For the same data, initial approximation, and convergence tolerance as in Example 5.11, the variable projections algorithm, using numerical approximation of the derivatives in combination with quasi-Newton method converges to a locally optimal solution with approximation error 0.1477—the same as the one found by the alternating projections algorithm. The optimal parameters found by the two algorithms are equivalent up to the nonuniqueness of a solution (Theorem 5.9).

Hankel low-rank approximation with centering

In the case of data centering we consider the following modified Hankel low-rank approximation problem:

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{w} \text{ and } c \quad \|w - c - \widehat{w}\|_2 \\ &\text{subject to} \quad \operatorname{rank}\left(\mathscr{H}_{n+1}(\widehat{w})\right) \leq r. \end{aligned} \qquad (\text{HLRA}_c)$$

Algorithm

Consider the kernel representation of the rank constraint

$$\operatorname{rank}\left(\mathscr{H}_{n+1}(\widehat{w})\right) \leq r \quad \iff \quad \begin{array}{c}\text{there is full rank matrix } R \in \mathbb{R}^{\mathtt{p}\times(\mathtt{n}+1)\mathtt{q}} \\ \text{such that } R\mathscr{H}_{n+1}(w_\mathrm{d}) = 0.\end{array}$$

We have

$$R\mathscr{H}_{n+1}(\widehat{w}) = 0 \quad \iff \quad \mathscr{T}(R)\widehat{w} = 0,$$

where

$$\mathscr{T}(R) = \begin{bmatrix} R_0 & R_1 & \cdots & R_\mathtt{n} & & & \\ & R_0 & R_1 & \cdots & R_\mathtt{n} & & \\ & & \ddots & \ddots & & \ddots & \\ & & & R_0 & R_1 & \cdots & R_\mathtt{n} \end{bmatrix}$$

(all missing elements are zeros). Let P be a full rank matrix, such that

$$\operatorname{image}(P) = \ker\left(\mathscr{T}(R)\right).$$

Then the constraint of (HLRA$_c$) can be replaced by

$$\text{there is } \ell\text{, such that } \widehat{w} = P\ell,$$

which leads to the following problem equivalent to (LRA$_c$)

$$\text{minimize} \quad \text{over } R \quad f(R),$$

where

$$f(R) := \min_{c,\ell} \left\| w - \begin{bmatrix} \mathbf{1}_N \otimes I_\mathtt{q} & P \end{bmatrix} \begin{bmatrix} c \\ \ell \end{bmatrix} \right\|_2.$$

The latter is a standard least squares problem, so that the evaluation of f for a given R can be done efficiently. Moreover, one can exploit the Toeplitz structure of the matrix $\mathscr{T}$ in the computation of P and in the solution of the least squares problem.

Example 5.13. The data sequence is

$$w(t) = 0.9^t + 1, \qquad t = 1, \ldots, 10.$$

The sequence $(0.9^1, \ldots, 0.9^{10})$ satisfies a difference equation

$$\sigma w = aw$$

(a first order autonomous linear time-invariant model), however, a shifted sequence $w(t) = 0.9^t + c$, with $c \neq 0$, does not satisfy such an equation. The mean of the data is $\mathbf{E}(w) = 1.5862$, so that the centered data $w(t) - \mathbf{E}(D)$ is not a trajectory of a first order autonomous linear time-invariant model. Solving the Hankel structured low-rank approximation problem with centering (HLRA$_c$), however, yields the exact solution $\widehat{c} = 1$.

Preprocessing by centering the data is common in system identification. Example 5.13 shows that preprocessing can lead to suboptimal results. Therefore, there is need for methods that combine data preprocessing with the existing identification methods. The algorithm derived in this section is such a method for identification in the errors-in-variables setting. It can be modified for output error identification, *i.e.*, assuming that the input of the system is known exactly.

5.3 Complex least squares problem with constrained phase

Problem formulation

The problem considered in this section is defined as follows.

Problem 5.14. Given a complex valued $m \times n$ matrix A and an $m \times 1$ vector b, find a real valued $n \times 1$ vector x and a number ϕ, such that the equation's error or residual of the overdetermined system of linear equations

$$Axe^{\mathbf{i}\phi} \approx b, \qquad (\mathbf{i} \text{ is the imaginary unit})$$

is minimized in the least squares sense, *i.e.*,

$$\text{minimize} \quad \text{over } x \in \mathbb{R}^n \text{ and } \phi \in (-\pi, \pi] \quad \|Axe^{\mathbf{i}\phi} - b\|_2. \qquad \text{(CLS)}$$

□

Problem (CLS) is a complex linear least squares problem with constraint that all elements of the solution have the same phase.

As formulated, (CLS) is a nonlinear optimization problem. General purpose local optimization methods can be used for solving it, however, this approach has the usual disadvantages of local optimization methods: need of initial approximation, no guarantee of global optimality, convergence issues, and no insight in the geometry of the solutions set. In (Bydder, 2010) the following closed form solution of (CLS) is derived

$$\widehat{x} = \big(\Re(A^H A)\big)^+ \Re(A^H b e^{-\mathbf{i}\phi}) \qquad (\text{SOL1 } \widehat{x})$$

$$\widehat{\phi} = \frac{1}{2} \angle\big((A^H b)^\top \Re(A^H A)^+ (A^H b)\big), \qquad (\text{SOL1 } \widehat{\phi})$$

where $\Re(A)/\Im(A)$ is the real/imaginary part, $\angle(A)$ is the angle, A^H is the complex conjugate transpose, and A^+ is the pseudoinverse of A. Moreover, in the case when a solution of (CLS) is not unique, (SOL1 $\widehat{x}$, SOL1 $\widehat{\phi}$) is a least norm element of the solution set, *i.e.*, a solution (x, ϕ), such that $\|x\|_2$ is minimized. Expression (SOL1

$\widehat{x}$) is the result of minimizing the cost function $\|Axe^{\mathbf{i}\phi} - b\|_2$ with respect to x, for a fixed ϕ. This is a linear least squares problems (with complex valued data and real valued solution). Then minimization of the cost function with respect to ϕ, for x fixed to its optimal value (SOL1 $\widehat{x}$), leads through a nontrivial chain of steps to (SOL1 $\widehat{\phi}$).

Solution

Problem (CLS) is equivalent[1] to the problem

$$\text{minimize} \quad \text{over } x \in \mathbb{R}^n \text{ and } \phi' \in (-\pi, \pi] \quad \|Ax - be^{\mathbf{i}\phi'}\|_2, \qquad \text{(CLS')}$$

where $\phi' = -\phi$. With

$$y_1 := \Re(e^{\mathbf{i}\phi'}) = \cos(\phi') = \cos(\phi) \qquad \text{and} \qquad y_2 := \Im(e^{\mathbf{i}\phi'}) = \sin(\phi') = -\sin(\phi),$$

we have

$$\begin{bmatrix} \Re(be^{\mathbf{i}\phi'}) \\ \Im(be^{\mathbf{i}\phi'}) \end{bmatrix} = \begin{bmatrix} \Re(b) & -\Im(b) \\ \Im(b) & \Re(b) \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}.$$

Then, (CLS') is furthermore equivalent to the problem

$$\begin{aligned} &\text{minimize} \quad \text{over } x \in \mathbb{R}^n \text{ and } y \in \mathbb{R}^2 \quad \left\| \begin{bmatrix} \Re(A) \\ \Im(A) \end{bmatrix} x - \begin{bmatrix} \Re(b) & -\Im(b) \\ \Im(b) & \Re(b) \end{bmatrix} y \right\| \\ &\text{subject to} \quad \|y\|_2 = 1, \end{aligned}$$

or

$$\text{minimize} \quad \text{over } z \in \mathbb{R}^{n+2} \quad z^\top C^\top C z \quad \text{subject to} \quad z^\top D^\top D z = 1, \qquad \text{(CLS'')}$$

with

$$C := \begin{bmatrix} \Re(A) & \Re(b) & -\Im(b) \\ \Im(A) & \Im(b) & \Re(b) \end{bmatrix} \in \mathbb{R}^{2m \times (n+2)} \quad \text{and} \quad D := \begin{bmatrix} 0 & 0 \\ 0 & I_2 \end{bmatrix} \in \mathbb{R}^{(n+2) \times (n+2)}. \qquad (C, D)$$

It is well known that a solution of problem (CLS'') can be obtained from the generalized eigenvalue decomposition of the pair of matrices $(C^\top C, D)$. More specifically, the smallest generalized eigenvalue $\lambda_{\min}$ of $(C^\top C, D)$ is equal to the minimum value of (CLS''), *i.e.*,

$$\lambda_{\min} = \|A\widehat{x}e^{\mathbf{i}\widehat{\phi}} - b\|_2^2.$$

If $\lambda_{\min}$ is simple, a corresponding generalized eigenvector $z_{\min}$ is of the form

[1] Two optimization problems are equivalent if the solution of the first can be obtained from the solution of the second by a one-to-one transformation. Of practical interest are equivalent problems for which the transformation is "simple".

$$z_{\min} = \alpha \begin{bmatrix} \widehat{x} \\ -\cos(\widehat{\phi}) \\ \sin(\widehat{\phi}) \end{bmatrix},$$

for some $\alpha \in \mathbb{R}$. We have the following result.

Theorem 5.15. *Let $\lambda_{\min}$ be the smallest generalized eigenvalue of the pair of matrices $(C^\top C, D)$, defined in (C, D), and let $z_{\min}$ be a corresponding generalized eigenvector. Assuming that $\lambda_{\min}$ is a simple eigenvalue, problem (CLS) has unique solution, given by*

$$\widehat{x} = \frac{1}{\|z_2\|_2} z_1, \quad \widehat{\phi} = \angle(-z_{2,1} + \mathbf{i} z_{2,2}), \qquad where \quad z_{\min} =: \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \begin{matrix} \}n \\ \}2 \end{matrix}. \qquad \text{(SOL2)}$$

Remarks:

1. *Generalized eigenvalue decomposition vs generalized singular value decomposition* Since the original data are the matrix A and the vector b, the generalized singular value decomposition of the pair (C,D) can be used instead of the generalized eigenvalue decomposition of the pair $(C^\top C, D)$. This avoids “squaring” the data and is recommended from a numerical point of view.
2. *Link to low-rank approximation and total least squares* Problem (CLS”) is equivalent to the generalized low-rank approximation problem

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{C} \in \mathbb{R}^{2m\times(n+2)} \quad \big\|(C-\widehat{C})D\big\|_F \\ &\text{subject to} \quad \operatorname{rank}(\widehat{C}) \le n+1 \quad \text{and} \quad \widehat{C}D^\perp = CD^\perp, \end{aligned} \qquad \text{(GLRA)}$$

where

$$D^\perp = \begin{bmatrix} I_n & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{(n+2)\times(n+2)}$$

and $\|\cdot\|_F$ is the Frobenius norm. Indeed, the constraints of (GLRA) imply that

$$\big\|(C-\widehat{C})D\big\|_F = \|b-\widehat{b}\|_2, \qquad \text{where} \quad \widehat{b} = Axe^{\mathbf{i}\phi}.$$

The normalization (SOL2) is reminiscent to the generic solution of the total least squares problems. The solution of total least squares problems, however, involves a normalization by scaling with the last element of a vector $z_{\min}$ in the approximate kernel of the data matrix C, while the solution of (CLS) involves normalization by scaling with the norm of the last two elements of the vector $z_{\min}$.
3. *Uniqueness of the solution and minimum norm solutions* A solution x of (CLS) is nonunique when A has nontrivial null space. This source of nonuniqueness is fixed in (Bydder, 2010) by choosing from the solutions set a least norm solution. A least norm solution of (CLS), however, may also be nonunique due to possible nonuniquess of ϕ. Consider the following example,

$$A = \begin{bmatrix} 1 & \mathbf{i} \\ -\mathbf{i} & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ -\mathbf{i} \end{bmatrix},$$

which has two least norm solutions

$$\widehat{x}e^{\mathbf{i}\phi_1} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \text{and} \qquad \widehat{x}' e^{\mathbf{i}\phi_2} = \begin{bmatrix} 0 \\ -\mathbf{i} \end{bmatrix}.$$

Moreover, there is a trivial source of nonuniqueness in x and ϕ due to

$$xe^{\mathbf{i}\phi} = -xe^{\mathbf{i}(\phi\pm\pi)}$$

with both ϕ and one of the angles $\phi \pm \pi$ in the interval $(-\pi, \pi]$.

Computational algorithms

Solution (SOL1 $\widehat{x}$, SOL1 $\widehat{\phi}$) gives a straightforward procedure for computing a least norm solution of problem (CLS).

162a ⟨*Complex least squares, solution by (SOL1 $\widehat{x}$, SOL1 $\widehat{\phi}$)* 162a⟩≡
```
function cx = cls1(A, b)
invM = pinv(real(A' * A)); Atb = A' * b;
phi  = 1 / 2 * angle((Atb).' * invM * Atb);
x    = invM * real(Atb * exp(-i * phi));
cx   = x * exp(i * phi);
```
Defines:
`cls1`, used in chunk 165b.

The corresponding computational cost is

$$\texttt{cls1} — O(n^2 m + n^3).$$

Theorem 5.15 gives two alternative procedures—one based on the generalized eigenvalue decomposition:

162b ⟨*Complex least squares, solution by generalized eigenvalue decomposition* 162b⟩≡
```
function cx = cls2(A, b)
⟨define C, D, and n 162c⟩
[v, l] = eig(C' * C, D); l = diag(l);
l(find(l < 0)) = inf; % ignore nevative values
[ml, mi] = min(l); z = v(:, mi);
phi = angle(-z(end - 1) + i * z(end));
x   = z(1:(end - 2)) / norm(z((end - 1):end));
cx  = x * exp(i * phi);
```
Defines:
`cls2`, used in chunk 165b.

162c ⟨*define C, D, and n* 162c⟩≡ (162 163)
```
C = [real(A) real(b) -imag(b);
     imag(A) imag(b)  real(b)];
n = size(A, 2); D = diag([zeros(1, n), 1, 1]);
```

and the other one based on the generalized singular value decomposition:

163a ⟨*Complex least squares, solution by generalized singular value decomposition* 163a⟩≡
```
function cx = cls3(A, b)
⟨define C, D, and n 162c⟩
[u, v] = gsvd(C, D); z = v(:, 1);
phi = angle(-z(end - 1) + i * z(end));
x   = pinv(C(:, 1:n)) * [real(b * exp(- i * phi));
                         imag(b * exp(- i * phi))];
cx  = x * exp(i * phi);
```
Defines:
  `cls3`, used in chunk 165b.

The computational costs are

$$\texttt{cls2} — O\big((n+2)^2m+(n+2)^3\big)$$

and

$$\texttt{cls3} — O\big(m^3+(n+2)^2m^2+(n+2)^2m+(n+2)^3\big).$$

Note, however, that `cls2` and `cls3` compute the full generalized eigenvalue decomposition and generalized singular value decomposition, respectively, while only the smallest generalized eigenvalue/eigenvector or singular value/singular vector pair is needed for solving (CLS). This suggests a way of reducing the computational complexity by a factor of magnitude.

The equivalence between problem (CLS) and the generalized low-rank approximation problem (GLRA), noted in remark 2 above, allows us to use the algorithm from (Golub et al, 1987) for solving problem (CLS). The resulting Algorithm 5 is implemented in the function `cls4`.

163b ⟨*Complex least squares, solution by Algorithm 5* 163b⟩≡
```
function cx = cls4(A, b)
⟨define C, D, and n 162c⟩
R   = triu(qr(C, 0));
[u, s, v] = svd(R((n + 1):(n + 2), (n + 1):end));
phi = angle(v(1, 2) - i * v(2, 2));
x   = R(1:n, 1:n) \ (R(1:n, (n + 1):end) * [v(1, 2); v(2, 2)]);
cx  = x * exp(i * phi);
```
Defines:
  `cls4`, used in chunk 165b.

Its computational cost is

$$\texttt{cls4} — O\big((n+2)^2m\big).$$

Table 5.5 Summary of methods for solving the complex least squares problem (CLS).

function	method	computational cost
`cls1`	(SOL1 $\widehat{x}$, SOL1 $\widehat{\phi}$)	$O(n^2m+n^3)$
`cls2`	full generalized eigenvalue decomp.	$O\big((n+2)^2m+(n+2)^3\big)$
`cls3`	full generalized singular value decomp.	$O\big(m^3+(n+2)^2m^2+(n+2)^2m+(n+2)^3\big)$
`cls4`	Algorithm 5	$O\big((n+2)^2m\big)$

Algorithm 5 Solution of problem (CLS) using generalized low-rank approximation.

```
Input: $A \in \mathbb{C}^{m\times n}$, $b \in \mathbb{C}^{m\times 1}$
1: QR factorization of $C$, $QR = C$.
2: Define $R =: \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \begin{matrix} \}\,n \\ \}\,2 \end{matrix}$, where $R_{11} \in \mathbb{R}^{n\times n}$.
3: Singular value decomposition of $R_{22}$, $U\Sigma V^\top = R_{22}$.
4: Let $\widehat{\phi} := \angle(v_{12} - \mathbf{i}v_{22})$ and $\widehat{x} := R_{11}^{-1}R_{12}\begin{bmatrix} v_{12} \\ v_{22} \end{bmatrix}$.
Output: $\widehat{x}e^{\mathbf{i}\widehat{\phi}}$
```

Numerical examples

Generically, the four solution methods implemented in the functions `cls1`, ..., `cls4` compute the same result, which is equal to the unique solution of problem (CLS). As predicted by the theoretical computation costs, the method based on Algorithm 5 is the fastest of the four methods when both the number of equations and the number of unknowns is growing, see Figure 5.2.

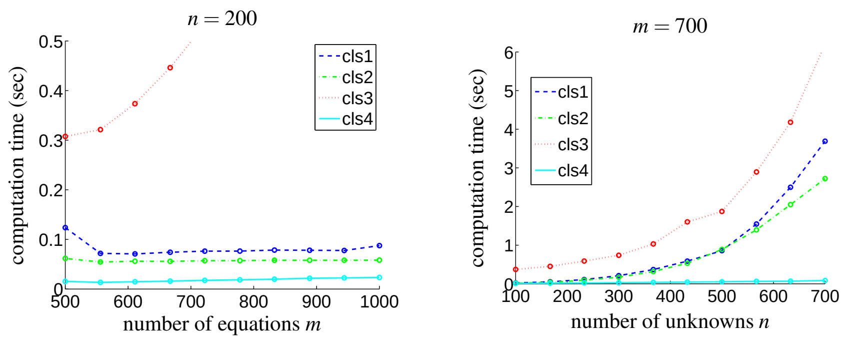

Fig. 5.2 Computation time for the four methods, implemented in the functions `cls1`, ..., `cls4`.

The figures are generated by using random test data

164a ⟨*Computation time for* `cls1-4` 164a⟩≡ 164b▷
```
⟨initialize the random number generator 91d⟩
mm = 1000; nm = 1000; s = {'b-' 'g-.' 'r:' 'c-'};
Am = rand(mm, nm) + i * rand(mm, nm);
bm = rand(mm, 1 ) + i * rand(mm, 1 );
```
Defines:
  `test_cls`, never used.

and solving problems with increasing number of equations m

164b ⟨*Computation time for* `cls1-4` 164a⟩+≡ ◁164a 165a▷
```
Nm = 10; M = round(linspace(500, 1000, Nm)); n = 200;
for j = 1:Nm, m = M(j); ⟨call cls1-4 165b⟩ end
k = 1; x = M; ax = [500 1000 0 0.5]; name = 'cls-f1';
⟨plot cls results 165c⟩
```

as well as increasing number of unknowns n

165a ⟨*Computation time for* `cls1-4` 164a⟩+≡ ◁164b
```
Nn = 10; N = round(linspace(100, 700, Nn)); m = 700;
for j = 1:Nn, n = N(j); ⟨call cls1-4 165b⟩ end
k = 2; x = N; ax = [100 700 0 6]; name = 'cls-f2';
⟨plot cls results 165c⟩
```

165b ⟨*call* `cls1-4` 165b⟩≡ (164b 165a)
```
A = Am(1:m, 1:n); b = bm(1:m);
for i = 1:4 % cls1, cls2, cls3, cls4
  eval(sprintf('tic, x = cls%d(A, b); t(%d) = toc;', i, i))
end
T(:, j) = t';
```
Uses `cls1` 162a, `cls2` 162b, `cls3` 163a, and `cls4` 163b.

165c ⟨*plot* `cls` *results* 165c⟩≡ (164b 165a)
```
figure(k), hold on
for i = 1:4 plot(x, T(i, :), s{i}, 'linewidth', 2), end
legend('cls1', 'cls2', 'cls3', 'cls4')
for i = 1:4, plot(x, T(i, :), [s{i}(1) 'o']), end
axis(ax), print_fig(name)
```
Uses `print_fig` 25a.

5.4 Approximate low rank factorization with structured factors

Problem formulation

Rank estimation

Consider an $\mathtt{q} \times N$ real matrix D_0 with rank $\mathtt{m}_0 < \mathtt{q}$ and let

$$D_0 = P_0 L_0, \qquad \text{where} \quad P_0 \in \mathbb{R}^{\mathtt{q}\times \mathtt{m}_0} \text{ and } L_0 \in \mathbb{R}^{\mathtt{m}_0 \times N}$$

be a *rank revealing* factorization of D_0. Suppose that instead of D_0 a matrix

$$D := D_0 + \widetilde{D}$$

is observed, where $\widetilde{D}$ is a perturbation, *e.g.*, $\widetilde{D}$ can represent rounding errors in a finite precision arithmetic or measurement errors in data acquisition. The rank of the perturbed matrix D may not be equal to $\mathtt{m}_0$. If $\widetilde{D}$ is random, generically, D is full rank, so that from a practical point of view, a nonzero perturbation $\widetilde{D}$ makes the matrix D full rank. If, however, $\widetilde{D}$ is "small", in the sense that its Frobenius norm $\|\widetilde{D}\|_{\mathrm{F}}$ is less than a constant ε (defining the perturbation size), then D will be "close" to a rank-$\mathtt{m}_0$ matrix in the sense that the distance of D to the manifold of rank-$\mathtt{m}_0$ matrices

$$\operatorname{dist}(D,\mathtt{m}_0) := \min_{\widehat{D}} \quad \|D-\widehat{D}\|_{\mathrm{F}} \quad \text{subject to} \quad \operatorname{rank}(\widehat{D}) = \mathtt{m}_0 \tag{5.2}$$

is less than the perturbation size ε. Therefore, provided that the size ε of the perturbation $\widetilde{D}$ is known, the distance measure $\operatorname{dist}(D,\mathtt{m})$, for $\mathtt{m} = 1,2,\ldots$, can be used to estimate the rank of the unperturbed matrix as follows

$$\widehat{\mathtt{m}} = \arg\min\{\,\mathtt{m} \mid \operatorname{dist}(D,\mathtt{m}) < \varepsilon\,\}.$$

Problem (5.2) has analytic solution in terms of the singular values $\sigma_1,\ldots,\sigma_{\mathtt{q}}$ of D

$$\operatorname{dist}(D,\mathtt{m}_0) := \sqrt{\sigma^2_{\mathtt{m}_0+1} + \cdots + \sigma^2_{\mathtt{q}}}, \tag{dist}$$

and therefore the rank of D_0 can be estimated from the decay of the singular values of D (find the largest singular value that is sufficiently small compared to the perturbation size ε). This is the standard way for rank estimation in numerical linear algebra, where the estimate $\widehat{\mathtt{m}}$ is called *numerical rank* of D, *cf.*, page 40. The question occurs:

Given a perturbed matrix $D := D_0 + \widetilde{D}$, is the numerical rank of D the "best" estimate for the rank of D_0, and if so, in what sense?

The answer to the above question depends on the type of the perturbation $\widetilde{D}$. If $\widetilde{D}$ is a random matrix with zero mean elements that are normally distributed, independent, and with equal variances, then the estimate $\widehat{D}$, defined by (5.2) is a maximum likelihood estimator of D_0, *i.e.*, it is statistically optimal. If, however, one or more of the above assumptions are not satisfied, $\widehat{D}$ is not optimal and can be improved by modifying problem (5.2). Our objective is to justify this statement in a particular case when there is prior information about the true matrix D_0 in the form of structure in a normalized rank-revealing factorization and the elements of the perturbation $\widetilde{D}$ are independent but possibly with different variances.

Prior knowledge in the form of structure

In applications often there is prior knowledge about the unperturbed matrix D_0, apart from the basic one that D_0 is rank deficient. Whenever available, such prior knowledge is beneficial to use in the computation of the distance measure $\operatorname{dist}(D,\mathtt{m})$. Using the prior knowledge amounts to modification of problem (5.2). For example, common prior information in image and text classification is nonnegativity of the elements of D_0. In this case, we require the approximation $\widehat{D}$ to be nonnegative and in order to achieve this, we impose nonnegativity of the estimate $\widehat{D}$ as an extra constraint in (5.2). Similarly, in signal processing and system theory the matrix D_0 is Hankel or Toeplitz structured and the relevant modification of (5.2) is to constrain $\widehat{D}$

to have the same structure. In chemometrics, the measurement errors $\widetilde{d}_{ij}$ may have different variances $\sigma^2 v_{ij}$, which are known (up to a scaling factor) from the measurement setup or from repeated experiments. Such prior information amounts to changing the cost function $\|D-\widehat{D}\|_{\mathrm{F}}$ to the weighted norm $\|D-\widehat{D}\|_{\Sigma}$ of the error matrix $D-\widehat{D}$, where the elements of the weight matrix Σ are up to a scaling factor equal to the inverse square root of the error variance $\sigma^2 V$. In general, either the addition of constraints on $\widehat{D}$ or the replacement of the Frobenius norm with a weighted norm, renders the modified distance problem (5.2) difficult to solve. A globally optimal solution can no longer be given in terms of the singular values of D and the resulting optimization problem is nonconvex.

A factorization $D = PL$ is nonunique; for any $r \times r$ nonsingular matrix T, we obtain a new factorization $D = P'L'$, where $P' := PT^{-1}$ and $L' = TL$. Obviously, this imposes a problem in estimating the factors P and L from the data D. In order to resolve the nonuniqueness problem, we assume that

$$P = \begin{bmatrix} I_{\mathtt{m}} \\ P' \end{bmatrix}.$$

Next, we present an algorithm for approximate low rank factorization with structured factors and test its performance on synthetic data. We use the alternating projections approach, because it is easier to modify for constrained optimization problems. Certain constrained problems can be treated also using a modification of the variable projections.

Statistical model and maximum likelihood estimation problem

Consider the errors-in-variables model

$$\begin{aligned} D = D_0 + \widetilde{D}, \quad \text{where} \quad & D_0 = P_0 L_0, \quad \text{with} \\ & P_0 \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}, \quad L_0 \in \mathbb{R}^{\mathtt{m}\times N}, \quad \mathtt{m} < \mathtt{q} \qquad (\mathrm{EIV}_0) \\ & \text{and } \operatorname{vec}(\widetilde{D}) \sim \mathrm{N}\big(0, \sigma^2 \operatorname{diag}(v)\big). \end{aligned}$$

The *true data matrix* D_0 has rank equal to $\mathtt{m}$ and the measurement errors $\widetilde{d}_{ij}$ are zero mean, normal, and uncorrelated, with covariance $\sigma^2 v_{i+\mathtt{q}(j-1)}$. The vector $v \in \mathbb{R}^{\mathtt{q}N}$ specifies the element-wise variances of the measurement error matrix $\widetilde{D}$ up to an unknown factor σ^2.

In order to make the parameters P_0 and L_0 unique, we impose the normalization constraint (or assumption on the "true" parameter values)

$$P_0 = \begin{bmatrix} I_{\mathtt{m}} \\ P_0' \end{bmatrix}. \qquad (\mathrm{A}_1)$$

In addition, the block P_0' of P_0 has elements (specified by a selector matrix S) equal to zero

$$S \operatorname{vec}(P_0') = 0. \qquad (\mathrm{A}_2)$$

The parameter L_0 is periodic with a period $l \in \mathbb{Z}_+$

$$L_0 = \mathbf{1}_l^\top \otimes L_0', \qquad (\mathrm{A}_3)$$

nonnegative

$$L_0' \geq 0, \qquad (\mathrm{A}_4)$$

and with smooth rows in the sense that

$$\|L_0' \mathbf{D}\|_{\mathrm{F}}^2 \leq \delta, \qquad (\mathrm{A}_5)$$

where $\delta > 0$ is a smoothness parameter and $\mathbf{D}$ is a finite difference matrix

$$\mathbf{D} := \begin{bmatrix} 1 & & & -1 \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}.$$

Define the $\mathtt{q} \times N$ matrix

$$\Sigma = \operatorname{vec}^{-1}\left(\begin{bmatrix} v_1^{-1/2} & \cdots & v_{\mathtt{q}N}^{-1/2} \end{bmatrix}\right) := \begin{bmatrix} v_1^{-1/2} & v_{\mathtt{q}+1}^{-1/2} & \cdots & v_{\mathtt{q}(N-1)+1}^{-1/2} \\ v_2^{-1/2} & v_{\mathtt{q}+2}^{-1/2} & \cdots & v_{\mathtt{q}(N-1)+2}^{-1/2} \\ \vdots & \vdots & & \vdots \\ v_{\mathtt{q}}^{-1/2} & v_{2\mathtt{q}}^{-1/2} & \cdots & v_{\mathtt{q}N}^{-1/2} \end{bmatrix}. \qquad (\Sigma)$$

The maximum likelihood estimator for the parameters P_0 and L_0 in (EIV$_0$) under assumptions (A$_1$–A$_5$), with known parameters $\mathtt{m}$, v, S, and δ, is given by the following optimization problem:

$$\begin{array}{llll} \text{minimize} \quad \text{over } P', L', \text{and } \widehat{D} & \|D-\widehat{D}\|_{\Sigma}^2 & \text{(cost function)} & (\mathrm{C}_0) \\ \text{subject to} & \widehat{D} = CP & \text{(rank constraint)} & \\ & P = \begin{bmatrix} I_{\mathtt{m}} \\ P' \end{bmatrix} & \text{(normalization of } P) & (\mathrm{C}_1) \\ & S\operatorname{vec}(P') = 0 & \text{(zero elements of } P') & (\mathrm{C}_2) \\ & L = \mathbf{1}_l^\top \otimes L' & \text{(periodicity of } L) & (\mathrm{C}_3) \\ & L' \geq 0 & \text{(nonnegativity of } L) & (\mathrm{C}_4) \\ & \|L'\mathbf{D}\|_{\mathrm{F}}^2 \leq \delta & \text{(smoothness of } L) & (\mathrm{C}_5) \end{array}$$

The rank and measurement errors assumptions in the model (EIV$_0$) imply the weighted low-rank approximation nature of the estimation problem (C$_0$–C$_5$) with weight matrix given by (Σ). Furthermore, the assumptions (A_1–A_5) about the true data matrix D_0 correspond to the constraints (C_1–C_5) in the estimation problem.

Computational algorithm

Algorithm 6 Alternating projections algorithm for solving problem (C_0–C_5).

```
• Find an initial approximation $(P'^{(0)}, L'^{(0)})$.
• For $k = 0, 1, \dots$ till convergence do
    1. $P'^{(k+1)} := \arg\min_{P'} \|D - PL\|_\Sigma^2$  subject to  ($C_1$–$C_2$) with $L' = L'^{(k)}$
    2. $L'^{(k+1)} := \arg\min_{L'} \|D - PL\|_\Sigma^2$  subject to  ($C_3$–$C_5$) with $P' = P'^{(k+1)}$
```

The alternating projections algorithm, see Algorithm 6, is based on the observation that the cost function (C_0) is quadratic and the constraints (C_1–C_5) are linear in either P or L. Therefore, for a fixed value of P, (C_0–C_5) is a nonnegativity constrained least squares problem in L and vice verse, for a fixed value of L, (C_0–C_5) is a constrained least squares problem in P. These problems correspond to, respectively, steps 1 and 2 of the algorithm. Geometrically they are projections. In the unweighted (*i.e.*, $\Sigma = \mathbf{1}_{\mathtt{q}}\mathbf{1}_N^\top$) and unconstrained case, the problem on step 1 is the orthogonal projection

$$\widehat{D} = DL^\top (LL^\top)^{-1} L^\top = D\Pi_L$$

of the row of D on the span of the rows of L, and problem on step 2 is the orthogonal projection

$$\widehat{D} = P(P^\top P)^{-1} P^\top D = \Pi_P D$$

of the columns of D on the span of the column of P. The algorithm iterates the two projections.

Note 5.16 (Rank deficient factors P and L). If the factor L is rank deficient, the indicated inverse in the computation of the projected matrix P^* does not exist. (This happens when the rank of the approximation $\widehat{D}$ if less than $\mathtt{m}$.) The projection P^*, however, is still well defined by the optimization problem on step 1 of the algorithm and can be computed in closed form by replacing the inverse with the pseudo inverses. The same is true when the factor L is rank deficient.

Theorem 5.17. *Algorithm 6 is globally and monotonically convergent in the $\|\cdot\|_\Sigma$ norm,* i.e., *if*

$$\widehat{D}^{(k)} := P^{(k)} L^{(k)}$$

is the approximation on the kth step of the algorithm, then

$$f(k) := \|D - \widehat{D}^{(k)}\|_\Sigma^2 \to f^*, \qquad \text{as } k \to \infty. \tag{$f(k) \to f^*$}$$

Assuming that there exists a solution to the problem (C_0–C_5) and any (locally optimal) solution is unique (i.e., *it is a strict minimum), the sequences $\widehat{D}^{(k)}$, $P^{(k)}$, and $L^{(k)}$ converge element-wise,* i.e.,

$$\widehat{D}^{(k)} \to D^*, \quad P^{(k)} \to P^*, \quad \text{and} \quad L^{(k)} \to L^*, \qquad \text{as } k \to \infty, \tag{$D^{(k)} \to D^*$}$$

where $\widehat{D}^* := P^* L^*$ is a (locally optimal) solution of (C_0–C_5).

The proof is given in Appendix B.

Simulation results

In this section, we show empirically that exploiting prior knowledge ((Σ) and assumptions (A_1–A_5)) improves the performance of the estimator. The data matrix D is generated according to the errors-in-variables model (EIV_0) with parameters $N = 100$, $\mathtt{q} = 6$, and $\mathtt{m} = 2$. The true low rank matrix $D_0 = P_0 L_0$ is random and the parameters P_0 and L_0 are normalized according to assumption (A_1) (so that they are unique). For the purpose of validating the algorithm, the element $p_{0,\mathtt{q}N}$ is set to zero but this prior knowledge is not used in the parameter estimation.

The estimation algorithm is applied on $M = 100$ independent noise realizations of the data D. The estimated parameters on the ith repetition are denoted by $P^{(i)}$, $L^{(i)}$ and $\widehat{D}^{(i)} := P^{(i)} L^{(i)}$. The performance of the estimator is measured by the following average relative estimation errors:

$$e_D = \frac{1}{M}\sum_{i=1}^{M} \frac{\|D_0 - \widehat{D}^{(i)}\|_F^2}{\|D_0\|_F^2}, \qquad e_P = \frac{1}{M}\sum_{i=1}^{M} \frac{\|P_0 - P^{(i)}\|_F^2}{\|P_0\|_F^2},$$

$$e_L = \frac{1}{M}\sum_{i=1}^{M} \frac{\|L_0 - L^{(i)}\|_F^2}{\|L_0\|_F^2}, \quad \text{and} \quad e_z = \frac{1}{M}\sum_{i=1}^{M} |p_{\mathtt{q}N}^{(i)}|.$$

For comparison the estimation errors are reported for the low-rank approximation algorithm, using only the normalization constraint (A_1), as well as for the proposed algorithm, exploiting the available prior knowledge. The difference between the two estimation errors is an indication of how important is the prior knowledge in the estimation.

Lack of prior knowledge is reflected by specific choice of the simulation parameters as follows:

homogeneous errors	$\leftrightarrow$	$\Sigma = \mathtt{ones(q,N)}$
no periodicity	$\leftrightarrow$	$l = 1$
no zeros in P'	$\leftrightarrow$	$S = [\,]$
no sign constraint on L'	$\leftrightarrow$	$\mathtt{nonneg} = 0$

We perform the following experiments: which test individually the effect of (Σ), assumptions (A_2), (A_3), (A_4), and their combined effect on the estimation error.

Σ	l	$S = [\,]$	`nonneg`
`rand`(q, N)	1	yes	0
`ones`(q, N)	3	yes	0
`ones`(q, N)	1	no	0
`ones`(q, N)	1	yes	1
`rand`(q, N)	3	no	1

Figures 5.3–5.7 show the average relative estimation errors (solid line is the estimator that exploits prior knowledge and dashed line is the estimator that does not exploit prior knowledge) versus the measurement noise standard deviation σ, for the five experiments. The vertical bars on the plots visualize the standard deviation of the estimates. The results indicate that main factors for the improved performance of the estimator are:

1. assumption (A_3) — known zeros in the P_0' and
2. (Σ) — known covariance structure of the measurement noise.

Files reproducing the numerical results and figures presented are available from the book's web page.

Implementation of Algorithm 6

Initial approximation

For initial approximation $(P'^{(0)}, L'^{(0)})$ we choose the normalized factors of a rank revealing factorization of the solution $\widehat{D}$ of (5.2). Let

$$D = U\Sigma V^{\top}$$

be the singular value decomposition of D and define the partitioning

$$U =: \begin{array}{cc} \mathtt{m} & \mathtt{q}-\mathtt{m} \\ \big[U_1 & U_2\big] \end{array}, \quad \Sigma =: \begin{array}{ccc} \mathtt{m} & \mathtt{q}-\mathtt{m} & \\ \Sigma_1 & 0 & \mathtt{m} \\ 0 & \Sigma_2 & \mathtt{q}-\mathtt{m} \end{array}, \quad V =: \begin{array}{cc} \mathtt{m} & N-\mathtt{m} \\ \big[V_1 & V_2\big] \end{array}.$$

Furthermore, let

$$\begin{bmatrix} U_{11} \\ U_{21} \end{bmatrix} := U, \qquad \text{with} \quad U_{11} \in \mathbb{R}^{\mathtt{m}\times\mathtt{m}}.$$

Then

$$P'^{(0)} := U_{21}U_{11}^{-1} \qquad \text{and} \qquad L^{(0)} := U_{11}\Sigma V^{\top}$$

define the Frobenius-norm optimal unweighted and unconstrained low-rank approximation

$$\widehat{D}^{(0)} := \begin{bmatrix} I \\ P'^{(0)} \end{bmatrix} L^{(0)}.$$

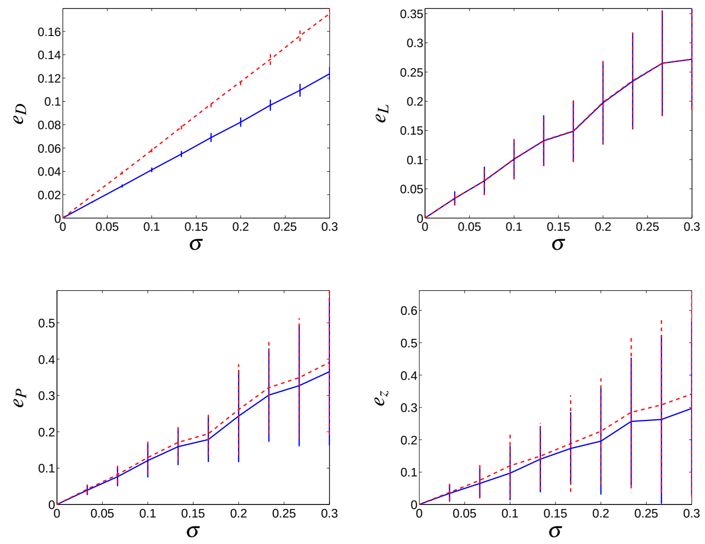

Fig. 5.3 Effect of weighting (solid line — exploiting prior knowledge, dashed line — without exploiting prior knowledge, vertical bars — standard deviations).

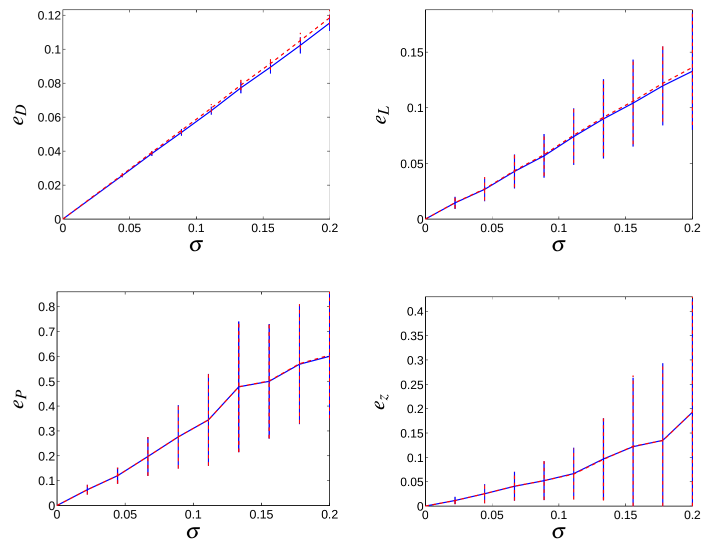

Fig. 5.4 Effect of periodicity of L (solid line — exploiting prior knowledge, dashed line — without exploiting prior knowledge, vertical bars — standard deviations).

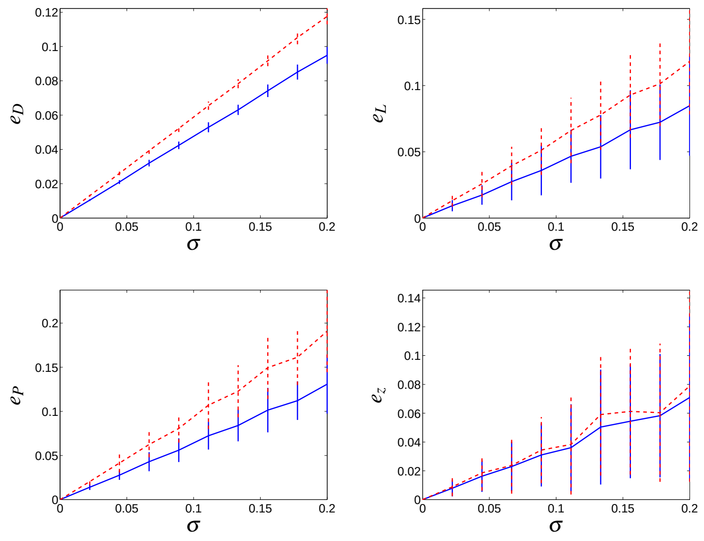

Fig. 5.5 Effect of zero elements in P (solid line — exploiting prior knowledge, dashed line — without exploiting prior knowledge, vertical bars — standard deviations).

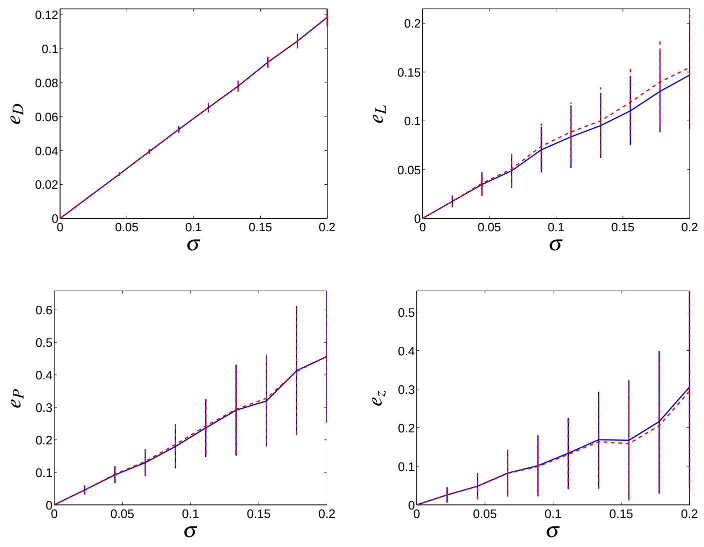

Fig. 5.6 Effect of nonnegativity of L (solid line — exploiting prior knowledge, dashed line — without exploiting prior knowledge, vertical bars — standard deviations).

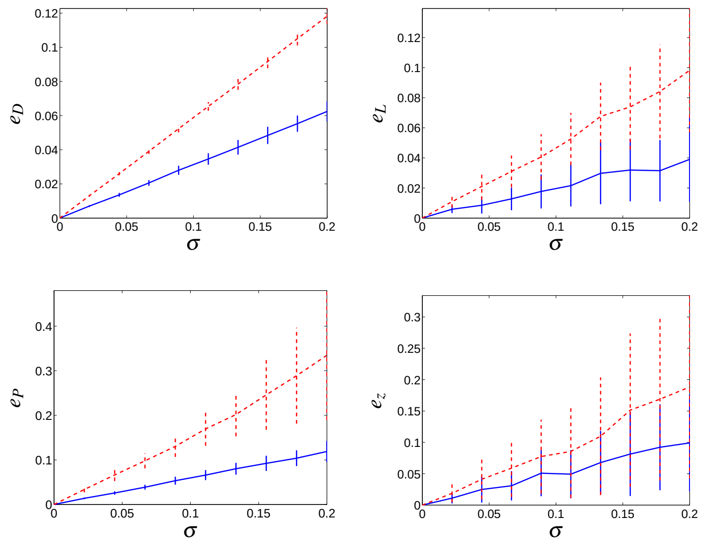

Fig. 5.7 Effect of weighting, periodicity, and nonnegativity of L, and zero elements in P (solid line — exploiting prior knowledge, dashed line — without exploiting prior knowledge, vertical bars — standard deviations).

More sophisticated choices for the initial approximation that take into account the weight matrix Σ are described in Section 2.4.

Separable least squares problem for P

In the weighted case, the projection on step 1 of the algorithm is computed separately for each row p^i of P. Let d^i be the ith row of D and w^i be the ith row of Σ. The problem

$$\text{minimize} \quad \text{over } P \quad \|D - PL\|_\Sigma^2 \quad \text{subject to} \quad (\text{C}_1\text{–C}_2)$$

is equivalent to the problem

$$\begin{aligned} &\text{minimize} \quad \text{over } p^i \quad \|(d^i - p^i L)\,\text{diag}(w^i)\|_2^2 \\ &\text{subject to} \quad (\text{C}_1\text{–C}_2), \quad \text{for } i = 1, \dots, \mathtt{m}. \end{aligned} \tag{$*$}$$

The projection on step 2 of the algorithm is not separable due to constraint (C_5).

Taking into account constraint (C$_1$)

Since the first $\mathtt{m}$ rows of P are fixed, we do not solve $(*)$ for $i = 1, \dots, \mathtt{m}$, but define

$$p^i := e_i^\top, \qquad \text{for} \quad i = 1, \dots, \mathtt{m},$$

where e_i is the ith unit vector (the ith column of the identity matrix $I_\mathtt{m}$).

Taking into account constraint (C$_2$)

Let S_i be a selector matrix for the zeros in the ith row of P

$$S\operatorname{vec}(P') = 0 \quad \iff \quad p^i S_i = 0, \quad \text{for } i = \mathtt{m}+1, \dots, \mathtt{q}.$$

(If there are no zeros in the ith row, then S_i is skipped.) The ith problem in $(*)$ becomes

$$\text{minimize} \quad \text{over } p^i \qquad \|(d^i - p^i L)\operatorname{diag}(w^i)\|_2^2 \quad \text{subject to} \quad p^i S_i = 0. \qquad (**)$$

Let the rows of the matrix N_i form a basis for the left null space of S_i. Then $p^i S_i = 0$ if and only if $p^i = z_i N_i$, for certain z_i, and problem $(**)$ becomes

$$\text{minimize} \quad \text{over } z_i \quad \|(d^i - z_i N_i L)\operatorname{diag}(w^i)\|_2^2.$$

Therefore, the solution of $(*)$ is

$$p^{i,*} = d^i L^\top N_i^\top (N_i L L^\top N_i^\top)^{-1} N_i.$$

Note 5.18. It is not necessary to explicitly construct the matrices S_i and compute basis N_i for their left null spaces. Since S_i is a selector matrix, it is a submatrix of the identity matrix $I_\mathtt{m}$. The rows of the complementary submatrix of $I_\mathtt{m}$ form a basis for the left null space of S_i. This particular matrix N_i is also a selector matrix, so that the product $N_i L$ need not be computed explicitly.

Taking into account constraint (C$_3$)

We have,

$$\begin{aligned} D - PL &= D - P(\mathbf{1}_l^\top \otimes L') = \begin{bmatrix} D_1 & \cdots & D_l \end{bmatrix} - P \begin{bmatrix} L' & \cdots & L' \end{bmatrix} \\ &= \begin{bmatrix} D_1 \\ \vdots \\ D_l \end{bmatrix} - \begin{bmatrix} P \\ \vdots \\ P \end{bmatrix} L' =: D' - \underbrace{(\mathbf{1}_l \otimes P)}_{P'} L' = D' - P'L'. \end{aligned}$$

Let

$$\Sigma' := \begin{bmatrix} \Sigma_1 \\ \vdots \\ \Sigma_l \end{bmatrix}, \qquad \text{where } \Sigma =: \begin{bmatrix} \Sigma_1 & \cdots & \Sigma_N \end{bmatrix}.$$

Then the problem

$$\text{minimize} \quad \text{over } L \quad \|D - PL\|_\Sigma^2 \quad \text{subject to} \quad (\text{C}_3\text{–C}_5)$$

is equivalent to the problem

$$\text{minimize} \quad \text{over } L' \quad \|D' - P'L'\|_{\Sigma'}^2 \quad \text{subject to} \quad (\text{C}_4\text{–C}_5).$$

Taking into account constraint (C$_4$)

Adding the nonnegativity constraint changes the least squares problem to a nonnegative least squares problem, which is a standard convex optimization problem for which robust and efficient methods and software exist.

Taking into account constraint (C$_5$)

The problem

$$\text{minimize} \quad \text{over } L \quad \|D - PL\|_\Sigma^2 \quad \text{subject to} \quad \|L\mathbf{D}\|_\text{F}^2 \le \delta$$

is equivalent to a regularized least squares problem

$$\text{minimize} \quad \text{over } L \qquad \|D - PL\|_\Sigma^2 + \gamma \|L\mathbf{D}\|_\text{F}^2$$

for certain regularization parameter γ. The latter problem is equivalent to the standard least squares problem

$$\text{minimize} \quad \text{over } L \quad \left\| \begin{bmatrix} \operatorname{diag}\big(\operatorname{vec}(\Sigma)\big)\operatorname{vec}(D) \\ 0 \end{bmatrix} - \begin{bmatrix} \operatorname{diag}\big(\operatorname{vec}(\Sigma)\big)(I \otimes P) \\ \sqrt{\gamma}(\mathbf{D}^\top \otimes I) \end{bmatrix} \operatorname{vec}(L) \right\|_2^2.$$

Stopping criteria

The iteration is terminated when the following stopping criteria are satisfied

$$\begin{aligned} \|P^{(k+1)}L^{(k+1)} - P^{(k)}L^{(k)}\|_\Sigma / \|P^{(k+1)}L^{(k+1)}\|_\Sigma &< \varepsilon_D, \\ \|(P^{(k+1)} - P^{(k)})L^{(k+1)}\|_\Sigma / \|P^{(k+1)}L^{(k+1)}\|_\Sigma &< \varepsilon_P, \text{ and} \\ \|L^{(k+1)}(L^{(k+1)} - L^{(k)})\|_\Sigma / \|P^{(k+1)}L^{(k+1)}\|_\Sigma &< \varepsilon_L. \end{aligned}$$

Here ε_D, ε_P, and ε_L are user defined relative convergence tolerances for D, P, and L, respectively.

5.5 Notes and references

Missing data

Optimization methods for solving weighted low-rank approximation problems with nonsingular weight matrix have been considered in the literature under different names:

- criss-cross multiple regression (Gabriel and Zamir, 1979),
- Riemannian singular value decomposition (De Moor, 1993),
- maximum likelihood principal component analysis (Wentzell et al, 1997),
- weighted low-rank approximation (Manton et al, 2003), and
- weighted low-rank approximation (Markovsky et al, 2005).

Gabriel and Zamir (1979) consider an element-wise weighted low-rank approximation problem with diagonal weight matrix W, and propose an iterative solution method. Their method, however, does not necessarily converge to a minimum point, see the discussion in (Gabriel and Zamir, 1979, Section 6, page 491). Gabriel and Zamir (1979)) proposed an alternating projections algorithm for the case of unweighted approximation with missing values, *i.e.*, $w_{ij} \in \{0,1\}$. Their method was further generalized by Srebro (2004) for arbitrary weights.

The Riemannian singular value decomposition framework of De Moor (1993) includes the weighted low-rank approximation problem with rank specification $r = \min(m,n) - 1$ and a diagonal weight matrix W as a special case. In (De Moor, 1993), an algorithm resembling the inverse power iteration algorithm is proposed. The method, however, has no proven convergence properties.

Manton et al (2003) treat the problem as an optimization over a Grassman manifold and propose steepest decent and Newton type algorithms. The least squares nature of the problem is not exploited in this work and the proposed algorithms are not globally convergent.

The maximum likelihood principal component analysis method of Wentzell et al (1997) is developed for applications in chemometrics, see also (Schuermans et al, 2005). This method is an alternating projections algorithm. It applies to the general weighted low-rank approximation problems and is globally convergent. The convergence rate, however, is linear and the method could be rather slow when the $r+1$st and the rth singular values of the data matrix D are close to each other. In the unweighted case this situation corresponds to lack of uniqueness of the solution, *cf.*, Theorem 2.23. The convergence properties of alternating projections algorithms are studied in (Kiers, 2002; Krijnen, 2006)

An implementation of the singular value thresholding method in MATLAB is available at `http://svt.caltech.edu/` Practical methods for solving the recommender system problem are given in (Segaran, 2007). The MovieLens data set is available from (GroupLens, 2009).

Nonnegative low-rank approximation

The notation $D \geq 0$ is used for a matrix $D \in \mathbb{R}^{\mathtt{q}\times N}$ whose elements are nonnegative. A low-rank approximation problem with element-wise nonnegativity constraint

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{D} \quad \|D-\widehat{D}\| \\ &\text{subject to} && \operatorname{rank}(\widehat{D}) \leq \mathtt{m} \quad \text{and} \quad \widehat{D} \geq 0 \end{aligned} \tag{NNLRA}$$

arises in Markov chains (Vanluyten et al, 2006) and image mining (Lee and Seung, 1999). Using the image representation, we obtain the following problem

$$\begin{aligned} &\text{minimize} && \text{over } \widehat{D},\, P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}, \text{ and } L \in \mathbb{R}^{\mathtt{m}\times N} \quad \|D-\widehat{D}\| \\ &\text{subject to} && \widehat{D} = PL \quad \text{and} \quad P, L \geq 0, \end{aligned} \tag{NNLRA$_P$}$$

which is a relaxation of problem (NNLRA). The minimal $\mathtt{m}$, for which (NNLRA$_P$) has a solution, is called the *positive rank* of $\widehat{D}$ (Berman and Shaked-Monderer, 2003). In general, the positive rank is less than or equal to the rank.

Note that due to the nonnegativity constraint on $\widehat{D}$, the problem can not be solved using the variable projections method. (There is no closed form solution for the equivalent problem with $\widehat{D}$ eliminated.) The alternating projections algorithm, however, can be used almost without modification for the solution of the relaxed problem (NNLRA$_P$). Let the norm $\|\cdot\|$ in (NNLRA) be the Frobenius norm. (In the context of Markov chains more adequate is the choice of the Kullback–Leibler divergence as a distance measure between D and $\widehat{D}$.) Then at each iteration step of the algorithm two least squares problems with nonnegativity constraint (*i.e.*, standard optimization problems) are solved. The resulting alternating least squares algorithm is Algorithm 7.

Algorithm 7 Alternating projections algorithm for nonnegative low-rank approximation

```
Input: Data matrix $D$, desired rank $\mathtt{m}$, and convergence tolerance $\varepsilon$.
1: Set $k := 0$ and compute an initial approximation $\widehat{D}^{(0)} := P^{(0)}L^{(0)}$ from the singular value de-
   composition by setting all negative elements to zero.
2: repeat
3:     $k := k+1$.
4:     Solve: $L^{(k)} := \arg\min_L \|D - P^{(k-1)}L\|$ subject to $L \geq 0$.
5:     Solve: $P^{(k)} := \arg\min_P \|D - PL^{(k)}\|$ subject to $P \geq 0$.
6: until $\|P^{(k-1)}L^{(k-1)} - P^{(k)}L^{(k)}\| < \varepsilon$
Output: A locally optimal solution $\widehat{D}^* := P^{(k)}L^{(k)}$ to problem (NNLRA$_P$).
```

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Chapter 6
Nonlinear static data modeling

Summary: Algebraic and geometric data fitting problems for a model class of affine varieties with bounded complexity (dimension and degree) are equivalent to low-rank approximation of a polynomially structured matrix constructed from the data. In algebraic fitting problems, the approximating matrix is unstructured and the corresponding low-rank approximation problem can be solved analytically by the singular value decomposition. In geometric fitting problems, the approximating matrix is polynomially structured and, except for the case of an affine model class, no analytic solution is know. The equivalence of nonlinear data modeling and low-rank approximation unifies existing curve fitting methods, showing that algebraic fitting is a relaxation of geometric fitting, obtained by removing the structure constraint, and reveals new solution approaches.

6.1 A framework for nonlinear static data modeling

Introduction

Identifying a curve in a set of curves that best fits given data points is a common problem in computer vision, statistics, and coordinate metrology. More abstractly, approximation by Fourier series, wavelets, splines, and sum-of-exponentials are also curve fitting problems. In the applications, the fitted curve is a model for the data and, correspondingly, the set of candidate curves is a model class.

Data modeling problems are specified by choosing a model class and a fitting criterion. The fitting criterion is maximisation of a measure for fit between the data and a model. Equivalently, the criterion can be formulated as minimization of a measure for lack of fit (misfit) between the data and a model. Data modeling problems can be classified according to the type of model and the type of fitting criterion as follows:

- linear/affine vs nonlinear model class,
- algebraic vs geometric fitting criterion.

A model is a subset of the data space. The model is linear/affine if it is a subspace/affine set. Otherwise, it is nonlinear. A geometric fitting criterion minimises the sum-of-squares of the Euclidean distances from the data points to a model. An algebraic fitting criterion minimises an equation error (residual) in a representation of the model. In general, the algebraic fitting criterion has no simple geometric interpretation. Problems using linear model classes and algebraic criteria are easier to solve numerically than problems using nonlinear model classes and geometric criteria.

In this chapter, a nonlinear model class of bounded complexity, consisting of affine varieties, *i.e.*, kernels of systems of multivariable polynomials is considered. The complexity of an affine variety is defined as the pair of the variety's dimension and the degree of its polynomial representation. In Section 6.2, an equivalence is established between the data modeling problem and low-rank approximation of a polynomially structured matrix constructed from the data. Algorithms for solving nonlinearly structured low-rank approximation problems are presented in Section 6.3. As illustrated in Section 6.4, the low-rank approximation setting makes possible to use a single algorithm and a piece of software for solving a wide variety of curve fitting problems.

Data, model class, and model complexity

We consider static multivariate modeling problems. The to-be-modelled data $\mathscr{D}$ is a set of N observations (also called data points)

$$\mathscr{D} = \{ d_1, \dots, d_N \} \subset \mathbb{R}^{\mathtt{q}}.$$

The observations $d_1, \dots, d_N$ are real $\mathtt{q}$-dimensional vectors. A model for the data $\mathscr{D}$ is a subset of the data space $\mathbb{R}^{\mathtt{q}}$ and a model class $\mathscr{M}^{\mathtt{q}}$ for $\mathscr{D}$ is a set of subsets of the data space $\mathbb{R}^{\mathtt{q}}$, *i.e.*, $\mathscr{M}^{\mathtt{q}}$ is an element of the powerset $2^{\mathbb{R}^{\mathtt{q}}}$. For example, the linear model class in $\mathbb{R}^{\mathtt{q}}$ consists of the subspaces of $\mathbb{R}^{\mathtt{q}}$. An example of a nonlinear model class in $\mathbb{R}^2$ is the set of the conic sections. When the dimension $\mathtt{q}$ of the data space is understood from the context, it is skipped from the notation of the model class.

In nonlinear data modeling problems, the model is usually represented by a function $y = f(u)$, where $d = \Pi \operatorname{col}(u, y)$, with Π a permutation matrix. The corresponding statistical estimation problem is regression. As in the linear case, we call the functional relation $y = f(u)$ among the variables u and y, an input/output representation of the model

$$\mathscr{B} = \{ \Pi \operatorname{col}(u, y) \mid y = f(u) \} \tag{I/O}$$

that this relation defines. The input/output representation $y = f(u)$ implies that the variables u are inputs and the variables y are outputs of the model $\mathscr{B}$.

Input-output representations are appealing because they are *explicit functions*, mapping some variables (inputs) to other variables (outputs) and thus display a causal relation among the variables (the inputs cause the outputs). The alternative kernel representation

$$\mathscr{B} = \ker(R) := \{\, d \in \mathbb{R}^{\mathtt{q}} \mid R(d) = 0 \,\} \tag{KER}$$

defines the model via an *implicit function* $R(d) = 0$, which does not a priori bound one set of variables as a cause and another set of variables as an effect.

A priori fixed causal relation, imposed on the model by an input/output representation, is restrictive. Consider, for example, data fitting by a model that is a conic section. Only parabolas and lines can be represented by functions. Hyperbolas, ellipses, and the vertical line $\{\,(u,y) \mid u = 0\,\}$ are not graphs of a function $y = f(u)$ and therefore can not be modeled by an input/output representation.

The complexity of a linear static model $\mathscr{B}$ is defined as the dimension of $\mathscr{B}$, *i.e.*, the smallest number $\mathtt{m}$, such that there is a linear function $P : \mathbb{R}^{\mathtt{m}} \to \mathbb{R}^{\mathtt{q}}$, for which

$$\mathscr{B} = \operatorname{image}(P) := \{\, P(\ell) \mid \ell \in \mathbb{R}^{\mathtt{m}} \,\}. \tag{IMAGE}$$

Similarly, the dimension of a nonlinear model $\mathscr{B}$ is defined as the smallest natural number $\mathtt{m}$, such that there is a (possibly nonlinear) function $P : \mathbb{R}^{\mathtt{m}} \to \mathbb{R}^{\mathtt{q}}$, for which (IMAGE) holds. In the context of nonlinear models, however, the model dimension alone is not sufficient to define the model complexity. For example, in $\mathbb{R}^2$ both a linear model (a line passing through the origin) and an ellipse have dimension equal to one, however, it is intuitively clear that the ellipse is a more "complex" model than the line.

The missing element in the definition of the model complexity in the nonlinear case is the "complexity" of the function P. In what follows, we restrict to models that can be represented as kernels of polynomial functions, *i.e.*, we consider models that are *affine varieties*. Complexity of an affine variety (IMAGE) is defined as the pair $(\mathtt{m},\mathtt{d})$, where $\mathtt{m}$ is the dimension of $\mathscr{B}$ and $\mathtt{d}$ is the degree of R. This definition allows us to distinguish a linear or affine model ($\mathtt{d} = 1$) from a nonlinear model ($\mathtt{d} > 1$) with the same dimension. For a model $\mathscr{B}$ with complexity $(\mathtt{m},\mathtt{d})$, we call $\mathtt{d}$ the degree of $\mathscr{B}$.

The complexity of a model class is the maximal complexity (in a lexicographic ordering of the pairs $(\mathtt{m},\mathtt{d})$) over all models in the class. The model class of complexity bounded by $(\mathtt{m},\mathtt{d})$ is denoted by $\mathscr{P}_{\mathtt{m},\mathtt{d}}$.

Special cases

The model class $\mathscr{P}^{\mathtt{q}}_{\mathtt{m},\mathtt{d}}$ and the related exact and approximate modeling problems (EM) and (AM) have as an important special case the linear model class and linear data modeling problems.

1. *Linear/affine model class of bounded complexity.* An affine model $\mathscr{B}$ (*i.e.*, an affine set in $\mathbb{R}^{\mathtt{q}}$) is an affine variety, defined by a first order polynomial through kernel or image representation. The dimension of the affine variety coincides

with the dimension of the affine set. Therefore, $\mathscr{P}^{\mathtt{q}}_{\mathtt{m},1}$ is an affine model class in $\mathbb{R}^{\mathtt{q}}$ with complexity bounded by $\mathtt{m}$. The linear model class in $\mathbb{R}^{\mathtt{q}}$, with dimension bounded by $\mathtt{m}$, is a subset $\mathscr{L}^{\mathtt{q}}_{\mathtt{m},0}$ of $\mathscr{P}^{\mathtt{q}}_{\mathtt{m},1}$.
2. *Geometric fitting by a linear model.* Approximate data modeling using the linear model class $\mathscr{L}^{\mathtt{q}}_{\mathtt{m}}$ and the geometric fitting criterion (dist) is a low-rank approximation problem

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{\mathscr{D}} \quad \big\|\Phi(\mathscr{D}) - \Phi(\widehat{\mathscr{D}})\big\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank}\big(\Phi(\widehat{\mathscr{D}})\big) \le \mathtt{m}, \end{array} \tag{LRA}$$

where

$$\Phi(\mathscr{D}) := \begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix}.$$

The rank constraint in (LRA) is equivalent to the constraint that the data $\widehat{\mathscr{D}}$ is exact for a linear model of dimension bounded by $\mathtt{m}$. This justifies the statement that exact modeling is an ingredient of approximate modeling.
3. *Algebraic curves.* In the special case of a curve in the plane, we use the notation

$$x := \text{first component } d_{1\cdot} \text{ of } d \quad \text{and} \quad y := \text{second component } d_{2\cdot} \text{ of } d.$$

Note that $w = \operatorname{col}(x,y)$ is not necessarily an input/output partitioning of the variables. An affine variety of dimension one is called an algebraic curve.
A second order algebraic curve

$$\mathscr{B} = \{\, d = \operatorname{col}(x,y) \mid d^\top A d + b^\top d + c = 0 \,\},$$

where $A = A^\top$, b, and c are parameters, is a conic section. Examples of 3rd order algebraic curves, see Figure 6.1, are the cissoid

$$\mathscr{B} = \{\, \operatorname{col}(x,y) \mid y^2(1+x) - (1-x)^3 = 0 \,\},$$

and the folium of Descartes

$$\mathscr{B} = \{\, \operatorname{col}(x,y) \mid x^3 + y^3 - 3xy = 0 \,\},$$

Examples of 4rd order algebraic curves, see Figure 6.2, are the eight curve

$$\mathscr{B} = \{\, \operatorname{col}(x,y) \mid y^2 - x^2 + x^4 = 0 \,\}$$

and the limacon of Pascal

$$\mathscr{B} = \{\, \operatorname{col}(x,y) \mid y^2 + x^2 - (4x^2 - 2x + 4y^2)^2 = 0 \,\},$$

The four-leaved rose, see Figure 6.3,

$$\mathscr{B} = \{\, \operatorname{col}(x,y) \mid (x^2 + y^2)^3 - 4x^2y^2 = 0 \,\}$$

is a sixth order algebraic curve.

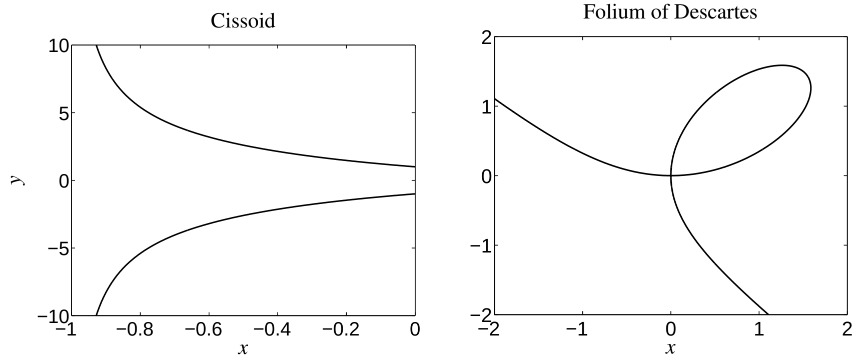


Fig. 6.1 Examples of algebraic curves of 3rd order.

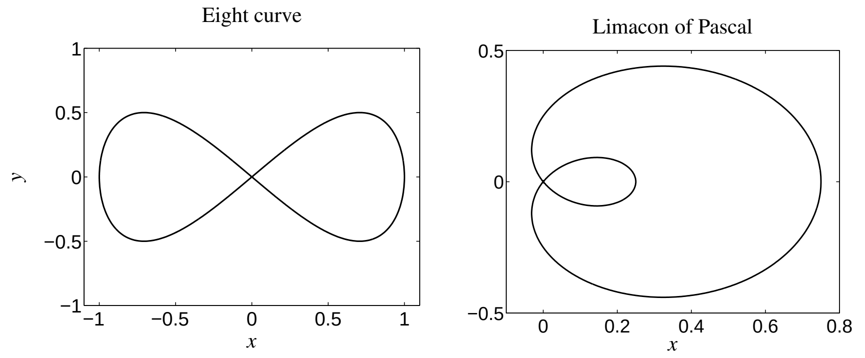


Fig. 6.2 Examples of algebraic curves of 4th order.

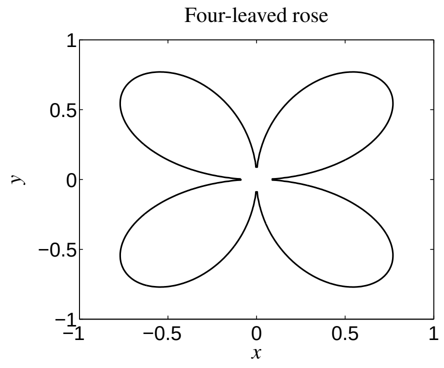


Fig. 6.3 Example of an algebraic curve of 6th order.

6.2 Nonlinear low-rank approximation

Parametrisation of the kernel representations

Consider a kernel representation (KER) of an affine variety $\mathscr{B} \in \mathscr{P}^{\mathtt{q}}_{\mathtt{m},\mathtt{d}}$, parametrized by a $\mathtt{p} \times 1$ multivariable polynomial R. The number of monomials in $\mathtt{q}$ variables with degree $\mathtt{d}$ or less is

$$\mathtt{q}_{\text{ext}} := \binom{\mathtt{q}+\mathtt{d}}{\mathtt{d}} = \frac{(\mathtt{q}+\mathtt{d})!}{\mathtt{d}!\mathtt{q}!}. \qquad (\mathtt{q}_{\text{ext}})$$

Define the vector of all such monomials

$$\phi(d) := \begin{bmatrix} \phi_1(d) & \cdots & \phi_{\mathtt{q}_{\text{ext}}}(d) \end{bmatrix}^\top.$$

The polynomial R can be written as

$$R_\Theta(d) = \sum_{k=1}^{\mathtt{q}_{\text{ext}}} \Theta_k \phi_k(d) = \Theta\phi(d), \qquad (R_\Theta)$$

where Θ is an $\mathtt{p} \times \mathtt{q}_{\text{ext}}$ parameter matrix.

In what follows, we assume that the monomials are ordered in $\phi(d)$ in decreasing degree according to the lexicographic ordering (with alphabet the indexes of d). For example, with $\mathtt{q} = 2$, $\mathtt{d} = 2$, and $d = \operatorname{col}(x,y)$,

$$\mathtt{q}_{\text{ext}} = 6 \qquad \text{and} \qquad \begin{aligned} \phi^\top(x,y) &= [\,\phi_1 \ \phi_2 \ \phi_3 \ \phi_4 \ \phi_5 \ \phi_6\,] \\ &= [\,x^2 \ xy \ x \ y^2 \ y \ 1\,] \end{aligned}$$

In general,

$$\phi_k(d) = d_{1\cdot}^{\mathtt{d}_{k1}} \cdots d_{\mathtt{q}\cdot}^{\mathtt{d}_{k\mathtt{q}}}, \qquad \text{for} \quad k = 1,\ldots,\mathtt{q}_{\text{ext}}, \qquad (\phi_k)$$

where

- $d_{1\cdot},\ldots,d_{\mathtt{q}\cdot} \in \mathbb{R}$ are the elements of $d \in \mathbb{R}^{\mathtt{q}}$, and
- $\mathtt{d}_{ki} \in \mathbb{Z}_+$, is the degree of the ith element of d in the kth monomial ϕ_k.

The matrix formed from the degrees $\mathtt{d}_{ki}$

$$\mathtt{D} = \begin{bmatrix} \mathtt{d}_{ki} \end{bmatrix} \in \mathbb{R}^{\mathtt{q}_{\text{ext}} \times \mathtt{q}}$$

uniquely defines the vector of monomials ϕ. The degrees matrix $\mathtt{D}$ depends only on the number of variables $\mathtt{q}$ and the degree $\mathtt{d}$. For example, with $\mathtt{q} = 2$ and $\mathtt{d} = 2$,

$$\mathtt{D}^\top = \begin{bmatrix} 2 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2 & 1 & 0 \end{bmatrix}.$$

The function `monomials` generates an implicit function `phi` that evaluates the 2-variate vector of monomials ϕ, with degree $\mathtt{d}$.

187a ⟨*Monomials constructor* 187a⟩≡ 187b▷

```
function [Deg, phi] = monomials(deg)
```

Defines:
`monomials`, used in chunks 192a and 194e.

First an extended degrees matrix $\mathtt{D}_{\text{ext}} \in \{0,1,\dots,\mathtt{d}\}^{(\mathtt{d}+1)^2\times 2}$, corresponding to all monomials $x^{\mathtt{d}_x}y^{\mathtt{d}_y}$ with degrees at most $\mathtt{d}$, is generated. It can be verified that

$$\mathtt{D}_{\text{ext}} = \begin{bmatrix} \mathbf{r}_{\mathtt{d}} \otimes \mathbf{1}_{\mathtt{d}+1} & \mathbf{1}_{\mathtt{d}+1} \otimes \mathbf{r}_{\mathtt{d}} \end{bmatrix}, \qquad \text{where} \quad \mathbf{r}_{\mathtt{d}} := \begin{bmatrix} 0 & 1 & \cdots & \mathtt{d} \end{bmatrix}^\top$$

is such a matrix; moreover, the monomials are ordered in decreasing degree.

187b ⟨*Monomials constructor* 187a⟩+≡ ◁187a 187c▷

```
Deg_ext = [kron([0:deg]', ones(deg + 1, 1)), ...
                  kron(ones(deg + 1, 1), [0:deg]')];
```

Then the rows of $\mathtt{D}_{\text{ext}}$ are scanned and those with degree less than or equal to $\mathtt{d}$ are selected to form a matrix $\mathtt{D}$.

187c ⟨*Monomials constructor* 187a⟩+≡ ◁187b

```
str = []; Deg = []; q = 2;
for i = 1:size(Deg_ext, 1)
    if (sum(Deg_ext(i, :)) <= deg)
        for k = q:-1:1,
            str = sprintf('.* d(%d,:) .^ %d %s', ...
                          k, Deg_ext(i, k), str);
        end
        str = sprintf('; %s', str(4:end));
        Deg = [Deg_ext(i, :); Deg];
    end
end
eval(sprintf('phi = @(d) [%s];', str(2:end)))
```

Minimality of the kernel representation is equivalent to the condition that the parameter Θ is full row rank. The nonuniqueness of R_Θ corresponds to a nonuniqueness of Θ. The parameters Θ and $Q\Theta$, where Q is a nonsingular matrix, define the same model. Therefore, without loss of generality, we can assume that the representation is minimal and normalise it, so that

$$\Theta\Theta^\top = I_{\mathtt{p}}.$$

Note that a $\mathtt{p}\times \mathtt{q}_{\text{ext}}$ full row rank matrix Θ defines via (R_Θ) a polynomial matrix R_Θ, which defines a minimal kernel representation (KER) of a model $\mathscr{B}_\Theta$ in $\mathscr{P}^{\mathtt{q}}_{\mathtt{m},\mathtt{d}}$. Therefore, Θ defines a function

$$\mathscr{B}_\Theta : \mathbb{R}^{\mathtt{p}\times\mathtt{q}_{\text{ext}}} \to \mathscr{P}^{\mathtt{q}}_{\mathtt{m},\mathtt{d}}.$$

Vice verse, a model $\mathscr{B}$ in $\mathscr{P}^{\mathtt{q}}_{\mathtt{m},\mathtt{d}}$ corresponds to a (nonunique) $\mathtt{p}\times\mathtt{q}_{\text{ext}}$ full row rank matrix Θ, such that $\mathscr{B} = \mathscr{B}_\Theta$. For a given $\mathtt{q}$, there are one-to-one mappings

$$\mathtt{q}_{\text{ext}} \leftrightarrow \mathtt{d} \qquad \text{and} \qquad \mathtt{p} \leftrightarrow \mathtt{m},$$

defined by ($\mathtt{q}_{\text{ext}}$) and $\mathtt{p} = \mathtt{q} - \mathtt{m}$, respectively.

Main results

We show a relation of the approximate modeling problems (AM) and (EM) for the model class $\mathscr{P}_{\mathtt{m},\mathtt{d}}$ to low-rank approximation problems.

Proposition 6.1 (Algebraic fit $\iff$ unstructured low-rank approximation) *The algebraic fitting problem for the model class of affine varieties with bounded complexity $\mathscr{P}_{\mathtt{m},\mathtt{d}}$*

$$\begin{aligned} &\text{minimize} \quad \text{over } \Theta \in \mathbb{R}^{\mathtt{p}\times\mathtt{q}_{\text{ext}}} \quad \sqrt{\sum_{j=1}^{N} \big\|R_\Theta(d_j)\big\|_{\text{F}}^2} \\ &\text{subject to} \quad \Theta\Theta^\top = I_{\mathtt{p}} \end{aligned} \tag{AM$'_\Theta$}$$

is equivalent to the unstructured low-rank approximation problem

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{\Phi} \in \mathbb{R}^{\mathtt{q}\times\mathtt{p}} \quad \|\Phi_{\mathtt{d}}(\mathscr{D}) - \widehat{\Phi}\|_{\text{F}} \\ &\text{subject to} \quad \operatorname{rank}(\widehat{\Phi}) \leq \mathtt{q}_{\text{ext}} - \mathtt{p}. \end{aligned} \tag{LRA}$$

Proof. Using the polynomial representation (R_Θ), the squared cost function of (AM$'_\Theta$) can be rewritten as a quadratic form

$$\begin{aligned} \sum_{j=1}^{N} \big\|R_\Theta(d_j)\big\|_{\text{F}}^2 &= \big\|\Theta\Phi_{\mathtt{d}}(\mathscr{D})\big\|_{\text{F}}^2 \\ &= \operatorname{trace}\big(\Theta\Phi_{\mathtt{d}}(\mathscr{D})\Phi_{\mathtt{d}}^\top(\mathscr{D})\Theta^\top\big) = \operatorname{trace}\big(\Theta\Psi_{\mathtt{d}}(\mathscr{D})\Theta^\top\big). \end{aligned}$$

Therefore, the algebraic fitting problem is equivalent to an eigenvalue problem for $\Psi_{\mathtt{d}}(\mathscr{D})$ or, equivalently (see the Notes and References section of Chapter 2), to low-rank approximation problem for $\Phi_{\mathtt{d}}(\mathscr{D})$. □

Proposition 6.2 (Geometric fit $\iff$ polynomial structured low rank approx.) *The geometric fitting problem for the model class of affine varieties with bounded complexity $\mathscr{P}_{\mathtt{m},\mathtt{d}}$*

$$\text{minimize} \quad \text{over } \mathscr{B} \in \mathscr{P}_{\mathtt{m},\mathtt{d}} \quad \operatorname{dist}(\mathscr{D},\mathscr{B}) \tag{AM}$$

is equivalent to the polynomially structured low-rank approximation problem

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{D} \in \mathbb{R}^{\mathtt{q}\times N} \quad \|D - \widehat{D}\|_{\text{F}} \\ &\text{subject to} \quad \operatorname{rank}\big(\Phi_{\mathtt{d}}(\widehat{D})\big) \leq \mathtt{q}_{\text{ext}} - \mathtt{p}. \end{aligned} \tag{PSLRA}$$

Proof. Problem (AM) is equivalent to

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{\mathscr{D}} \text{ and } \mathscr{B} \quad \sqrt{\sum_{j=1}^{N} \|d_j - \widehat{d}_j\|_2^2} \\ &\text{subject to} \quad \widehat{\mathscr{D}} \subset \mathscr{B} \in \mathscr{P}_{\mathtt{m},\mathtt{d}}. \end{aligned} \qquad (*)$$

Using the condition

$$\widehat{\mathscr{D}} \subset \mathscr{B} \in \mathscr{P}_{\mathtt{m},\mathtt{d}} \quad \Longrightarrow \quad \operatorname{rank}\big(\Phi_{\mathtt{d}}(\widehat{\mathscr{D}})\big) \leq \mathtt{q}_{\text{ext}} - \mathtt{p} \qquad \text{(MPUM)}$$

to replace the constraint of $(*)$ with a rank constraint for the structured matrix $\Phi_{\mathtt{d}}(\widehat{\mathscr{D}}) = \Phi_{\mathtt{d}}(\widehat{D})$, this latter problem becomes a polynomially structured low-rank approximation problem (PSLRA). □

Propositions 6.1 and 6.2 show a relation between the algebraic and geometric fitting problems.

Corollary 6.3. *The algebraic fitting problem (AM$'_\Theta$) is a relaxation of the geometric fitting problem (AM), obtained by removing the structure constraint of the approximating matrix $\Phi_{\mathtt{d}}(\widehat{D})$.*

6.3 Algorithms

In the linear case, the misfit computation problem is a linear least norm problem. This fact is effectively used in the variable projections method. In the nonlinear case, the misfit computation problem is a nonconvex optimization problem. Thus the elimination step of the variable projections approach is not possible in the nonlinear case. This requires the data approximation $\widehat{\mathscr{D}} = \{\widehat{d}_1, \ldots, \widehat{d}_N\}$ to be treated as an extra optimization variable together with the model parameter Θ. As a result, the computational complexity and sensitivity to local minima increases in the nonlinear case.

The above consideration makes critical the choice of the initial approximation. The default initial approximation is obtained from a direct method such as the algebraic fitting method. Next, we present a modification of the algebraic fitting method that is motivated by the objective of obtaining an unbiased estimate in the errors-in-variables setup.

Bias corrected low-rank approximation

Assume that the data $\mathscr{D}$ is generated according to the errors-in-variables model

$$d_j = d_{0,j} + \widetilde{d}_j, \qquad \text{where} \quad d_{0,j} \in \mathscr{B}_0 \in \mathscr{P}_{\mathtt{m},\mathtt{q}}$$
$$\text{and} \quad \operatorname{vec}\Big(\big[\widetilde{d}_1 \ \cdots \ \widetilde{d}_N\big]\Big) \sim \mathrm{N}(0, \sigma^2 I_{\mathtt{q}N}). \qquad \text{(EIV)}$$

Here $\mathscr{B}_0$ is the to-be-estimated true model. The estimate $\widehat{\mathscr{B}}$ obtained by the algebraic fitting method (AM$'_\Theta$) is biased, *i.e.*, $\mathbf{E}(\widehat{\mathscr{B}}) \neq \mathscr{B}_0$. In this section, we derive a bias correction procedure. The correction depends on the noise variance σ^2, however, the noise variance can be estimated from the data $\mathscr{D}$ together with the model parameter $\widehat{\Theta}$. The resulting bias corrected estimate $\widehat{\mathscr{B}}_{\mathrm{c}}$ is invariant to rigid transformations. Simulation results show that $\widehat{\mathscr{B}}_{\mathrm{c}}$ has smaller orthogonal distance to the data than alternative direct methods.

Define the matrices

$$\Psi := \Phi_{\mathtt{d}}(\mathscr{D})\Phi_{\mathtt{d}}^{\top}(\mathscr{D}) \qquad \text{and} \qquad \Psi_0 := \Phi_{\mathtt{d}}(\mathscr{D}_0)\Phi_{\mathtt{d}}^{\top}(\mathscr{D}_0)$$

The algebraic fitting method computes the rows of parameter estimate $\widehat{\Theta}$ as eigenvectors related to the $\mathtt{p}$ smallest eigenvalues of Ψ. We construct a "corrected" matrix Ψ_{c}, such that

$$\mathbf{E}(\Psi_{\mathrm{c}}) = \Psi_0. \qquad (*)$$

This property ensures that the corrected estimate $\widehat{\Theta}_{\mathrm{c}}$, obtained from the eigenvectors related to the $\mathtt{p}$ smallest eigenvalues of Ψ_{c}, is unbiased.

190a ⟨*Bias corrected low-rank approximation* 190a⟩≡
```
function [th, sh] = bclra(D, deg)
[q, N] = size(D); qext = nchoosek(q + deg, deg);
```
⟨*construct the corrected matrix Ψ_c* 192a⟩
⟨*estimate σ^2 and θ* 192c⟩

Defines:
`bclra`, used in chunk 194e.

The key tool to achieve bias correction is the sequence of the Hermite polynomials, defined by the recursion

$$h_0(x) = 1, \quad h_1(x) = x, \quad \text{and}$$
$$h_k(x) = x h_{k-1}(x) - (k-2) h_{k-2}(x), \quad \text{for } k = 2, 3, \ldots$$

(See Table 6.1 for explicit expressions of $h_2, \ldots, h_{10}$.) The Hermite polynomials have the deconvolution property

$$\mathbf{E}\big(h_k(x_0 + \widetilde{x})\big) = x_0^k, \qquad \text{where} \quad \widetilde{x} \sim \mathrm{N}(0, 1). \qquad (**)$$

The following code generates a cell array `h` of implicit function that evaluate the sequence of Hermite polynomials: `h{k+1}(d)` $= h_k(d)$. (The difference in the indexes of the `h` and h is due to MATLAB convention indexes to be positive integers.)

190b ⟨*define the Hermite polynomials* 190b⟩≡ (192a)
```
h{1} = @(x) 1; h{2} = @(x) x;
for k = 3:(2 * deg + 1)
  h{k} = @(x) [x * h{k - 1}(x) zeros(1, mod(k - 2, 2))] ...
```

Table 6.1 Explicit expressions of the Hermite polynomials $h_2, \dots, h_{10}$.

$$\begin{aligned}
h_2(x) &= x^2 - 1\\
h_3(x) &= x^3 - 3x\\
h_4(x) &= x^4 - 6x^2 + 3\\
h_5(x) &= x^5 - 10x^3 + 15x\\
h_6(x) &= x^6 - 15x^4 + 45x^2 - 15\\
h_7(x) &= x^7 - 21x^5 + 105x^3 - 105x\\
h_8(x) &= x^8 - 28x^6 + 210x^4 - 420x^2 + 105\\
h_9(x) &= x^9 - 36x^7 + 378x^5 - 1260x^3 + 945x\\
h_{10}(x) &= x^{10} - 45x^8 + 630x^6 - 3150x^4 + 4725x^2 - 945
\end{aligned}$$

```
          - [0 (k - 2) * h{k - 2}(x)];
end
```

We have,

$$\Psi = \sum_{\ell=1}^{N} \phi(d_\ell)\phi^\top(d_\ell) = \sum_{\ell=1}^{N} \left[\phi_i(d_\ell)\phi_j(d_\ell)\right],$$

and, from (ϕ_k), the (i,j)th element of Ψ is

$$\psi_{ij} = \sum_{\ell=1}^{N} d_{1\ell}^{\mathtt{d}_{i1}+\mathtt{d}_{j1}} \cdots d_{\mathtt{q}\ell}^{\mathtt{d}_{i\mathtt{q}}+\mathtt{d}_{j\mathtt{q}}} = \sum_{\ell=1}^{N} \prod_{k=1}^{\mathtt{q}} (d_{0,k\ell} + \widetilde{d}_{k\ell})^{\mathtt{d}_{i\mathtt{q}}+\mathtt{d}_{j\mathtt{q}}}.$$

By the data generating assumption (EIV), $\widetilde{d}_{k\ell}$ are independent, zero mean, normally distributed. Then, using the deconvolution property $(**)$ of the Hermit polynomials, we have that

$$\psi_{\mathrm{c},ij} := \sum_{\ell=1}^{N} \prod_{k=1}^{\mathtt{q}} h_{\mathtt{d}_{ik}+\mathtt{d}_{jk}}(d_{k\ell}) \qquad (\psi_{ij})$$

has the unbiasness property $(*)$, *i.e.*,

$$\mathbf{E}(\psi_{\mathrm{c},ij}) = \sum_{\ell=1}^{N} \prod_{k=1}^{\mathtt{q}} d_{0,k\ell}^{\mathtt{d}_{ik}+\mathtt{d}_{jk}} =: \psi_{0,ij}.$$

The elements $\psi_{\mathrm{c},ij}$ of the corrected matrix are even polynomials of σ of degree less than or equal to

$$\mathtt{d}_\psi = \left\lceil \frac{\mathtt{qd}+1}{2} \right\rceil.$$

The following code constructs a $1 \times (\mathtt{d}_\psi + 1)$ vector of the coefficients of $\psi_{\mathrm{c},ij}$ as a polynomial of σ^2. Note that the product of Hermite polynomials in (ψ_{ij}) is a convolution of their coefficients.

191 ⟨*construct* $\psi_{c,ij}$ 191⟩≡ (192a)

```
Deg_ij = Deg(i, :) + Deg(j, :);
for l = 1:N
  psi_ijl = 1;
  for k = 1:q
```

```
    psi_ijl  = conv(psi_ijl, h{Deg_ij(k) + 1}(D(k, l)));
  end
  psi_ijl = [psi_ijl zeros(1, dpsi - length(psi_ijl))];
  psi(i, j, :) = psi(i, j, :) + ...
                reshape(psi_ijl(1:dpsi), 1, 1, dpsi);
end
```

The corrected matrix

$$\Psi_{\mathrm{c}}(\sigma^2) = \Psi_{\mathrm{c},0} + \sigma^2 \Psi_{\mathrm{c},1} + \cdots + \sigma^{2\mathtt{d}_\psi} \Psi_{\mathrm{c},\mathtt{d}_\psi}$$

is then obtained by computing its elements in the lower triangular part

192a ⟨*construct the corrected matrix* Ψ_c 192a⟩≡ (190a) 192b▷

```
⟨define the Hermite polynomials 190b⟩
Deg  = monomials(deg);
dpsi = ceil((q * deg + 1) / 2);
psi  = zeros(qext, qext, dpsi);
for i = 1:qext
  for j = 1:qext
    if i >= j
      ⟨construct ψc,ij 191⟩
    end
  end
end
```

Uses `monomials` 187a.

and using the symmetry property to fill in the upper triangular part

192b ⟨*construct the corrected matrix* Ψ_c 192a⟩+≡ (190a) ◁192a

```
for k = 1:dpsi,
  psi(:, :, k) = psi(:, :, k) + triu(psi(:, :, k)', 1);
end
```

The rows of the parameter $\widehat{\Theta}$ form a basis for the p-dimensional (approximate) null space of $\Psi_{\mathrm{c}}(\sigma^2)$

$$\Theta \Psi_{\mathrm{c}}(\sigma^2) = 0.$$

Computing simultaneously σ and Θ is a *polynomial eigenvalue problem:* the noise variance estimate is the minimum eigenvalue and the parameter estimate is a corresponding eigenvector.

192c ⟨*estimate* σ^2 *and* θ 192c⟩≡ (190a)

```
[evec, ev] = polyeig_(psi); ev(find(ev < 0)) = inf;
[sh2, min_ind]  = min(ev);
sh = sqrt(sh2); th = evec(:, min_ind);
```

(The function `polyeig_` is a minor modification of the standard MATLAB function `polyeig`. The input to `polyeig_` is a 3-dimensional tensor while the input to `polyeig` is a sequence of matrices—the slices of the tensor in the third dimension.)

Method based on local optimization

The nonlinearly structured low-rank approximation problem (PSLRA) is solved numerically using Optimization Toolbox.

193a ⟨*Polynomially structured low-rank approximation* 193a⟩≡ 193b▷
```
function [th, Dh, info] = pslra(D, phi, r, xini)
[q, N] = size(D); nt = size(phi(D), 1);
```
Defines:
`pslra`, used in chunk 194e.

If not specified, the initial approximation is taken as the algebraic fit and the noisy data points.

193b ⟨*Polynomially structured low-rank approximation* 193a⟩+≡ ◁193a 193c▷
```
if (nargin < 4) | isempty(xini)
    tini = lra(phi(D), r); xini = [D(:); tini(:)];
end
```
Uses `lra` 66.

Anonymous functions that extract the data approximation $\widehat{\mathscr{D}}$ and the model parameter θ from the optimization parameter `x` are defined next.

193c ⟨*Polynomially structured low-rank approximation* 193a⟩+≡ ◁193b 193d▷
```
Dh = @(x) reshape(x(1:(q * N)), q, N);
th = @(x) reshape(x((q * N + 1):end), nt - r, nt)';
```
The optimization problem is set and solved, using the Optimization Toolbox:

193d ⟨*Polynomially structured low-rank approximation* 193a⟩+≡ ◁193c
```
⟨set optimization solver and options 87a⟩
prob.objective = @(x) norm(D - Dh(x), 'fro');
prob.nonlcon   = @(x) deal([], ...
                  [th(x)' * phi(Dh(x)), th(x)' * th(x) - eye(nt - r)]);
prob.x0 = xini;
⟨call optimization solver 87b⟩ Dh = Dh(x); th = th(x);
```

6.4 Examples

In this section, we apply the algebraic and geometric fitting methods on a range of algebraic curve fitting problems. In all examples, except for the last one, the data $\mathscr{D}$ is simulated in the errors-in-variables setup, see (EIV) on page 190. The perturbations $\widetilde{d}_j$, $j = 1, \ldots, N$ are independent, zero mean, normally distributed 2×1 vectors with covariance matrix $\sigma^2 I_2$. The true model $\mathscr{B}_0 = \ker(r_0)$, the number of data points N, and the perturbation standard deviation σ are simulation parameters. The true model is plotted by a solid line, the data points by circles, the algebraic fit by a dotted line, the bias corrected fit by dashed dotted line, and the geometric fit by a dashed line.

Test function

The test script `test_curve_fitting` assumes that the simulation parameters:

- polynomial r in x and y, defined as a symbolic object;
- degree `d` of r;
- number of data points N;
- noise standard deviation σ; and
- coordinates `ax` of a rectangle for plotting the results

are already defined.

194a ⟨*Test curve fitting* 194a⟩≡
```
⟨initialize the random number generator 91d⟩
⟨default parameters 194b⟩
⟨generate data 194c⟩
⟨fit data 194e⟩
⟨plot results 195a⟩
```
Defines:
`test_curve_fitting`, used in chunks 195–97.

If not specified, `q` = 2, `m` = 1.

194b ⟨*default parameters* 194b⟩≡ (194a)
```
if ~exist('q'), q = 2; end
if ~exist('m'), m = 1; end
if ~exist('xini'), xini = []; end
```
The true (`D0`) and noisy (`D`) data points are generated by plotting the true model

194c ⟨*generate data* 194c⟩≡ (194a) 194d▷
```
figure,
H = plot_model(r, ax, 'LineStyle', '-', 'color', 'k');
```
Uses `plot_model` 195b.

and sampling N equidistant points on the curve

194d ⟨*generate data* 194c⟩+≡ (194a) ◁194c
```
D0 = [];
for h = H',
  D0 = [D0 [get(h, 'XData'); get(h, 'YData')]];
end
D0 = D0(:, round(linspace(1, size(D0, 2), N)));
D  = D0 + s * randn(size(D0));
```
The data is fitted by the algebraic (`lra`), bias corrected (`bclra`), and geometric (`pslra`) fitting methods:

194e ⟨*fit data* 194e⟩≡ (194a 198)
```
qext  = nchoosek(q + deg, deg); p = q - m;
[Deg, phi] = monomials(deg);
th_exc   = lra(phi(D), qext - p)';
th_ini   = bclra(D, deg);
[th, Dh] = pslra(D, phi, qext - p, xini);
```
Uses `bclra` 190a, `lra` 66, `monomials` 187a, and `pslra` 193a.

The noisy data and the fitted models are plotted on top of the true model:

195a ⟨*plot results* 195a⟩≡ (194a 198)
```
hold on; plot(D(1,:), D(2,:), 'o', 'markersize', 7);
plot_model(th2poly(th_exc, phi), ax, ...
                  'LineStyle', ':', 'color', 'k');
plot_model(th2poly(th_ini, phi), ax, ...
                  'LineStyle', '-.', 'color', 'r');
plot_model(th2poly(th, phi), ax, ...
                  'LineStyle', '-', 'color', 'b');
axis(ax); print_fig(sprintf('%s-est', name))
```
Uses `plot_model` 195b, `print_fig` 25a, and `th2poly` 195c.

Plotting the algebraic curve

$$\mathscr{B} = \{\, d \mid \phi(d)\theta = 0 \,\}$$

in a region, defined by the vector `rect`, is done with the function `plot_model`.

195b ⟨*Plot the model* 195b⟩≡
```
function H = plot_model(r, rect, varargin)
H = ezplot(r, rect);
if nargin > 2, for h = H', set(h, varargin{:}); end, end
```
Defines:
`plot_model`, used in chunks 194c and 195a.

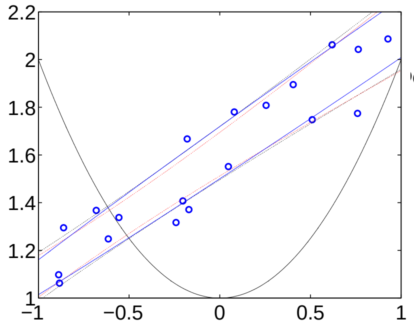
The function `th2poly` converts a vector of polynomial coefficients to a function that evaluates that polynomial.

195c ⟨$\Theta \mapsto R_\Theta$ 195c⟩≡
```
function r = th2poly(th, phi), r = @(x, y) th' * phi([x y]');
```
Defines:
`th2poly`, used in chunk 195a.

Fitting algebraic curves in $\mathbb{R}^2$

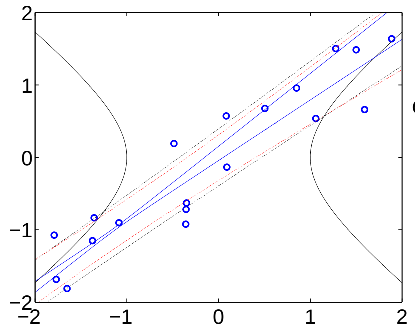
Simulation 1: Parabola
$\mathscr{B} = \{\, \mathrm{col}(x,y) \mid y = x^2 + 1 \,\}$

195d ⟨*Curve fitting examples* 195d⟩≡ 196a▷
```
clear all
name = 'parabola';
N = 20; s = 0.1;
deg = 2; syms x y;
r = x^2 - y + 1;
ax = [-1 1 1 2.2];
test_curve_fitting
```
Uses `test_curve_fitting` 194a.



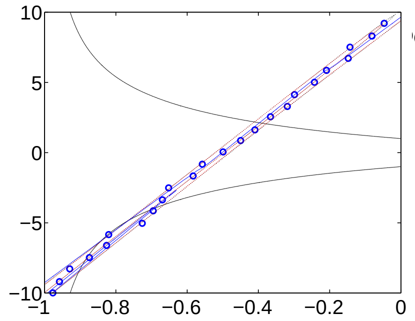
Simulation 2: Hyperbola
$\mathscr{B} = \{\, \mathrm{col}(x,y) \mid x^2 - y^2 - 1 = 0 \,\}$

196a ⟨*Curve fitting examples* 195d⟩+≡ ◁195d 196b▷
```
name = 'hyperbola';
N = 20; s = 0.3;
deg = 2; syms x y;
r = x^2 - y^2 - 1;
ax = [-2 2 -2 2];
test_curve_fitting
```
Uses `test_curve_fitting` 194a.



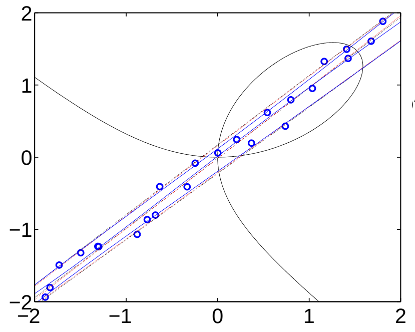
Simulation 3: Cissoid
$\mathscr{B} = \{\, \mathrm{col}(x,y) \mid y^2(1+x) = (1-x)^3 \,\}$

196b ⟨*Curve fitting examples* 195d⟩+≡ ◁196a 196c▷
```
name = 'cissoid';
N = 25; s = 0.02;
deg = 3; syms x y;
r = y^2 * (1 + x) ...
    - (1 - x)^3;
ax = [-1 0 -10 10];
test_curve_fitting
```
Defines:
`examples_curve_fitting`, never used.
Uses `test_curve_fitting` 194a.



Simulation 4: Folium of Descartes
$\mathscr{B} = \{\, \mathrm{col}(x,y) \mid x^3 + y^3 - 3xy = 0 \,\}$

196c ⟨*Curve fitting examples* 195d⟩+≡ ◁196b 197a▷
```
name = 'folium';
N = 25; s = 0.1;
deg = 3; syms x y;
r = x^3 + y^3 - 3 * x * y;
ax = [-2 2 -2 2];
test_curve_fitting
```
Uses `test_curve_fitting` 194a.

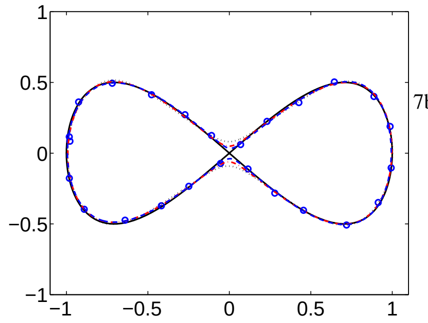


Simulation 5: Eight curve
$\mathscr{B} = \{\, \mathrm{col}(x,y) \mid y^2 - x^2 + x^4 = 0 \,\}$

197a ⟨*Curve fitting examples* 195d⟩+≡ 7b▷

```
name = 'eight';
N = 25; s = 0.01;
deg = 4; syms x y;
r = y^2 - x^2 + x^4;
ax = [-1.1 1.1 -1 1];
test_curve_fitting
```

Uses `test_curve_fitting` 194a.

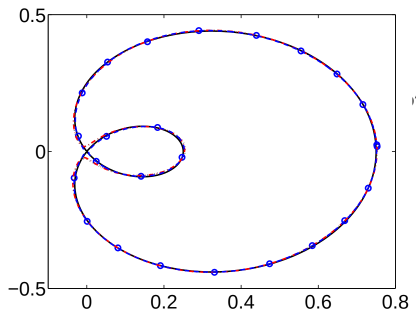


Simulation 6: Limacon of Pascal
$\mathscr{B} = \{\, \mathrm{col}(x,y) \mid y^2 + x^2 - (4x^2 - 2x + 4y^2)^2 = 0 \,\}$

197b ⟨*Curve fitting examples* 195d⟩+≡ 7c▷

```
name = 'limacon';
N = 25; s = 0.002;
deg = 4; syms x y;
r = y^2 + x^2 - (4 * x^2 ...
    - 2 * x + 4 * y^2)^2;
ax = [-.1 .8 -0.5 .5];
test_curve_fitting
```

Uses `test_curve_fitting` 194a.

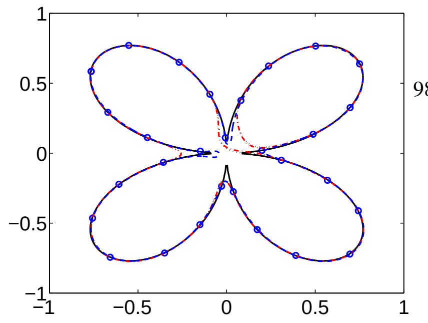


Simulation 7: Four-leaved rose
$\mathscr{B} = \{\, (x,y) \mid (x^2 + y^2)^3 - 4x^2y^2 = 0 \,\}$

197c ⟨*Curve fitting examples* 195d⟩+≡ 98▷

```
name = 'rose';
N = 30; s = 0.002;
deg = 6; syms x y;
r = (x^2 + y^2)^3 ...
    - 4 * x^2 * y^2;
ax = [-1 1 -1 1];
test_curve_fitting
```

Uses `test_curve_fitting` 194a.

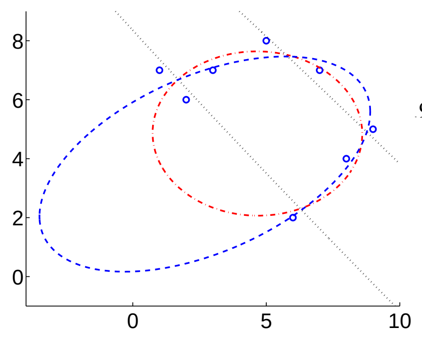


Simulation 8: "Special data" example from (Gander et al, 1994)

198 ⟨*Curve fitting examples* 195d⟩+≡ 97c

```
name = 'special-data';
D = [1 2 5 7 9 3 6 8 ;
     7 6 8 7 5 7 2 4 ];
D0 = D; deg = 2;
xini = [D(:)' 1 0 0 1 0 -1]'
figure, ax = [-4 10 -1 9];
```

⟨*fit data* 194e⟩ ⟨*plot results* 195a⟩



6.5 Notes and references

Fitting curves to data is a basic problem in coordinate metrology, see (Van Huffel, 1997, Part IV). In the computer vision literature, there is a large body of work on ellipsoid fitting (see, *e.g.*, (Bookstein, 1979; Fitzgibbon et al, 1999; Gander et al, 1994; Kanatani, 1994; Markovsky et al, 2004)), which is a special case of the considered in this chapter data fitting problem when the degree of the polynomial is equal to two.

In the systems and control literature, the geometric distance is called misfit and the algebraic distance is called latency, see (Lemmerling and De Moor, 2001). Identification of a linear time-invariant dynamical systems, using the latency criterion leads to the autoregressive moving average exogenous setting, see (Ljung, 1999; Söderström and Stoica, 1989). Identification of a linear time-invariant dynamical systems, using the misfit criterion leads to the errors-in-variables setting, see (Söderström, 2007).

State-of-the art image segmentation methods are based on the *level set* approach (Sethian, 1999). Level set methods use implicit equations to represent a contour in the same way we use kernel representations to represent a model in this chapter. The methods used for parameter estimation in the level set literature, however, are based on solution of partial differential equations while we use classical parameter estimation/optimization methods.

Relaxation of the nonlinearly structured low-rank approximation problem, based on ignoring the nonlinear structure and thus solving the problem as unstructured low-rank approximation, (*i.e.*, the algebraic fitting method) is known in the machine learning literature as *kernel principal component analysis* (Schölkopf et al, 1999). The *principal curves*, introduced in (Hastie and Stuetzle, 1989), lead to a problem of minimizing the sum of squares of the distances from data points to a curve. This is a polynomially structured low-rank approximation problem. More generally, dimensionality reduction by manifold learning, see, *e.g.*, (Zhang and Zha, 2005) is related to the problem of fitting an affine variety to data, which is also polynomially structured low-rank approximation.

Nonlinear (Vandermonde) structured total least squares problems are discussed in (Lemmerling et al, 2002; Rosen et al, 1998) and are applied to fitting a sum of damped exponentials model to data. Fitting a sum of damped exponentials to data, however, can be solved as a linear (Hankel) structured approximation problem. In contrast, the geometric data fitting problem considered in this chapter in general can not be reduced to a linearly structured problem and is therefore a genuine application of nonlinearly structured low-rank approximation.

The problem of passing from image to kernel representation of the model is known as the *implicialization problem* (Cox et al, 2004, Page 96) in computer algebra. The reverse transformation—passing from a kernel to an image representation of the model, is a problem of solving a system of multivariable polynomial equations.

References

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Chapter 7
Fast measurements of slow processes

Summary: Motivated by an application in metrology for speed up of measurement devices, the following problem is considered: given output observations of a stable linear time-invariant system with known dc-gain, generated by a step input, find the input. If a model of the data generating process is available, the input estimation problem is solved as an equivalent state estimation problem for an autonomous system. Otherwise, the input estimation problem is reduced to standard system identification problems: 1) identification from step response data and 2) autonomous system identification. The link to autonomous system identification suggests a data-driven solution, *i.e.*, an algorithm for computation of the input value without identifying a representation of the system. The data-driven algorithm is a structured low-rank approximation problem.

7.1 Introduction

The core idea developed in this chapter is expressed in the following problem from (Luenberger, 1979, Page 53):

Problem 7.1. A thermometer reading 21°C, which has been inside a house for a long time, is taken outside. After one minute the thermometer reads 15°C; after two minutes it reads 11°C. What is the outside temperature? (According to Newton's law of cooling, an object of higher temperature than its environment cools at a rate that is proportional to the difference in temperature.) □

The solution of the problem shows that measurement of a signal from a "slow" processes can be speeded up by data processing. The solution applies to the special case of exact data from a first order single input single output linear time-invariant system. Our purpose is to generalize Problem 7.1 and its solution to multi input multi output processes with higher order linear time-invariant dynamics and to make the solution a practical tool for improvement of the speed-accuracy characteristics of measurement devices by signal processing.

A method for speeding up of measurement devices is of generic interest. Specific applications can be found in process industry where the process, the measurement device, or both have slow dynamics, *e.g.*, processes in biotechnology that involve chemical reactions and convection. Of course, the notion of "slow process" is relative. There are applications, *e.g.*, weight measurement, where the dynamics may be fast according to the human perception but slow according to the state-of-the-art technological requirements.

The dynamics of the process is assumed to be linear time-invariant but otherwise it need not be known. Knowledge of the process dynamics simplifies considerably the problem. In some applications, however, such knowledge is not available a priori. For example, in Problem 7.1 the heat exchange coefficient (cooling time constant) depends on unknown environmental factors, such as pressure and humidity. As another example, consider the dynamic weighing problem, where the unknown mass of the measured object affects the dynamics of the weighting process. The linearity assumption is justifiable on the basis that nonlinear dynamical processes can be approximated by linear models, and existence of an approximate linear model is often sufficient for solving the problem to a desirable accuracy. The time-invariance assumption can be relaxed in the recursive estimation algorithms proposed by using windowing of the processed signal and forgetting factor in the recursive update formula.

Although only the steady-state measurement value is of interest, the solution of Problem 7.1 identifies explicitly the process dynamics as a byproduct. The proposed methods for dynamic weighing (see the notes and references section) are also model-based and involve estimation of model parameters. Similarly, the generalized problem considered reduces to a system identification question—find a system from step response data. Off-line and recursive methods for solving this latter problem, under different noise assumptions, exist in the literature, so that these methods can be readily used for input estimation.

In this chapter, a method for estimation of the parameter of interest—the input step value—without identifying a model of the measurement process is described. The key idea that makes model-free solution possible comes from work on data-driven estimation and control. The method proposed requires only a solution of a system of linear equations and is computationally more efficient and less expensive to implement in practice than the methods based on system identification. Modifications of the model-free algorithm compute approximate solutions that are optimal for different noise assumptions. The modifications are obtained by replacing exact solution of a system of linear equations with approximate solution by the least squares method or one of its variations. On-line versions of the data-driven method, using ordinary or weighted least squares approximation criterion, are obtained by using a standard recursive least squares algorithms. Windowing of the processed signal and forgetting factor in the recursive update allow us to make the algorithm adaptive to time-variation of the process dynamics.

The possibility of using theoretical results, algorithms, and software for different standard identification methods in the model based approach and approximation methods in the data-driven approach lead to a range of new methods for speedup of measurement devices. These new methods inherit desirable properties (such as consistency, statistical and computational efficiency) from the identification or approximation methods being used.

The generalization of Problem 7.1 considered is defined in this section. In Section 7.2, the simpler version of the problem when the measurement process dynamics is known is solved by reducing the problem to an equivalent state estimation problem for an augmented autonomous system. Section 7.3 reduces the general problem without known model to standard identification problems—identification from step response data as well as identification in a model class of autonomous system (sum-of-damped exponentials modeling). Then the data-driven method is derived as a modification of the method based on autonomous system identification. Examples and numerical results showing the performance of the methods are presented in Section 7.4. The proofs of the statements are almost identical for the continuous and discrete-time cases, so that only the proof for the discrete-time case is given.

Problem formulation

Problem 7.1 can be restated more abstractly as follows.

Problem 7.2. A step input $u = \bar{u}s$, where $\bar{u} \in \mathbb{R}$, is applied to a first order stable linear time-invariant system with unit dc-gain[1]. Find the input step level $\bar{u}$ from the output values $y(0) = 21$, $y(1) = 15$, and $y(2) = 11$. □

The heat exchange dynamics in Problem 7.1 is indeed a first order stable linear time-invariant system with unit dc-gain and step input. The input step level $\bar{u}$ is therefore equal to the steady-state value of the output and is the quantity of interest. Stating Problem 7.1 in system theoretic terms opens a way to generalizations and makes clear the link of the problem to system identification. The general problem considered is defined as follows.

Problem 7.3. Given output observations

$$y = \big(y(t_1), \dots, y(t_T)\big), \qquad \text{where} \quad y(t) \in \mathbb{R}^{\mathtt{p}}$$

at given moments of time $0 \leq t_1 < \cdots < t_T$, of a stable linear time-invariant system $\mathscr{B} \in \mathscr{L}^{\mathtt{p}+\mathtt{m}}_{\mathtt{m},\mathtt{n}}$ with known dc-gain $G \in \mathbb{R}^{\mathtt{p}\times\mathtt{m}}$, generated by a step input $u = \bar{u}s$ (but not necessarily zero initial conditions), find the input step value $\bar{u} \in \mathbb{R}^{\mathtt{m}}$. □

The known dc-gain assumption imposed in Problem 7.3 corresponds to calibration of the measurement device in real-life metrological applications. Existence of a dc-

[1] The dc (or steady state) gain of a linear time-invariant system, defined by an input/output representation with transfer function H, is $G = H(0)$ in the continuous-time case and $G = H(1)$ in the discrete-time case. As the name suggest the dc gain G is the input-output amplification factor in a steady state regime, *i.e.*, constant input and output.

gain, however, requires stability hence the process is assumed to be a stable dynamical system. By this assumption, in a steady-state regime, the output of the device is $\bar{y} = G\bar{u}$, so that, provided G is a full column rank matrix, the value of interest is uniquely determined as $\bar{u} = G^{+}\bar{y}$, where G^{+} is a left inverse of G. Obviously, without prior knowledge of G and without G beginning full column rank, $\bar{u}$ can not be inferred from $\bar{y}$. Therefore, we make the following standing assumption.

Assumption 7.4 *The measurement process dynamics $\mathscr{B}$ is a stable linear time-invariant system with full column rank dc-gain,* i.e.,

$$\operatorname{rank}(G) = \mathtt{m}, \qquad \textit{where} \quad G := \textit{dcgain}(\mathscr{B}) \in \mathbb{R}^{\mathtt{p}\times\mathtt{m}}.$$

Note 7.5 (Exact vs noisy observations). Problem 7.3, aims to determine the *exact* input value $\bar{u}$. Correspondingly, the given observations y of the sensor are assumed to be exact. Apart from the problem of finding the exact value of $\bar{u}$ from exact data y, the practically relevant estimation and approximation problems are considered, where the observations are subject to measurement noise

$$y = y_0 + \widetilde{y}, \qquad \text{where} \quad y_0 \in \mathscr{B} \text{ and } \widetilde{y} \text{ is white process with } \widetilde{y}(t) \sim \mathrm{N}(0, V) \quad \text{(OE)}$$

and/or the process dynamics is not finite dimensional linear time-invariant.

Despite the unrealistic assumption of exact observations, Problem 7.3 poses a valid theoretical question that needs to be answered before more realistic approximate and stochastic versions are considered. In addition to its theoretical (and pedagogical) value, the solution of Problem 7.3 leads to algorithms for computation of $\bar{u}$ that with small modifications (approximate rather than exact identification and approximate solution of an overdetermined system of equations) produce approximations of $\bar{u}$ in the case of noisy data and/or process dynamics that is not linear time-invariant.

We start in the next section by solving the simpler problem of speed-up of a sensor when the measurement process dynamics $\mathscr{B}$ is known.

Problem 7.6. Given a linear time-invariant system $\mathscr{B} \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}}$ and an output trajectory y of $\mathscr{B}$, obtained from a step input $u = \bar{u}s$, find the step level $\bar{u} \in \mathbb{R}^{\mathtt{m}}$. □

7.2 Estimation with known measurement process dynamics

Proposition 7.7 *Define the maps between an* $\mathtt{n}$*th order linear time-invariant system with* $\mathtt{m}$ *inputs and an* $\mathtt{n}+\mathtt{m}$*th order autonomous system with* $\mathtt{m}$ *poles at 0 in the continuous-time case, or at 1 in the discrete-time case:*

$$\mathscr{B} \mapsto \mathscr{B}_{\text{aut}} \quad \textit{by} \quad \mathscr{B}_{\text{aut}} := \{\, y \mid \textit{there is } \bar{u}, \textit{ such that } (\bar{u}s, y) \in \mathscr{B} \,\}$$

and

$\mathscr{B}_{\text{aut}} \mapsto \mathscr{B}$ by $\mathscr{B} := \mathscr{B}_{\text{i/s/o}}(A,B,C,D)$, where $\mathscr{B}_{\text{aut}} = \mathscr{B}_{\text{i/s/o}}(A_{\text{aut}}, B_{\text{aut}})$,

with

$$A_{\text{aut}} := \begin{bmatrix} A & B \\ 0 & I_{\mathtt{m}} \end{bmatrix} \qquad \textit{and} \qquad C_{\text{aut}} := \begin{bmatrix} C & D \end{bmatrix}. \tag{$*$}$$

Then

$$(\bar{u}s, y) \in \mathscr{B} \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}} \iff y \in \mathscr{B}_{\text{aut}} \in \mathscr{L}^{\mathtt{p}}_{0,\mathtt{n}+\mathtt{m}} \textit{ and } \mathscr{B}_{\text{aut}} \textit{ has}$$
$$\mathtt{m} \textit{ poles at 0 in the continuous-time case, or at 1 in the discrete-time case.}$$

The state vector x of $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ and the state vector x_{aut} of $\mathscr{B}_{\text{i/s/o}}(A_{\text{aut}},C_{\text{aut}})$, are related by $x_{\text{aut}} = (x, \bar{u})$.

Proof.

$$\begin{aligned}
&(\bar{u}s, y) \in \mathscr{B} = \mathscr{B}_{\text{i/s/o}}(A,B,C,D) \\
\iff\quad & \sigma x = Ax + B\bar{u}s,\ y = Cx + D\bar{u}s, \quad x(0) = x_{\text{ini}} \\
\iff\quad & \sigma x = Ax + B\bar{u}s,\ \sigma\bar{u} = \bar{u},\ y = Cx + D\bar{u}s, \quad x(0) = x_{\text{ini}} \\
\iff\quad & \sigma x_{\text{aut}} = A_{\text{aut}} x_{\text{aut}},\ y = C_{\text{aut}} x_{\text{aut}}, \quad x_{\text{aut}}(0) = (x_{\text{ini}}, \bar{u}) \\
\iff\quad & y \in \mathscr{B}_{\text{aut}} = \mathscr{B}_{\text{i/s/o}}(A_{\text{aut}}, B_{\text{aut}}) \qquad \square
\end{aligned}$$

Proposition 7.7 shows that Problem 7.6 can be solved as a state estimation problem for the augmented system $\mathscr{B}_{\text{i/s/o}}(A_{\text{aut}}, B_{\text{aut}})$. In the case of discrete-time exact data y, a dead-beat observer computes the exact state vector in a finite (less than $\mathtt{n}+\mathtt{m}$) time steps. In the case of noisy observations (OE), the maximum likelihood state estimator is the Kalman filter.

The algorithm for input estimation, resulting from Proposition 7.7 is:

205a ⟨*Algorithm for sensor speedup in the case of known dynamics* 205a⟩≡
```
function uh = stepid_kf(y, a, b, c, d, v, x0, p0)
[p, m] = size(d); n = size(a, 1);
if nargin == 6,
  x0 = zeros(n + m, 1); p0 = 1e8 * eye(n + m);
end
```
⟨*model augmentation: $\mathscr{B} \mapsto \mathscr{B}_{\text{aut}}$* 205b⟩
⟨*state estimation: $(y, \mathscr{B}_{\text{aut}}) \mapsto x_{\text{aut}} = (x, \bar{u})$* 206⟩

Defines:
`stepid_kf`, used in chunks 214c, 215b, and 223b.

The obligatory inputs to the function `stepid_kf` are a $T \times \mathtt{p}$ matrix `y` of uniformly sampled outputs ($y(t) =$ `y(t,:)'`), parameters `a`, `b`, `c`, `d` of a state space representation $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$ of the measurement process, and the output noise variance `v`. The output `uh` is a $T \times \mathtt{m}$ matrix of the sequence of parameter $\bar{u}$ estimates $\widehat{u}(t) =$ `uh(t,:)'`. The first step $\mathscr{B} \mapsto \mathscr{B}_{\text{aut}}$ of the algorithm is implemented as follows, see ($*$).

205b ⟨*model augmentation: $\mathscr{B} \mapsto \mathscr{B}_{\text{aut}}$* 205b⟩≡ (205a)
```
a_aut = [a b; zeros(m, n) eye(m)]; c_aut = [c d];
```

Using the function `tvkf_oe`, which implements the time-varying Kalman filter for an autonomous system with output noise, the second step

$$(y, \mathscr{B}_{\text{aut}}) \mapsto x_{\text{aut}} = (x, \bar{u})$$

of the algorithm is implemented as follows.

206 ⟨*state estimation: $(y, \mathscr{B}_{\text{aut}}) \mapsto x_{\text{aut}} = (x, \bar{u})$* 206⟩≡ (205a)
```
xeh = tvkf_oe(y, a_aut, c_aut, v, x0, p0);
uh = xeh((n + 1):end, :)';
```
Uses `tvkf_oe` 224a.

The optional parameters `x0` and `p0` of `stepid_kf` specify prior knowledge about mean and covariance of the initial state $x_{\text{aut}}(0)$. The default value is a highly uncertain initial condition.

Denote by $\mathtt{n}_{\text{f}}$ the order of the Kalman filter. We have that $\mathtt{n}_{\text{f}} = \mathtt{n} + \mathtt{m}$. The computational cost of processing the data by the time-varying Kalman filter is $O(\mathtt{n}_{\text{f}}^2 + \mathtt{n}_{\text{f}}\mathtt{p})$ floating point operations per discrete-time step, provided the filter gain is precomputed and stored off-line. Note, however, that in the solution of Problem 7.3, presented in Section 7.3, the equivalent autonomous model has state dimension $\mathtt{n}+1$, independent of the value of $\mathtt{m}$.

Note 7.8 (Comparison of other methods with `stepid_kf`*).* In the case of noisy data (OE), `stepid_kf` is a statistically optimal estimator for the parameter $\bar{u}$. Therefore, the performance of `stepid_kf` is an upper bound for the achievable performance with the methods described in the next section.

Although `stepid_kf` is theoretically optimal estimator of $\bar{u}$, in practice it need not be the method of choice even when an a priori given model for the measurement process and the noise covariance are available. The reason for this, perhaps paradoxical statement, is that in practice the model of the process and the noise covariance are not known exactly and the performance of the method may degrade significantly as a result of the uncertainty in the given prior knowledge. The alternative methods that do not relay on a priori given model, may be more robust in case of large uncertainty. In specific cases, this claim can be justified theoretically on the basis of the sensitivity of the Kalman filter to the model parameters. In general cases, the claim can be observed experimentally or by numerical simulation.

7.3 Estimation with unknown measurement process dynamics

Solution by reduction to identification from step response data

Problem 7.3 resembles a classical identification problem of finding a linear time-invariant system from step response data, except that

- the input is unknown,

- the dc-gain of the system is constrained to be equal to the given matrix G, and
- the goal of the problem is to find the input rather than the unknown system dynamics.

As shown next, the first two peculiarities of Problem 7.3 are easily dealt with. The third one is addressed by the data-driven algorithm.

The following proposition shows that Problem 7.3 can be solved equivalently as a standard system identification problem from step response data.

Proposition 7.9 *Let $P \in \mathbb{R}^{\mathtt{m}\times\mathtt{m}}$ be a nonsingular matrix and define the mappings*

$$(P,\mathscr{B}) \mapsto \mathscr{B}', \quad \text{by} \quad \mathscr{B}' := \{\, (Pu,y) \mid (u,y) \in \mathscr{B} \,\}$$

and

$$(P,\mathscr{B}') \mapsto \mathscr{B}, \quad \text{by} \quad \mathscr{B} := \{\, (P^{-1}u,y) \mid (u,y) \in \mathscr{B}' \,\}.$$

Then, under Assumption 7.4, we have that

$$(\bar{u}s,y) \in \mathscr{B} \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}} \quad \text{and} \quad \text{dcgain}(\mathscr{B}) = G$$
$$\iff \quad (\mathbf{1}_{\mathtt{m}}s,y) \in \mathscr{B}' \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}} \quad \text{and} \quad \text{dcgain}(\mathscr{B}') = G', \quad (*)$$

where $\bar{u} = P\mathbf{1}_{\mathtt{m}}$ and $GP = G'$.

Proof. Obviously, $\mathscr{B} \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}}$ and $\text{dcgain}(\mathscr{B}) = G$ implies $\mathscr{B}' \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}}$ and

$$\text{dcgain}(\mathscr{B}') = GP =: G'.$$

Vice verse, if $\mathscr{B}' \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}}$ and $\text{dcgain}(\mathscr{B}') = G'$, then $\mathscr{B} \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}}$ and

$$\text{dcgain}(\mathscr{B}) = P^{-1}G' = G.$$

With $\bar{y} := \lim_{t\to\infty} y(t)$, we have

$$(\mathbf{1}_{\mathtt{m}}s,y) \in \mathscr{B}' \implies G'\mathbf{1}_{\mathtt{m}} = \bar{y} \qquad \text{and} \qquad (\bar{u}s,y) \in \mathscr{B}' \implies G\bar{u} = \bar{y}.$$

Therefore, $G'\mathbf{1}_{\mathtt{m}} = GP\mathbf{1}_{\mathtt{m}} = G\bar{u}$. Finally, using Assumption 7.4, we obtain $P\mathbf{1}_{\mathtt{m}} = \bar{u}$. □

Note 7.10. The input value $\mathbf{1}_{\mathtt{m}}$ in $(*)$ is arbitrary. The equivalence holds for any nonzero vector $\bar{u}'$, in which case $\bar{u} = P\bar{u}'$.

The importance of Proposition 7.9 stems from the fact that while in the left hand side of $(*)$ the input $\bar{u}$ is unknown and the gain G is known, in the right hand side of $(*)$, the input $\mathbf{1}_{\mathtt{m}}$ is known and the gain G' is unknown. Therefore, for the case $\mathtt{p} = \mathtt{m}$, the standard identification problem of finding $\mathscr{B}' \in \mathscr{L}^{\mathtt{p}+\mathtt{m}}_{\mathtt{m},\mathtt{n}}$ from the data $(\mathbf{1}_{\mathtt{m}}s,y)$ is equivalent to Problem 7.3, *i.e.*, find $\bar{u} \in \mathbb{R}^{\mathtt{m}}$ and $\mathscr{B} \in \mathscr{L}^{\mathtt{p}+\mathtt{m}}_{\mathtt{m},\mathtt{n}}$, such that $(\mathbf{1}_{\mathtt{m}}s,y) \in \mathscr{B}$ and $\text{dcgain}(\mathscr{B}) = G$. (The $\mathtt{p} = \mathtt{m}$ condition is required in order to ensure that the system $GP = G'$ has a unique solution P for any $\mathtt{p}\times\mathtt{m}$ full column rank matrices G and G'.)

Next, we present an algorithm for solving Problem 7.3 using Proposition 7.9.

208a ⟨*Algorithm for sensor speedup based on reduction to step response system identification* 208a⟩≡
```
function [uh, sysh] = stepid_si(y, g, n)
⟨system identification: (1_m s, y) ↦ B' 208b⟩
⟨ū := G^{-1} G' 1_m, where G' := dcgain(B') 208c⟩
```
Defines:
`stepid_si`, never used.

The input to the function `stepid_si` is a $T \times \mathtt{p}$ matrix `y` of uniformly sampled output values ($y(t) =$ `y(t,:)'`), a nonsingular $\mathtt{p}\times\mathtt{m}$ matrix `g`, and the system order `n`. For simplicity, in `stepid_si` as well as in the following algorithms, the order `n` of the measurement process $\mathscr{B}$ is assumed known. In case of unknown system order, one of the many existing order estimation methods (see, (Stoica and Selén, 2004)) can be used.

For exact data, the map $(\mathbf{1}_{\mathtt{m}}s,y) \mapsto \mathscr{B}'$ is the exact identification problem of computing the most powerful unfalsified model of $(\mathbf{1}_{\mathtt{m}}s,y)$ in the model class of linear-time invariant systems. For noisy data, an approximation of the "true" system $\mathscr{B}'$ is obtained by an approximate identification method. The approximation criterion should reflect known properties of the noise, *e.g.*, in the case of observations corrupted by measurement noise (OE), an output error identification method should be selected.

Using the function `ident_oe`, the pseudo-code of `stepid_si` is completed as follows.

208b ⟨*system identification: $(\mathbf{1}_{\mathtt{m}}s,y) \mapsto \mathscr{B}'$* 208b⟩≡ (208a)
```
sysh = ident_oe([y ones(size(y))], n);
```
Uses `ident_oe` 119a.

and

208c ⟨*$\bar{u} := G^{-1}G'\mathbf{1}_{\mathtt{m}}$, where $G' :=$ dcgain$(\mathscr{B}')$* 208c⟩≡ (208a)
```
[p, m] = size(g); uh = sum(g \ dcgain(sysh), 2);
```

Note 7.11 (Output error identification). The shown implementation of `stepid_si` is optimal (maximum likelihood) for data y generated according to (OE).

Note 7.12 (Recursive implementation). The function `ident_oe` is an off-line identification method. Replacing it with the recursive identification methods results in a recursive algorithm for solution of Problem 7.3. The easy modification of the pseudo-code for different situations, such as different noise assumptions, different model class, and batch vs on-line implementation, is possible by the reduction of Problem 7.3 to a standard problem in system identification, for which well developed theory, algorithms, and software exist.

Solution by identification of an autonomous system

An alternative way of solving Problem 7.3 is to exploit its equivalence to autonomous system identification, stated in the following proposition.

Proposition 7.13 *Define the maps*

$$(\mathscr{B},\bar{u}) \mapsto \mathscr{B}'_{\text{aut}}, \quad \text{by} \quad \mathscr{B}'_{\text{aut}} := \{\, y \mid (s\bar{u},y) \in \mathscr{B} \,\}$$

and

$$(\mathscr{B}'_{\text{aut}},G) \mapsto \mathscr{B}, \quad \text{by} \quad \mathscr{B} := \mathscr{B}_{\text{i/s/o}}(A,B,C,D),$$
$$\text{where } \mathscr{B}'_{\text{aut}} = \mathscr{B}_{\text{i/s/o}}\left(\begin{bmatrix} A & B\bar{u} \\ 0 & \lambda_1 \end{bmatrix}, \begin{bmatrix} C & D\bar{u} \end{bmatrix}\right),$$
$$\lambda_1 = 0 \text{ in the continuous-time case or } \lambda_1 = 1 \text{ in the discrete-time case.}$$

We have that

$$(s\bar{u},y) \in \mathscr{B} \in \mathscr{L}^{\mathtt{m}+\mathtt{p}}_{\mathtt{m},\mathtt{n}} \quad \text{and} \quad \mathit{dcgain}(\mathscr{B}) = G \quad \Longleftrightarrow \quad y \in \mathscr{B}'_{\text{aut}} \in \mathscr{L}^{\mathtt{p}}_{0,\mathtt{n}+1} \quad \text{and}$$
$$\mathscr{B}'_{\text{aut}} \text{ has a pole at 0 in the continuous-time or 1 in the discrete-time.} \qquad (*)$$

Proof. Let $z_1,\dots,z_n$ be the poles of $\mathscr{B}$, *i.e.*,

$$\{z_1,\dots,z_n\} := \lambda(\mathscr{B}).$$

An output y of $\mathscr{B}$ to a step input $u = \bar{u}s$ is of the form

$$y(t) = \Big(\bar{u} + \sum_{i=1}^{n} \alpha_i p_i(t) z_i^t\Big) s(t), \qquad \text{for all } t,$$

where p_i is a polynomial function (of degree equal to the multiplicity of z_i minus one), and $\alpha_i \in \mathbb{R}^{\mathtt{n}}$. This shows that y is a response of an autonomous linear time-invariant system with poles $1 \cup \lambda(\mathscr{B})$.

A system $\mathscr{B}'_{\text{aut}} \in \mathscr{L}^{\mathtt{p}}_{0,\mathtt{n}+1}$ with a pole at 1, admits a minimal state space representation

$$\mathscr{B}_{\text{i/s/o}}\left(\begin{bmatrix} A & b \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} C & d \end{bmatrix}\right).$$

The "$\Rightarrow$" implication in $(*)$ follows from the definition of the map $(\mathscr{B},\bar{u}) \mapsto \mathscr{B}'_{\text{aut}}$. The "$\Leftarrow$" implication in $(*)$ follows from

$$y \in \mathscr{B}'_{\text{aut}} = \mathscr{B}_{\text{i/s/o}}\left(\begin{bmatrix} A & b \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} C & d \end{bmatrix}\right)$$
$$\Longrightarrow \quad \text{there exist initial conditions } x(0) \in \mathbb{R}^{\mathtt{n}} \text{ and } z(0) = z_{\text{ini}} \in \mathbb{R},$$
$$\text{such that} \quad \sigma x = Ax + bz, \quad y = Cx + dz, \quad \sigma z = z$$
$$\Longrightarrow \quad \text{there exist initial condition } x(0) = x_{\text{ini}} \in \mathbb{R}^{\mathtt{n}} \text{ and } z \in \mathbb{R},$$
$$\text{such that} \quad \sigma x = Ax + bz, \quad y = Cx + dz$$
$$\Longrightarrow \quad (zs,y) \in \mathscr{B} = \mathscr{B}_{\text{i/s/o}}(A,b,C,d).$$

Using the prior knowledge about the dc-gain of the system, we have

$$\bar{y} := \lim_{t\to\infty} y(t) = G\bar{u}.$$

On the other hand, $(zs,y) \in \mathscr{B} = \mathscr{B}_{\text{i/s/o}}(A,b,C,d)$ implies that

$$\bar{y} := \big(C(I-A)^{-1}b + d\big)\bar{z}.$$

These relations give us the system of linear equations for $\bar{u}$

$$\big(C(I-A)^{-1}b + d\big)\bar{z} = G\bar{u}. \qquad (**)$$

By Assumption 7.4, $\bar{u}$ is uniquely determined from $(**)$. □

The significance of Proposition 7.13 is that Problem 7.3 can be solved equivalently as an autonomous system identification problem with a fixed pole at 0 in the continuous-time case or at 1 in the discrete-time case. The following proposition shows how a preprocessing step makes possible standard methods for autonomous system identification (or equivalently sum-of-damped exponential modeling) to be used for identification of a system with a fixed pole at 0 or 1.

Proposition 7.14

$$y \in \mathscr{B}_{\text{i/s/o}}\left(\begin{bmatrix} A & b \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} C & d \end{bmatrix}\right) \quad \Longleftrightarrow \quad \Delta y := \frac{\mathrm{d}}{\mathrm{d}t} y \in \Delta\mathscr{B} := \mathscr{B}_{\text{i/s/o}}(A,C)$$
in the continuous-time case

$$y \in \mathscr{B}_{\text{i/s/o}}\left(\begin{bmatrix} A & b \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} C & d \end{bmatrix}\right) \quad \Longleftrightarrow \quad \Delta y := (1-\sigma^{-1}) y \in \Delta\mathscr{B} := \mathscr{B}_{\text{i/s/o}}(A,C)$$
in the discrete-time case

Proof. Let p be the characteristic polynomial of the matrix A.

$$y \in \mathscr{B}_{\text{i/s/o}}(A_{\text{e}},C_{\text{e}}) := \mathscr{B}_{\text{i/s/o}}\left(\begin{bmatrix} A & b \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} C & d \end{bmatrix}\right) \quad \Longleftrightarrow \quad p(\sigma^{-1})(1-\sigma^{-1})y = 0.$$

On the other hand, we have

$$\Delta y := (1-\sigma^{-1}) y \in \Delta\mathscr{B} := \mathscr{B}_{\text{i/s/o}}(A,C) \quad \Longleftrightarrow \quad p(\sigma^{-1})(1-\sigma^{-1})y = 0.$$

The initial conditions $(x_{\text{ini}},\bar{u})$ of $\mathscr{B}_{\text{i/s/o}}(A_{\text{e}},C_{\text{e}})$ and Δx_{ini} of $\mathscr{B}_{\text{i/s/o}}(A,C)$ are related by

$$(I-A)x_{\text{ini}} = \Delta x_{\text{ini}}. \qquad \square$$

Once the model parameters A and C are determined via autonomous system identification from Δy, the parameter of interest $\bar{u}$ can be computed from the equation

$$y = \bar{y} + y_{\text{aut}}, \qquad \text{where} \quad \bar{y} = G\bar{u} \quad \text{and} \quad y_{\text{aut}} \in \mathscr{B}_{\text{i/s/o}}(A,C) = \Delta\mathscr{B}. \qquad \text{(AUT)}$$

Using the fact that the columns of the extended observability matrix $\mathscr{O}_T(A,C)$ form a basis for $\Delta\mathscr{B}|_{[1,T]}$, we obtain the following system of linear equations for the estimation of $\bar{u}$

$$\begin{bmatrix}\mathbf{1}_T \otimes G & \mathscr{O}_T(A,C)\end{bmatrix} \begin{bmatrix}\bar{u} \\ x_{\text{ini}}\end{bmatrix} = \operatorname{col}\big(y(t_s),\dots,y(Tt_s)\big). \qquad \text{(SYS AUT)}$$

Propositions 7.13 and 7.14, together with (SYS AUT), lead to the following algorithm for solving Problem 7.3.

211a ⟨*Algorithm for sensor speedup based on reduction to autonomous system identification* 211a⟩≡
```
function [uh, sysh] = stepid_as(y, g, n)
```
⟨*preprocessing by finite difference filter* $\Delta y := (1-\sigma^{-1})y$ 211b⟩
⟨*autonomous system identification:* $\Delta y \mapsto \Delta\mathscr{B}$ 211c⟩
⟨*computation of* $\bar{u}$ *by solving (SYS AUT)* 211d⟩

Defines:
`stepid_as`, never used.

where

211b ⟨*preprocessing by finite difference filter* $\Delta y := (1-\sigma^{-1})y$ 211b⟩≡ (211a 212)
```
dy = diff(y);
```
and, using the function `ident_aut`

211c ⟨*autonomous system identification:* $\Delta y \mapsto \Delta\mathscr{B}$ 211c⟩≡ (211a)
```
sysh = ident_aut(dy, n);
```
Uses `ident_aut` 114a.

Notes 7.11 and 7.12 apply for `stepid_as` as well. Alternatives to the prediction error method in the second step are methods for sum-of-damped exponential modeling (*e.g.*, the Prony, Yule-Walker, or forward-backward linear prediction methods) and approximate system realization methods (*e.g.*, Kung's method, implemented in the function `h2ss`). Theoretical results and numerical studies justify different methods as being effective for different noise assumptions. This allows us to pick the "right" identification method, to be used in the algorithm for solving Problem 7.3 under additional assumptions or prior knowledge about the measurement noise.

Finally, the third step of `stepid_as` is implemented as follows.

211d ⟨*computation of* $\bar{u}$ *by solving (SYS AUT)* 211d⟩≡ (211a)
```
T = size(y, 1); [p, m] = size(g); yt = y'; O = sysh.c;
for t = 2:T
   O = [O; O(end - p + 1:end, :) * sysh.a];
end
xe = [kron(ones(T, 1), g) O] \ yt(:); uh = xe(1:m);
```

Data-driven solution

A signal w is persistently exciting of order $\mathtt{l}$ if the Hankel matrix $\mathscr{H}_{\mathtt{l}}(w)$ has full row rank. By Lemma 4.11, a persistently exciting signals of order $\mathtt{l}$ can not be fitted exactly by a system in the model class $\mathscr{L}_{0,\mathtt{l}}$. Persistency of excitation of the input is a necessary identifiability condition in exact system identification.

Assuming that Δy is persistently exciting of order $\mathtt{n}$,

$$\mathscr{B}_{\text{mpum}}(\Delta y) = \Delta\mathscr{B}.$$

Since,

$$\mathscr{B}_{\text{mpum}}(\Delta y) = \operatorname{span}\big(\{\,\sigma^\tau \Delta y \mid \tau \in \mathbb{R}\,\}\big),$$

we have that

$$\mathscr{B}_{\text{mpum}}(\Delta y)|_{[1,T-\mathtt{n}]} = \operatorname{span}\big(\mathscr{H}_{T-\mathtt{n}}(\Delta y)\big).$$

Then, from (AUT), we obtain the system of linear equations for $\bar{u}$

$$\underbrace{\begin{bmatrix}\mathbf{1}_{T-\mathtt{n}} \otimes G & \mathscr{H}_{T-\mathtt{n}}(\Delta y)\end{bmatrix}}_{H} \begin{bmatrix}\bar{u} \\ \ell\end{bmatrix} = \operatorname{col}\Big(y\big((\mathtt{n}+1)t_s\big),\dots,y(Tt_s)\Big), \qquad \text{(SYS DD)}$$

which depends only on the given output data y and gain matrix G. The resulting model-free algorithm is:

212 ⟨*Data-driven algorithm for sensor speedup* 212⟩≡
```
function uh = stepid_dd(y, g, n, ff)
if nargin == 3, ff = 1; end
```
⟨*preprocessing by finite difference filter* $\Delta y := (1-\sigma^{-1})y$ 211b⟩
⟨*computation of* $\bar{u}$ *by solving (SYS DD)* 213⟩

Defines:
`stepid_dd`, used in chunks 214c, 215b, and 223a.

As proved next, `stepid_dd` computes the correct parameter value $\bar{u}$ under less restrictive condition than identifiability of $\Delta\mathscr{B}$ from Δy, *i.e.*, persistency of excitation of Δy of order $\mathtt{n}$ is not required.

Proposition 7.15 *Let*

$$(u,y) := \Big(\big(\underbrace{\bar{u},\dots,\bar{u}}_{T\ \text{times}}\big), \big(y(1),\dots,y(T)\big)\Big) \in \mathscr{B}|_{[1,T]}, \qquad (*)$$

for some $\bar{u} \in \mathbb{R}^{\mathtt{m}}$. *Then, if the number of samples* T *is larger than or equal to* $2\mathtt{n}+\mathtt{m}$, *where* $\mathtt{n}$ *is the order of the data generating system* $\mathscr{B}$, *and Assumption 7.4 holds, the estimate computed by* `stepid_dd` *equals the true input value* $\bar{u}$.

Proof. The derivation of (SYS DD) and the exact data assumption $(*)$ imply that there exists $\bar{\ell} \in \mathbb{R}^n$, such that $(\bar{u},\bar{\ell})$ is a solution of (SYS DD). Our goal is to show that all solutions of (SYS DD) are of this form.

By Assumption 7.4, $\mathscr{B}$ is a stable system, so that $1 \notin \lambda(\mathscr{B})$. It follows that for any $\bar{y} \in \mathbb{R}^{\mathtt{p}}$,

$$\big(\underbrace{\bar{y},\dots,\bar{y}}_{T\ \text{times}}\big) \notin \mathscr{B}_{\text{aut}}|_{[1,T]} = \Delta\mathscr{B}|_{[1,T]}.$$

Therefore,

$$\operatorname{span}(\mathbf{1}_T \otimes G) \cap \mathscr{B}_{\text{aut}}|_{[1,T]} = \{0\}.$$

By the assumption $T \geq 2n + \mathtt{m}$, the matrix H in (SYS DD) has at least as many rows as columns. Then using the full column rank property of G (Assumption 7.4), it follows that a solution $\bar{u}$ of (SYS DD) is unique. □

Note 7.16 (Nonuniqueness of a solution ℓ of (SYS DD)). Under the assumptions of Proposition 7.15, the first $\mathtt{m}$ elements of a solution of (SYS DD) are unique. The solution for ℓ, however, may be nonunique. This happens if and only if the order of $\mathscr{B}_{\text{mpum}}(\Delta y)$ is less than $\mathtt{n}$, *i.e.*, $\mathscr{B}_{\text{mpum}}(\Delta y) \subset \Delta\mathscr{B}$. A condition on the data for $\mathscr{B}_{\text{mpum}}(\Delta y) \subset \Delta\mathscr{B}$ is that Δy is persistently exciting of order less than $\mathtt{n}$. Indeed,

$$\dim\left(\mathscr{B}_{\text{mpum}}(\Delta y)\right) = \operatorname{rank}\left(\mathscr{H}_{T-\mathtt{n}}(\Delta y)\right).$$

It follows from Note 7.16 that if the order $\mathtt{n}$ is not specified a priori but is estimated from the data by, *e.g.*, computing the numerical rank of $\mathscr{H}_{T-\mathtt{n}}(\Delta y)$, the system of equations (SYS DD) has a unique solution.

Note 7.17 (Relaxed assumption). The methods `stepid_si` and `stepid_as`, based on a model computed from the data y using a system identification method, require identifiability conditions. By Proposition 7.15, however, `stepid_dd` does not require identifiability. The order specification in `stepid_dd` can be relaxed to an upper bound of the true system order, in which case any solution of (SYS DD) recovers $\bar{u}$ from its unique first $\mathtt{m}$ elements.

The data-driven algorithm can be implemented recursively and generalized to estimation under different noise assumptions. The following code chunk uses a standard recursive least squares algorithm, implemented in the function `rls`, for approximate solution of (SYS DD).

213 ⟨*computation of $\bar{u}$ by solving (SYS DD)* 213⟩≡ (212)
```
T  = size(y, 1); [p, m] = size(g);
Tt = T - n; yt = y((n + 1):T, :)'; if n == 0, dy = [0; dy]; end
x  = rls([kron(ones(Tt, 1), g), blkhank(dy, Tt)], yt(:), ff);
uh = x(1:m, p:p:end)'; uh = [NaN * ones(n, m); uh];
```
Uses `blkhank` 25b and `rls` 225a.

The first estimated parameter `uh(1, :)` is computed at time

$$T_{\min} = \left\lceil \frac{\mathtt{n}+\mathtt{m}}{\mathtt{p}} \right\rceil + \mathtt{n}.$$

In `rls`, the first $\lceil(\mathtt{n}+\mathtt{m})/\mathtt{p}\rceil - 1$ samples are used for initialization, so that in order to match the index of `uh` with the actual discrete-time when the estimate is computed, `uh` is padded with $\mathtt{n}$ additional rows.

Using the recursive least squares algorithm `rls`, the computational cost of `stepid_dd` is $O\left((\mathtt{m}+\mathtt{n})^2\mathtt{p}\right)$. Therefore, its computational complexity compares favourably with the one of `stepid_kf` with precomputed filter gain (see Section 7.2). The fact that Problem 7.3 can be solved with the same order of computations with and without knowledge of the process dynamics is surprising and remarkable. We consider this fact as our main result.

In the next section, the performance of `stepid_dd` and `stepid_kf` is compared on test examples, where the data is generated according to the output error noise model (OE).

Note 7.18 (Mixed least squares Hankel structured total least squares approximation method). In case of noisy data (OE), the ordinary least squares approximate solution of (SYS DD) is not maximum likelihood. The reason for this is that the matrix in the left-hand-side of (SYS DD) depends on y, which is perturbed by the noise. A statistically better approach is to be used the mixed least squares total least squares approximation method that accounts for the fact that the block $\mathbf{1}_T \otimes G$ in H is exact but the block $\mathscr{H}_{T-\mathtt{n}}(\Delta y)$ of H as well as the right hand side of (SYS DD) are noisy. The least squares total least squares method, however, requires the more expensive singular value decomposition of the matrix $\begin{bmatrix} H & y \end{bmatrix}$ and is harder to implement as a recursive on-line method. In addition, although the mixed least squares total least squares approximation method improves on the standard least squares method it is also not maximum likelihood either, because it does not take into account the Hankel structure of the perturbations. A maximum-likelihood data-driven method requires an algorithm for structured total least squares.

7.4 Examples and real-life testing

Simulation setup

In the simulations, we use the output error model (OE). The exact data y_0 in the estimation problems is a uniformly sampled output trajectory $y_0 = \left(y_0(t_s), \ldots, y_0(Tt_s)\right)$ of a continuous-time system $\mathscr{B} = \mathscr{B}_{\text{i/s/o}}(A,B,C,D)$, obtained with input u_0 and initial condition x_{ini}.

214a ⟨*Test sensor speedup* 214a⟩≡ 214b▷
```
⟨initialize the random number generator 91d⟩
sys = c2d(ss(A, B, C, D), ts); G = dcgain(sys);
[p, m] = size(G); n = size(sys, 'order');
y0 = lsim(sys, u0, [], xini);
```
Defines:
`test_sensor`, used in chunks 217–22.

According to (OE), the exact trajectory `y0` is perturbed with additive noise $\widetilde{y}$, which is modelled as a zero mean, white, stationary, Gaussian process with standard deviation Σ.

214b ⟨*Test sensor speedup* 214a⟩+≡ ◁214a 214c▷
```
y = y0 + randn(T, p) * s;
```
After the data `y` is simulated, the estimation methods `stepid_kf` and `stepid_dd` are applied

214c ⟨*Test sensor speedup* 214a⟩+≡ ◁214b 215a▷
```
uh_dd = stepid_dd(y, G, n, ff);
uh_kf = stepid_kf(y, sys.a, sys.b, sys.c, sys.d, ...
                s^2 * eye(size(D, 1)));
```

Uses `stepid_dd` 212 and `stepid_kf` 205a.

and the corresponding estimates are plotted as functions of time, together with the "naive estimator"

$$\widehat{u} := G^{+}y, \qquad \text{where } G^{+} = (G^{\top}G)^{-1}G^{\top}.$$

215a ⟨*Test sensor speedup* 214a⟩+≡ ◁214c 215b▷

```
figure(2 * (exm_n - 1) + 1), hold on,
if n > 0, Tmin = 2 * n + 1; else Tmin = 2; end, t = Tmin:T;
plot(t, y0(t, :) / G', 'k-'), plot(t, y(t, :) / G', 'k:'),
plot(t, u0(t, :), 'k-'), plot(t, uh_dd(t, :), '-b'),
plot(t, uh_kf(t, :), '-.r'), ax = axis;
axis([Tmin T ax(3:4)]), print_fig(['example-' int2str(exm_n)])
```

Uses `print_fig` 25a.

The plotted results are in the interval $[2\mathtt{n}+\mathtt{m}, T]$, because $2\mathtt{n}+\mathtt{m}$ is the minimum number of samples needed for estimation of $\bar{u}$. The convention used to denote the different estimates by different line styles is summarized in Table 7.1.

Table 7.1 Legend for the line style styles in figures showing simulation results.

line style	—	corresponds to
dashed	—	true parameter value $\bar{u}$
solid	—	true output trajectory y_0
dotted	—	naive estimate $\widehat{u} = G^{+}y$
dashed	—	`stepid_kf`
dashed-dotted	—	`stepid_dd`

Let $\widehat{u}^{(i)}(t)$ be the estimate of $\bar{u}$, using the data $\big(y(1),\dots,y(t)\big)$ in an ith Monte Carlo repetition of the estimation experiment. In addition to the results for a specific noise realization, the average estimation errors of the compared methods

$$e = \frac{1}{N}\sum_{i=1}^{N} \|\bar{u} - \widehat{u}^{(i)}\|_1, \qquad \text{where} \quad \|x\|_1 := \sum_{i=1}^{\mathtt{n}} |x_i|$$

are computed and plotted over n independent noise realizations.

215b ⟨*Test sensor speedup* 214a⟩+≡ ◁215a

```
N = 100; clear e_dd e_kf e_nv
for i = 1:N
  y = y0 + randn(T, p) * s;
  e_nv(:, i) = sum(abs(u0 - y / G'), 2);
  uh_dd = stepid_dd(y, G, n, ff);
  e_dd(:, i) = sum(abs(u0 - uh_dd), 2);
  uh_kf = stepid_kf(y, sys.a, sys.b, sys.c, sys.d, ...
                    s^2 * eye(size(D, 1)));
  e_kf(:, i) = sum(abs(u0 - uh_kf), 2);
end
figure(2 * (exm_n - 1) + 2), hold on
```

```
plot(t, mean(e_dd(t, :), 2), '-b'),
plot(t, mean(e_kf(t, :), 2), '-.r'),
plot(t, mean(e_nv(t, :), 2), ':k'),
ax = axis; axis([Tmin T 0 ax(4)]),
print_fig(['example-error-' int2str(exm_n)])
exm_n = exm_n + 1;
```

Uses `print_fig` 25a, `stepid_dd` 212, and `stepid_kf` 205a.

The script file `examples_sensor_speedup.m`, listed in the rest of this section, reproduces the simulation results. The variable `exm_n` is the currently executed example.

216a ⟨*Sensor speedup examples* 216a⟩≡ 217a▷

```
clear all, close all, exm_n = 1;
```

Defines:
`examples_sensor_speedup`, never used.

Dynamic cooling

The first example is the temperature measurement problem from the introduction. The heat transfer between the thermometer and its environment is governed by Newton's law of cooling, *i.e.*, the changes in the thermometer's temperature y is proportional to the difference between the thermometer's temperature and the environment's temperature $\bar{u}$. We assume that the heat capacity of the environment is much larger than the heat capacity of the thermometer, so that the heat transfer between the thermometer and the environment does not change the environment's temperature. Under this assumption, the dynamics of the measurement process is given by the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}y = a\big(\bar{u}s - y\big),$$

where a is a positive constant that depends on the thermometer and the environment. The differential equation defines a first order linear time-invariant dynamical system $\mathscr{B} = \mathscr{B}_{\mathrm{i/s/o}}(-a, a, 1, 0)$ with input $u = \bar{u}s$.

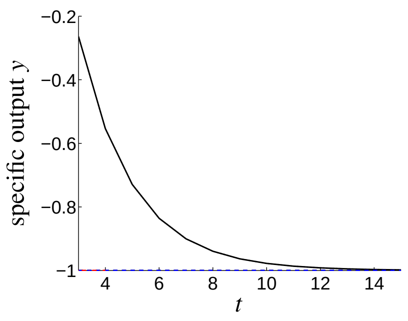
216b ⟨*cooling process* 216b⟩≡ (217 222)

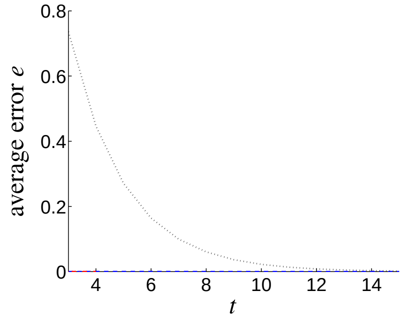
```
A = -a; B = a; C = 1; D = 0;
```

The dc-gain of the system is equal to 1, so that it can be assumed known, independent of the process's parameter a. This matches the setup of Problem 7.3, where the dc-gain is assumed a priori known but the process dynamics is not.

Simulation 1: exact data

217a ⟨*Sensor speedup examples* 216a⟩+≡ ◁216a 217b▷
```
  a = 0.5; ⟨cooling process 216b⟩ T = 15; ts = 1; s = 0.0;
  xini = 1; ff = 1; u0 = ones(T, 1) * (-1); test_sensor
```
Uses `test_sensor` 214a.



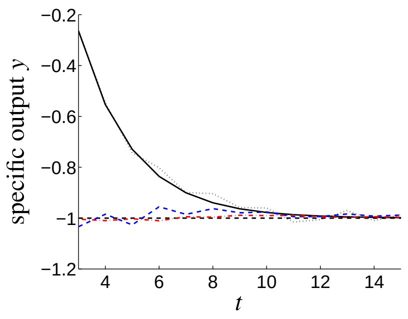


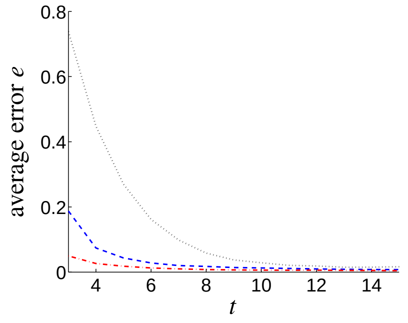
The average error for both `stepid_kf` and `stepid_dd` is zero (up to errors incurred by the numerical computation). The purpose of showing simulation results of an experiment with exact data is verification of the theoretical results stating that the methods solve Problem 7.3.

In the case of output noise (OE), `stepid_kf` is statistically optimal estimator, while `stepid_dd`, implemented with the (recursive) least squares approximation method, is not statistically optimal (see Note 7.18). In the next simulation example we show how far from optimal is `stepid_dd` in the dynamic colling example with the simulation parameters given below.

Simulation 2: noisy data

217b ⟨*Sensor speedup examples* 216a⟩+≡ ◁217a 218b▷
```
  a = 0.5; ⟨cooling process 216b⟩ T = 15; ts = 1; s = 0.02;
  xini = 1; ff = 1; u0 = ones(T, 1) * (-1); test_sensor
```
Uses `test_sensor` 214a.





Temperature-pressure measurement

Consider ideal gas in a closed container with a fixed volume. We measure the temperature (as described in the previous section) by a slow but accurate thermometer, and the pressure by fast but inaccurate pressure sensor. By Gay-Lussac's law, the temperature (measured in Kelvin) is proportional to the pressure, so by proper calibration, we can measure the temperature also with the pressure sensor. Since the pressure sensor is much faster than the thermometer, we model it as a static system. The measurement process in this example is a multivariable (one input, two outputs) system $\mathscr{B}_{\text{i/s/o}}(A,B,C,D)$, where

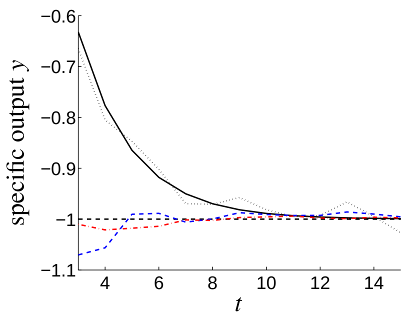
$$A=-a,\qquad B=a,\qquad C=\begin{bmatrix}1\\0\end{bmatrix},\qquad \text{and}\qquad D=\begin{bmatrix}0\\1\end{bmatrix}.$$

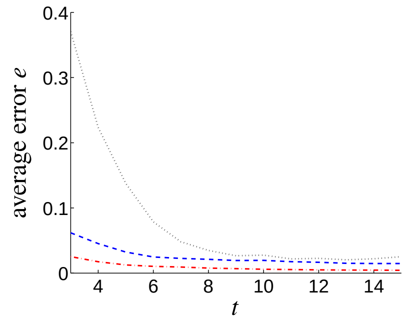
218a ⟨*temperature-pressure process* 218a⟩≡ (218b)
```
  A = -a; B = a; C = [1; 0]; D = [0; 1];
```

Problem 7.3 in this example can be viewed as a problem of "blending" the measurements of two sensors in such a way that a faster and more accurate measurement device is obtained. The algorithms developed can be applied directly to process the vector values data sequence y, thus solving the "data fusion" problem.

Simulation 3: using two sensors

218b ⟨*Sensor speedup examples* 216a⟩+≡ ◁217b 219▷
```
  a = 0.5; T = 15; ts = 1; ⟨temperature-pressure process 218a⟩ ff = 1;
  s = diag([0.02, 0.05]); xini = 1; u0 = ones(T, 1) * (-1);
  test_sensor
```
Uses `test_sensor` 214a.





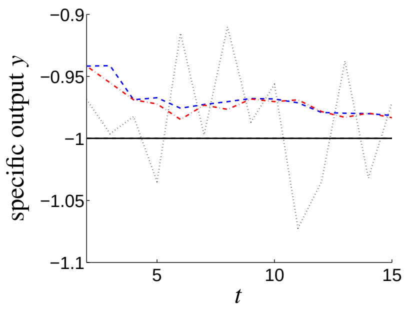
Comparing the results of Simulation 3 with the ones of Simulation 2 (experiment with the temperature sensor only), we see about two fold initial improvement of the average errors of all methods, however, in a long run the naive and `stepid_dd` methods show smaller improvement. The result is consistent with the intuition that the benefit in having fast but inaccurate second sensor is to be expected mostly in the beginning when the estimate of the slow but accurate sensor is still far off the true value. This intuitive explanation is confirmed by the results of an experiment in which only the pressure sensor is used.

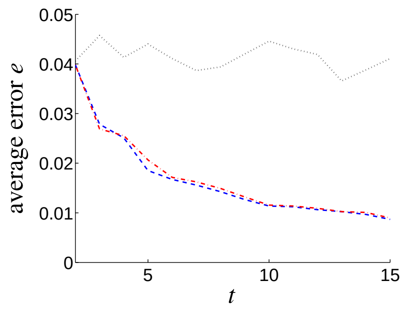
Simulation 4: pressure sensor only

219 ⟨*Sensor speedup examples* 216a⟩+≡ ◁218b 220c▷

```
A = []; B = []; C = []; D = 1; T = 15; ts = 1; s = 0.05;
xini = []; ff = 1; u0 = ones(T, 1) * (-1); test_sensor
```

Uses `test_sensor` 214a.





Dynamic weighing

The third example is the dynamic weighing problem. An object with mass M is placed on a weighting platform with mass m that is modelled as a mass, spring, damper system, see Figure 7.1.

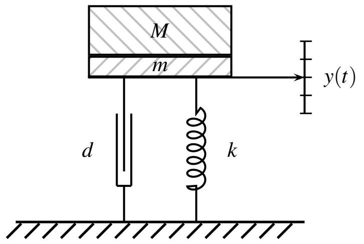


Fig. 7.1 Dynamic weighing setup.

At the time of placing the object, the platform is in a specified (in general nonzero) initial condition. The object placement has the effect of a step input as well as a step change of the total mass of the system—platform and object. The goal is to measure the object's mass while the platform is still in vibration.

We choose the origin of the coordinate system at the equilibrium position of the platform when there is no object placed on it with positive direction being upwards, perpendicular to the ground. With $y(t)$ being the platform's position at time t, the measurement process $\mathscr{B}$ is described by the differential equation

$$(M+m)\frac{\mathrm{d}^2}{\mathrm{d}t^2}y = -ky - d\frac{\mathrm{d}}{\mathrm{d}t}y - Mg,$$

where g is the gravitational constant,

220a ⟨*define the gravitational constant* 220a⟩≡ (220b)

```
g = 9.81;
```

k is the elasticity constant of the spring, and d is the damping constant of the damper. Defining the state vector $x = (y, \frac{\mathrm{d}}{\mathrm{d}t}y)$ and taking as an input $u_0 = Ms$, we obtain the following state space representation $\mathscr{B}_{\mathrm{i/s/o}}(A,b,c,0)$ of $\mathscr{B}$, where

$$A = \begin{bmatrix} 0 & 1 \\ \frac{k}{M+m} & \frac{d}{M+m} \end{bmatrix}, \qquad B = \begin{bmatrix} 0 \\ -\frac{g}{M+m} \end{bmatrix}, \qquad C = \begin{bmatrix} 1 & 0 \end{bmatrix}, \qquad \text{and} \qquad D = 0.$$

220b ⟨*weighting process* 220b⟩≡ (220 221)

```
⟨define the gravitational constant 220a⟩
A = [0, 1; -k / (m + M), -d / (m + M)];
B = [0; -g / (m + M)]; C = [1, 0]; D = 0;
u0 = ones(T, 1) * M;
```

Note that the process parameters and, in particular, its poles depend on the unknown parameter M, however, the dc-gain

$$\mathrm{dcgain}(\mathscr{B}) = -\frac{g}{k}$$

is independent of M. Therefore, the setup in Problem 7.3—prior knowledge of the dc-gain but unknown process dynamics—matches the actual setup of the dynamic weighing problem.

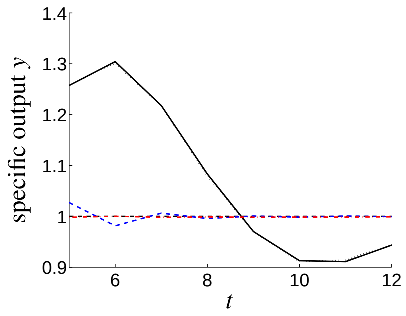
Next, we test the methods `stepid_kf` and `stepid_dd` on dynamic weighing problems with different object's masses.

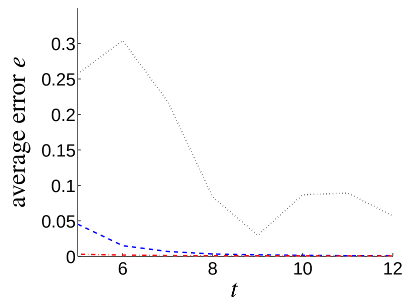
Simulation 5: $M = 1$

220c ⟨*Sensor speedup examples* 216a⟩+≡ ◁219 221a▷

```
m = 1; M = 1; k = 1; d = 1; T = 12; ⟨weighting process 220b⟩
ts = 1; s = 0.02; ff = 1; xini = 0.1 * [1; 1]; test_sensor
```

Uses `test_sensor` 214a.



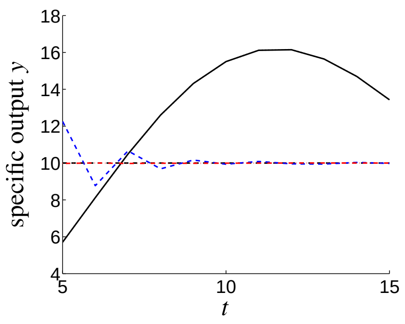


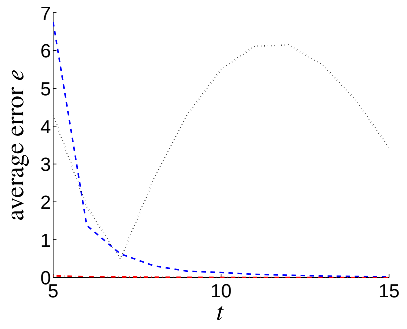
Simulation 6: $M = 10$

221a ⟨*Sensor speedup examples* 216a⟩+≡ ◁220c 221b▷

```
  m = 1; M = 10; k = 1; d = 1; T = 15; ⟨weighting process 220b⟩
  ts = 1; s = 0.05; ff = 1; xini = 0.1 * [1; 1]; test_sensor
```

Uses `test_sensor` 214a.



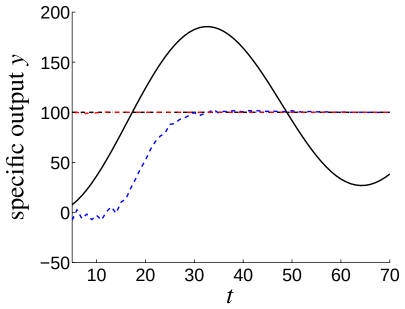


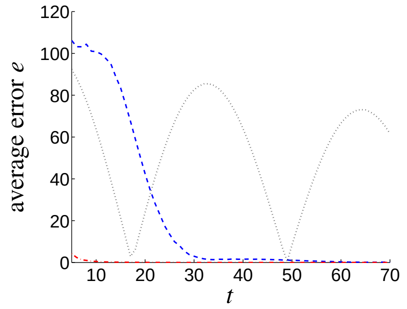
Simulation 7: $M = 100$

221b ⟨*Sensor speedup examples* 216a⟩+≡ ◁221a 222▷

```
  m = 1; M = 100; k = 1; d = 1; T = 70; ⟨weighting process 220b⟩
  ts = 1; s = 0.5; ff = 1; xini = 0.1 * [1; 1]; test_sensor
```

Uses `test_sensor` 214a.





Time-varying parameter

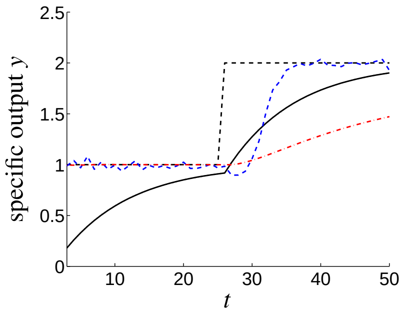
Finally, we show an example with a time-varying measured parameter $\bar{u}$. The measurement setup is the cooling process with the parameter a changing from 1 to 2 at time $t = 25$. The performance of the estimates in the interval $[1,25]$ (estimation of the initial value 1) was already observed in Simulations 1 and 2 for the exact and noisy case, respectively. The performance of the estimates in the interval $[26,50]$ (estimation of the new value $\bar{u} = 2$) is new characteristic for the adaptive properties of the algorithms.

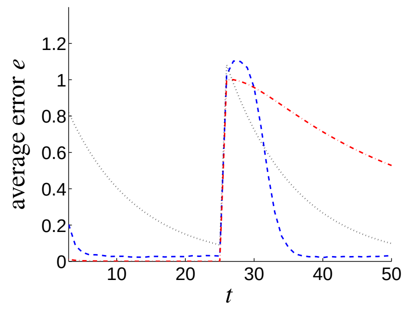
Simulation 8: parameter jump

222 ⟨*Sensor speedup examples* 216a⟩+≡ ◁221b

```
  a = 0.1; ⟨cooling process 216b⟩ T = 50; ts = 1; s = 0.001; ff = 0.5;
  u0 = [ones(T / 2, 1); 2 * ones(T / 2, 1)]; xini = 0;
  test_sensor
```

Uses `test_sensor` 214a.





The result shows that by choosing "properly" the forgetting factor f ($f = 0.5$ in Simulation 8), `stepid_dd` tracks the changing parameter value. In contrast, `stepid_kf` which assumes constant parameter value is much slower in correcting the old parameter estimate $\widehat{u} \approx 1$.

Currently the choice of a the forgetting factor f is based on the heuristic rule that "slowly" varying parameter requires value of f "close" to 1 and "quickly" changing parameter requires value of f close to 0. A suitable value is fine tuned by trail and error.

Another possibility for making `stepid_dd` adaptive is to include windowing of the data y by down-dating of the recursive least squares solution. In this case the tunable parameter (similar to the forgetting factor) is the window length. Again there is an obvious heuristic for choosing the window length but no systematic procedure. Windowing and exponential weighting can be combined, resulting in a method with two tunable parameter.

Real-life testing

The data-driven algorithms for input estimation are tested also on real-life data of the "dynamic cooling" application. The experimental setup for the data collection is based on the Lego NXT mindstorms digital signal processor and digital temperature sensor, see Figure 7.2.

As a true measured value $\bar{u}$, we take the (approximate) steady-state temperature $\bar{y} := y(40)$. In order to apply the model based `stepid_kf` method, the measured data is fitted by a first order model and an output error standard deviation $\sigma = 0.01$ is hypothesised. The fit of the model to the data is shown in Figure 7.3, left. The data-driven algorithm `stepid_dd` is applied with forgetting factor $f = 0.75$.

Fig. 7.2 Experimental setup: Lego NXT mindstorms brick (left) and temperature sensor (right).

The recursive estimation results are shown in Figure 7.3, right. Although initially the model based estimation method is more accurate, after 15 sec. the data-driven method outperforms it.

First, we load the data and apply the data-driven algorithm

223a ⟨*Test sensor speedup methods on measured data* 223a⟩≡ 223b▷

```
load('y-tea.mat'); ub = y(end);
T = length(y); G = 1; n = 1; ff = .75; s = 0.01;
uh_dd = stepid_dd(y, G, n, ff);
```

Defines:
  `test_lego`, never used.
Uses `stepid_dd` 212.

Then the data is modeled by removing the steady state value and fitting an exponential to the residual. The obtained model is a first order dynamical system, which is used for the model based input estimation method.

223b ⟨*Test sensor speedup methods on measured data* 223a⟩+≡ ◁223a 223c▷

```
yc = y - ub; f = yc(1:end - 1) \ yc(2:end);
yh = f .^ (0:(T - 1))' * yc(1) + ub;
sys = ss(f, 1 - f, 1, 0, t(2) - t(1));
uh_kf = stepid_kf(y, sys.a, sys.b, sys.c, sys.d, s^2);
```

Uses `stepid_kf` 205a.

Finally, the estimation results for the naive, model-based, and data-driven methods are plot for comparison.

223c ⟨*Test sensor speedup methods on measured data* 223a⟩+≡ ◁223b

```
figure(1), hold on, plot(t, y, 'b-', t, yh, 'r-')
axis([1 t(end) y(1) y(end)]), print_fig('lego-test-fit')

figure(2), hold on,
plot(t, abs(ub - y / G'), 'k-'),
plot(t, abs(ub - uh_dd), '-b'),
plot(t, abs(ub - uh_kf), '-.r'),
axis([t(10) t(end) 0 5]), print_fig('lego-test-est')
```

Uses `print_fig` 25a.

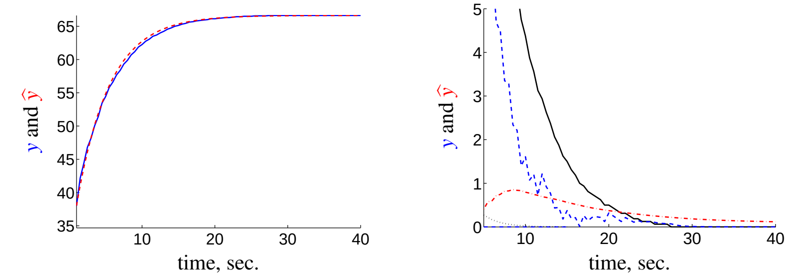


Fig. 7.3 Left: model fit to the data (solid blue—measured data, dashed red—model fit). Right: parameter estimates (solid black—naive estimator, dashed blue—`stepid_dd`, dashed dotted red—`stepid_kf`).

Auxiliary functions

Time-varying Kalman filter

The function `tvkf_oe` implements the time-varying Kalman filter for the discrete-time autonomous stochastic system, described by the state space representation

$$\sigma x = Ax, \qquad y = Cx + v,$$

where v is a stationary, zero mean, white, Gaussian noise with covariance V.

224a ⟨*Time-varying Kalman filter for autonomous output error model* 224a⟩≡ 224b▷

```
function x = tvkf_oe(y, a, c, v, x0, p)
T = size(y, 1); y = y';
```

Defines:
  `tvkf_oe`, used in chunk 206.

The optional parameters `x0` and `p` specify prior knowledge about the mean value of the initial state $x(0)$ and its error covariance matrix P. The default value is highly uncertain zero mean random vector.

The Kalman filter algorithm (see, (Kailath et al, 2000, Theorem 9.2.1)) is

$$\begin{aligned} K &:= APC^\top(V + CPC^\top)^{-1} \\ \sigma\hat{x} &= A\hat{x} + K\big(y - C\hat{x}\big), \qquad x(0) = x_{\text{ini}} \\ \sigma P &= APA^\top - K(V + CPC^\top)K^\top, \qquad P(0) = P_{\text{ini}}. \end{aligned}$$

224b ⟨*Time-varying Kalman filter for autonomous output error model* 224a⟩+≡ ◁224a

```
x = zeros(size(a, 1), T); x(:, 1) = x0;
for t = 1:(T-1)
  k    = (a * p * c') / (v + c * p * c');
  x(:, t + 1) = a * x(:, t) + k * (y(:, t) - c * x(:, t));
  p    = a * p * a' - k * (v + c * p * c') * k';
end
```

Recursive least squares

The function `rls` implements an (exponentially weighted) recursive least squares algorithm (see, (Kailath et al, 2000, Lemma 2.6.1 and Problem 2.6)) for a system of linear equations $Ax \approx b$, where $A \in \mathbb{R}^{m \times n}$, *i.e.*, `rls` computes the (exponentially weighted) least squares approximate solutions $x(n), \dots, x(m)$ of the sequence of problems $A_{1:i,:}x(i) \approx b_{1:i}$, for $i = n, \dots, m$.

225a ⟨*Recursive least squares* 225a⟩≡ 225b▷
```
function x = rls(a, b, f)
[m, n] = size(a); finv = 1 / f;
```
Defines:
`rls`, used in chunk 213.

The input parameter `f`, $f \in (0, 1]$, is called forgetting factor and specifies an exponential weighting $f^i r_i$ of the residual $r := Ax - b$ in the least squares approximation criterion.

Let $a(i)$ be the ith row of A and let $b(i) := b_i$. The (exponentially weighted) recursive least squares algorithm is

$$K := \frac{1}{f} P a^\top \left(1 + \frac{1}{f} a P a^\top\right)^{-1}$$

$$\sigma x = x + K(b - ax), \qquad x(0) = x_{\text{ini}}$$

$$\sigma P = \frac{1}{f}\big(P - KaP\big), \qquad P(0) = P_{\text{ini}}.$$

225b ⟨*Recursive least squares* 225a⟩+≡ ◁225a
```
⟨initialization 225c⟩
for i = (n + 1):m
  ai = a(i, :);
  k  = finv * p * ai' / (1 + finv * ai * p * ai');
  x(:, i) = x(:, i - 1) + k * (b(i) - ai * x(:, i - 1));
  p  = finv * (p - k * ai * p);
end
```

The algorithm is initialized with the solution of the system formed by the first `n` equations

$$x_{\text{ini}} := A_{1:n,:}^{-1} b_{1:n}, \qquad P_{\text{ini}} := (A_{1:n,:}^\top A_{1:n,:})^{-1}.$$

225c ⟨*initialization* 225c⟩≡ (225b)
```
ai = a(1:n, 1:n); x = zeros(n, m);
x(:, n) = ai \ b(1:n); p = inv(ai' * ai);
```

7.5 Notes and references

In metrology the problem considered in this chapter is called *dynamic measurement*. The methods proposed in the literature, see the survey (Eichstädt et al, 2010) and the

references there in, pose and solve the problem as a compensator design problem, *i.e.*, the input estimation problem is solved by:

1. designing off-line a dynamical system, called compensator, such that the series connection of the measurement process with the compensator is an identity, and
2. processing on-line the measurements by the compensator.

Most authors aim at a linear time-invariant compensator and assume that a model of the measurement process is a priori given. This is done presumably due to the simplification that the linear-time invariant assumption of the compensator brings in the design stage and the reduced computational cost in the on-line implementation compared to alternative nonlinear compensators. In the case of known model, step 1 of the dynamic measurement problem reduces to the classical problem of designing an inverse system (Sain and Massey, 1969). In the presence of noise, however, compensators that take into account the noise are needed. To the best of our knowledge, there is no theoretically sound solution of the dynamic measurement problem in the noisy case available in the literature although, as shown in Section 7.2, the problem reduces to a state estimation problem for a suitably defined autonomous linear time-invariant system. As a consequence, under standard assumptions about the measurement and process noises, the maximum likelihood solution is given by the Kalman filter, designed for the autonomous system.

More flexible is the approach of (Shu, 1993), where the compensator is tuned on-line by a parameter estimation algorithm. In this case, the compensator is a nonlinear system and an a priori given model of the process is no longer required. The solutions proposed in (Jafaripanah et al, 2005; Shu, 1993), however, are tailored to the dynamic weighing problem, where the measurement process dynamics is a specific second order system.

Compared with the existing results on the dynamic measurement problem in the literature the methods described in the chapter have the following advantages.

- The considered measurement process dynamics is a general linear multivariable system. This is a significant generalization of the previously considered dynamic measurement problems (single input single output, first and second order systems).
- In the case of known measurement process dynamics, the problem is shown to be equivalent to a state estimation problem for an augmented system, which implies that the standard Kalman filter, designed for the augmented system is the optimal estimator in the case of Gaussian noise. Efficient filtering algorithms for systems with `m` constant inputs that avoid the increase in the state dimension from the original system's order `n` to $\mathtt{n} + \mathtt{m}$ are described in (Friedland, 1969; Willman, 1969).
- In the case of unknown measurement process dynamics, the problem is solved as an input estimation problem. The solution leads to recursive on-line algorithms that can be interpreted as nonlinear compensators, however, we do not a priori restrict the solution to a special type of compensator, such as linear time-invariant system tuned by an adaptive filter of a specific type.

- The data-driven solution derived uses a recursive least squares algorithm, so that it can be viewed as a nonlinear compensator, similar to the one of (Shu, 1993) derived for the case of a second order single input single output system. The data-driven solution proposed, however, applies to higher order multivariable systems. In addition, unlike the use of recursive least squares in (Shu, 1993) for model parameter estimation, the data-driven algorithm estimates directly the parameter of interest. This leads to significant computational savings. The on-line computational cost of the data-driven algorithm is comparable to the one of running a full order linear time-invariant compensator in the case of known process model.
  The data driven method for estimation of the input value is similar to the data driven simulation and control methods of (Markovsky, 2010; Markovsky and Rapisarda, 2008). The key link between the set of system's trajectories and the image of the Hankel matrix requiring persistency of excitation of the input and controllability of the system is proven in (Willems et al, 2005), see also (Markovsky et al, 2006, Section 8.4).

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Appendix A
Approximate solution of an overdetermined system of equations

Approximate solution of an overdetermined system of linear equations $AX \approx B$ is one of the main topics in (numerical) linear algebra and is covered in any linear algebra textbook, see, *e.g.*, (Strang, 1976, Section 3.3), (Meyer, 2000, Sections 4.6 and 5.14), and (Trefethen and Bau, 1997, Lecture 11). The classical approach is approximate solution in the least squares sense:

$$\text{minimize} \quad \text{over } \widehat{B} \text{ and } X \quad \|B - \widehat{B}\|_{\mathrm{F}} \quad \text{subject to} \quad AX = \widehat{B}, \tag{LS}$$

where the matrix B is modified as little as possible in the sense of minimizing the correction size $\|B - \widehat{B}\|_{\mathrm{F}}$, so that the modified system of equations $AX = \widehat{B}$ is compatible. The classical least squares problem has an analytic solution: assuming that that the matrix A is full column rank, the unique least squares approximate solution is

$$\widehat{X}_{\mathrm{ls}} = (A^{\top}A)^{-1}A^{\top}B \qquad \text{and} \qquad \widehat{B}_{\mathrm{ls}} = A(A^{\top}A)^{-1}A^{\top}B.$$

In the case when A is rank deficient, the solution is either nonunique or does not exist. Such least squares problems are solved numerically by regularization techniques, see, *e.g.*, (Björck, 1996, Section 2.7).

There are many variations and generalizations of the least squares method for solving approximately an overdetermined system of equations. Well known ones are methods for recursive least squares approximation (Kailath et al, 2000, Section 2.6), regularized least squares (Hansen, 1997), linear and quadratically constrained least squares problems (Golub and Van Loan, 1996, Section 12.1).

Next, we list generalizations related to the class of the total least squares methods because of their close connection to corresponding low-rank approximation problems. Total least squares methods are low-rank approximation methods using an input/output representation of the rank constraint. In all these problems the basic idea is to modify the given data as little as possible, so that the modified data defines a consistent system of equations. In the different methods, however, the correction is done and its size is measured in different ways. This results in different properties of the methods in a stochastic estimation setting and motivates the use of the methods in different practical setups.

- The *data least squares* (Degroat and Dowling, 1991) method is the “reverse” of the least squares method in the sense that the matrix A is modified and the matrix B is not:

$$\text{minimize} \quad \text{over } \widehat{A} \text{ and } X \quad \|A - \widehat{A}\|_{\mathrm{F}} \quad \text{subject to} \quad \widehat{A}X = B. \tag{DLS}$$

  As in the least squares problem, the solution of the data least squares is computable in closed form.
- The classical *total least squares* (Golub, 1973; Golub and Reinsch, 1970; Golub and Van Loan, 1980) method modifies symmetrically the matrices A and B:

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{A}, \widehat{B}, \text{and } X \quad \big\| \begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} \big\|_{\mathrm{F}} \\ &\text{subject to} \quad \widehat{A}X = \widehat{B}. \end{aligned} \tag{TLS}$$

  Conditions for existence and uniqueness of a total least squares approximate solution are given in terms of the singular value decomposition of the augmented data matrix $\begin{bmatrix} A & B \end{bmatrix}$. In the generic case when a unique solution exists, that solution is given in terms of the right singular vectors of $\begin{bmatrix} A & B \end{bmatrix}$ corresponding to the smallest singular values. In this case, the optimal total least squares approximation $\begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix}$ of the data matrix $\begin{bmatrix} A & B \end{bmatrix}$ coincides with the Frobenius norm optimal low-rank approximation of $\begin{bmatrix} A & B \end{bmatrix}$, *i.e.*, in the generic case, the model obtained by the total least squares method coincides with the model obtained by the unstructured low-rank approximation in the Frobenius norm.

Theorem A.1. *Let $\widehat{D}^*$ be a solution to the low-rank approximation problem*

$$\text{minimize} \quad \textit{over } \widehat{D} \quad \|D - \widehat{D}\|_{\mathrm{F}} \quad \textit{subject to} \quad \operatorname{rank}(\widehat{D}) \leq \mathtt{m}$$

and let $\widehat{\mathscr{B}}^* = \operatorname{image}(\widehat{D}^*)$ be the corresponding optimal linear static model. The parameter $\widehat{X}^*$ of an input/output representation $\widehat{\mathscr{B}}^* = \mathscr{B}_{\mathrm{i/o}}(\widehat{X}^*)$ of the optimal model is a solution to the total least squares problem (TLS) with data matrices

$$\begin{array}{r} \mathtt{m} \; \{ \\ \mathtt{q}-\mathtt{m} \; \{ \end{array} \begin{bmatrix} A^{\top} \\ B^{\top} \end{bmatrix} = D \in \mathbb{R}^{\mathtt{q} \times N}.$$

A total least squares solution $\widehat{X}^*$ exists if and only if an input/output representation $\mathscr{B}_{\mathrm{i/o}}(\widehat{X}^*)$ of $\widehat{\mathscr{B}}^*$ exists and is unique if and only if an optimal model $\widehat{\mathscr{B}}^*$ is unique. In the case of existence and uniqueness of a total least squares solution

$$\widehat{D}^* = \begin{bmatrix} \widehat{A}^* & \widehat{B}^* \end{bmatrix}^{\top}, \qquad \textit{where} \quad \widehat{A}^*\widehat{X}^* = \widehat{B}^*.$$

The theorem makes explicit the link between low-rank approximation and total least squares. From a data modeling point of view, total least squares is low-rank approximation of the data matrix $D = \begin{bmatrix} A & B \end{bmatrix}^\top$, followed by input/output representation of the optimal model.

231a ⟨*Total least squares* 231a⟩≡
```
function [x, ah, bh] = tls(a, b)
n = size(a, 2); [r, p, dh] = lra([a b]', n);
⟨low-rank approximation ↦ total least squares solution 231b⟩
```
Defines:
`tls`, never used.
Uses `lra` 66.

231b ⟨*low-rank approximation ↦ total least squares solution* 231b⟩≡ (231a 232)
```
x = p2x(p); ah = dh(1:n, :); bh = dh((n + 1):end, :);
```

Lack of solution of the total least squares problem (TLS)—a case called nongeneric total least squares problem—is caused by lack of existence of an input/output representation of the model. Nongeneric total least squares problems are considered in (Paige and Strakos, 2005; Van Huffel and Vandewalle, 1988, 1991).

- The *generalized total least squares* (Van Huffel and Vandewalle, 1989) method measures the size of the data correction matrix

$$\begin{bmatrix} \Delta A & \Delta B \end{bmatrix} := \begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix}$$

after row and column weighting:

$$\text{minimize} \quad \text{over } \widehat{A}, \widehat{B}, \text{ and } X \quad \left\| W_\text{l} \left(\begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} \right) W_\text{r} \right\|_\text{F} \qquad \text{subject to} \quad \widehat{A}X = \widehat{B}. \tag{GTLS}$$

Here the matrices are W_l and W_r are positive semidefinite weight matrices—W_l corresponds to weighting of the rows and W_r to weighting of the columns of the correction $\begin{bmatrix} \Delta A & \Delta B \end{bmatrix}$. Similarly to the classical total least squares problem, the existence and uniqueness of a generalized total least squares approximate solution is determined from the singular value decomposition. The data least squares and total least squares problems are special cases of the generalized total least squares problem.

- The *restricted total least squares* (Van Huffel and Zha, 1991) method constrains the correction to be in the form

$$\begin{bmatrix} \Delta A & \Delta B \end{bmatrix} = P_\text{e} E L_\text{e}, \qquad \text{for some } E,$$

i.e., the row and column span of the correction matrix are constrained to be within the given subspaces image(P_e) and image$(L_\text{e}^\top)$, respectively. The restricted total least squares problem is:

$$\text{minimize} \quad \text{over } \widehat{A}, \widehat{B}, E, \text{ and } X \quad \|E\|_\text{F} \qquad \text{subject to} \quad \begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} = P_\text{e} E L_\text{e} \quad \text{and} \quad \widehat{A}X = \widehat{B}. \tag{RTLS}$$

The generalized total least squares problem is a special case of (RTLS).

- The *Procrustes problem*: given $m \times n$ real matrices A and B,

$$\text{minimize over } X \quad \|B - AX\|_\text{F} \quad \text{subject to} \quad X^\top X = I_\text{n}$$

is a least squares problem with a constraint that the unknown X is an orthogonal matrix. The solution is given by $X = UV^\top$, where $U\Sigma V^\top$ is the singular value decomposition of $AB^\top$, see (Golub and Van Loan, 1996, page 601).

- The *weighted total least squares* (De Moor, 1993, Section 4.3) method generalizes the classical total least squares problem by measuring the correction size by a weighted matrix norm $\|\cdot\|_W$

$$\text{minimize} \quad \text{over } \widehat{A}, \widehat{B}, \text{ and } X \quad \left\| \begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} \right\|_W \qquad \text{subject to} \quad \widehat{A}X = \widehat{B}. \tag{WTLS}$$

Special weighted total least squares problems correspond to weight matrices W with special structure, *e.g.*, diagonal W corresponds to *element-wise weighted total least squares* (Markovsky et al, 2005). In general, the weighted total least squares problem has no analytic solution in terms of the singular value decomposition, so that contrary to the above listed generalizations, weighted total least squares problems, in general, can not be solved globally and efficiently. Weighted low-rank approximation problems, corresponding to the weighted total least squares problem are considered in (Manton et al, 2003; Markovsky and Van Huffel, 2007a; Wentzell et al, 1997).

232 ⟨*Weighted total least squares* 232⟩≡
```
function [x, ah, bh, info] = wtls(a, b, s, opt)
n = size(a, 2);
[p, l, info] = wlra([a b]', n, s, opt); dh = p * l;
⟨low-rank approximation ↦ total least squares solution 231b⟩
```
Defines:
`wtls`, never used.
Uses `wlra` 142a.

- The *regularized total least squares* (Beck and Ben-Tal, 2006; Fierro et al, 1997; Golub et al, 1999; Sima, 2006; Sima et al, 2004) methods is defined as

$$\text{minimize} \quad \text{over } \widehat{A}, \widehat{B}, \text{ and } X \quad \left\| \begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} \right\|_\text{F} + \gamma \|DX\|_\text{F} \qquad \text{subject to} \quad \widehat{A}X = \widehat{B}. \tag{RegTLS}$$

Global and efficient solution methods for solving regularized total least squares problems are derived in (Beck and Ben-Tal, 2006).

- The *structured total least squares* method (Abatzoglou et al, 1991; De Moor, 1993) method is a total least squares method with the additional constraint that the correction should have certain specified structure

$$\begin{array}{lll} \text{minimize} & \text{over } \widehat{A}, \widehat{B}, \text{and } X & \left\| \begin{bmatrix} A & B \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} \right\|_{\mathrm{F}} \\ \text{subject to} & \widehat{A}X = \widehat{B} \quad \text{and} & \begin{bmatrix} \widehat{A} & \widehat{B} \end{bmatrix} \text{ has a specified structure.} \end{array} \tag{STLS}$$

Hankel and Toeplitz structured total least squares problems are the most often studied ones due to the their application in signal processing and system theory.

- The *structured total least norm* method (Rosen et al, 1996) is the same as the structured total least squares method with a general matrix norm in the approximation criterion instead of the Frobenius norm.

For generalizations and applications of the total least squares problem in the periods 1990–1996, 1996–2001, and 2001–2006, see respectively the edited books (Van Huffel, 1997), (Van Huffel and Lemmerling, 2002), and the special issues (Van Huffel et al, 2007a,b). An overview of total least squares problems is given in (Markovsky and Van Huffel, 2007b; Markovsky et al, 2010; Van Huffel and Zha, 1993).

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Appendix B
Proofs

. . . the ideas and the arguments with which the mathematician is concerned have physical, intuitive or geometrical reality long before they are recorded in the symbolism.

The proof is meaningful when it answers the students doubts, when it proves what is not obvious. Intuition may fly the student to a conclusion but where doubt remains he may then be asked to call upon plodding logic to show the overland route to the same goal.

Kline (1974)

Proof of Proposition 2.23

The proof is given in (Vanluyten et al, 2006). Let $\widehat{D}^*$ be a solution to

$$\widehat{D}^* := \arg\min_{\widehat{D}} \|D-\widehat{D}\| \quad \text{subject to} \quad \operatorname{rank}(\widehat{D}) \leq \mathtt{m}. \tag{LRA}$$

and let

$$\widehat{D}^* := U^* \Sigma^* (V^*)^\top$$

be a singular value decomposition of $\widehat{D}^*$. By the unitary invariance of the Frobenius norm, we have that

$$\|D-\widehat{D}^*\|_{\mathrm{F}} = \|(U^*)^\top (D-\widehat{D}^*)V^*\|_{\mathrm{F}} = \|\underbrace{(U^*)^\top DV^*}_{\widehat{D}} - \Sigma^*\|_{\mathrm{F}},$$

which shows that Σ^* is an optimal approximation of $\widehat{D}$. Partition

$$\widehat{D} =: \begin{bmatrix} \widehat{D}_{11} & \widehat{D}_{12} \\ \widehat{D}_{21} & \widehat{D}_{22} \end{bmatrix}$$

conformably with $\Sigma^* =: \left[\begin{smallmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{smallmatrix}\right]$ and observe that

$$\operatorname{rank}\left(\begin{bmatrix} \Sigma_1^* & \widehat{D}_{12} \\ 0 & 0 \end{bmatrix}\right) \leq \mathtt{m} \quad \text{and} \quad \widehat{D}_{12} \neq 0 \implies \left\|\widehat{D} - \begin{bmatrix} \Sigma_1^* & \widehat{D}_{12} \\ 0 & 0 \end{bmatrix}\right\|_{\mathrm{F}} < \left\|\widehat{D} - \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix}\right\|_{\mathrm{F}},$$

so that $\widehat{D}_{12} = 0$. Similarly $\widehat{D}_{21} = 0$. Observe also that

$$\operatorname{rank}\left(\begin{bmatrix} \widehat{D}_{11} & 0 \\ 0 & 0 \end{bmatrix}\right) \leq \mathtt{m} \quad \text{and} \quad \widehat{D}_{11} \neq \Sigma_1^* \implies \left\|\widehat{D} - \begin{bmatrix} \widehat{D}_{11} & 0 \\ 0 & 0 \end{bmatrix}\right\|_{\mathrm{F}} < \left\|\widehat{D} - \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix}\right\|_{\mathrm{F}},$$

so that $\widehat{D}_{11} = \Sigma_1^*$. Therefore,

$$\widehat{D} = \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & \widehat{D}_{22} \end{bmatrix}.$$

Let

$$\widehat{D}_{22} = U_{22} \Sigma_{22} V_{22}^\top$$

be the singular value decomposition of $\widehat{D}_{22}$. Then the matrix

$$\begin{bmatrix} I & 0 \\ 0 & U_{22}^\top \end{bmatrix} \widehat{D} \begin{bmatrix} I & 0 \\ 0 & V_{22} \end{bmatrix} = \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & \Sigma_{22} \end{bmatrix}$$

has optimal rank-$\mathtt{m}$ approximation $\Sigma^* =: \left[\begin{smallmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{smallmatrix}\right]$, so that

$$\min\big(\operatorname{diag}(\Sigma_1^*)\big) > \max\big(\operatorname{diag}(\Sigma_{22})\big)$$

Therefore,

$$D = U^* \begin{bmatrix} I & 0 \\ 0 & U_{22} \end{bmatrix} \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & \Sigma_{22} \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & V_{22}^\top \end{bmatrix} (V^*)^\top$$

is a singular value decomposition of D.

Then, if $\sigma_{\mathtt{m}} > \sigma_{\mathtt{m}+1}$, the rank-$\mathtt{m}$ truncated singular value decomposition

$$\widehat{D}^* = U^* \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix} (V^*)^\top = U^* \begin{bmatrix} I & 0 \\ 0 & U_{22} \end{bmatrix} \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & V_{22}^\top \end{bmatrix} (V^*)^\top$$

is unique and $\widehat{D}^*$ is the unique solution of (LRA). Moreover, $\widehat{D}^*$ is simultaneously optimal in any unitarily invariant norm.

Proof of Proposition 2.32

The probability density function of the observation vector $\operatorname{vec}(D)$ is

$$p_{\widehat{\mathscr{B}},\widehat{D}}\big(\operatorname{vec}(D)\big) = \begin{cases} \text{const} \cdot \exp\left(-\frac{1}{2\sigma^2}\|\operatorname{vec}(D) - \operatorname{vec}(\widehat{D})\|_{V^{-1}}^2\right), \\ \qquad \text{if } \operatorname{image}(\widehat{D}) \subset \widehat{\mathscr{B}} \text{ and } \dim(\widehat{\mathscr{B}}) \leq \mathtt{m} \\ 0, \quad \text{otherwise}, \end{cases}$$

where "const" is a term that does not depend on $\widehat{D}$ and $\widehat{\mathscr{B}}$. The log-likelihood function is

$$\ell(\widehat{\mathscr{B}},\widehat{D}) = \begin{cases} -\text{const} \cdot \frac{1}{2\sigma^2}\|\operatorname{vec}(D) - \operatorname{vec}(\widehat{D})\|_{V^{-1}}^2, \\ \qquad \text{if } \operatorname{image}(\widehat{D}) \subset \widehat{\mathscr{B}} \text{ and } \dim(\widehat{\mathscr{B}}) \leq \mathtt{m} \\ -\infty, \quad \text{otherwise}, \end{cases}$$

and the maximum likelihood estimation problem is

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{\mathscr{B}} \text{ and } \widehat{D} \quad \frac{1}{2\sigma^2}\|\operatorname{vec}(D)-\operatorname{vec}(\widehat{D})\|_{V^{-1}}^2 \\ \text{subject to} & \operatorname{image}(\widehat{D}) \subset \widehat{\mathscr{B}} \text{ and } \dim(\widehat{\mathscr{B}}) \leq \mathtt{m}, \end{array}$$

which is an equivalent problem to Problem 2.31 with $\|\cdot\| = \|\cdot\|_{V^{-1}}$.

Note B.1 (Weight matrix in the norm specification). The weight matrix W in the norm specification is the inverse of the measurement noise covariance matrix V. In case of singular covariance matrix (*e.g.*, missing data) the method needs modification.

Proof of Theorem 3.16

The polynomial equations (GCD) are equivalent to the following systems of algebraic equations

$$\begin{bmatrix} \widehat{p}_0 \\ \widehat{p}_1 \\ \vdots \\ \widehat{p}_n \end{bmatrix} = \mathscr{T}_{\mathtt{d}+1}^{\top}(u) \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_{\mathtt{d}} \end{bmatrix}, \qquad \begin{bmatrix} \widehat{q}_0 \\ \widehat{q}_1 \\ \vdots \\ \widehat{q}_n \end{bmatrix} = \mathscr{T}_{\mathtt{d}+1}^{\top}(v) \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_{\mathtt{d}} \end{bmatrix},$$

where the Toeplitz matrix constructor $\mathscr{T}$ is defined in ($\mathscr{T}$) on page 88. Rewriting and combining the above equations, we have that a polynomial c is a common factor of $\widehat{p}$ and $\widehat{q}$ with $\operatorname{degree}(c) \leq \mathtt{d}$ if and only if the system of equations

$$\begin{bmatrix} \widehat{p}_0 & \widehat{q}_0 \\ \widehat{p}_1 & \widehat{q}_1 \\ \vdots & \vdots \\ \widehat{p}_n & \widehat{q}_n \end{bmatrix} = \mathscr{T}_{n-\mathtt{d}+1}^{\top}(c) \begin{bmatrix} u_0 & v_0 \\ u_1 & v_1 \\ \vdots & \vdots \\ u_{n-\mathtt{d}} & v_{n-\mathtt{d}} \end{bmatrix}$$

has a solution.

The condition $\operatorname{degree}(c) = \mathtt{d}$ implies that the highest power coefficient $c_{\mathtt{d}}$ of c is different from 0. Since c is determined up to a scaling factor, we can impose the normalization $c_{\mathtt{d}} = 1$. Conversely, imposing the constraint $c_{\mathtt{d}} = 1$ in the optimization problem to be solved ensures that $\operatorname{degree}(c) = \mathtt{d}$. Therefore, Problem 3.13 is equivalent to

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{p}, \widehat{q} \in \mathbb{R}^{n+1},\ u, v \in \mathbb{R}^{n-\mathtt{d}+1}, \text{ and } c_0, \ldots, c_{\mathtt{d}-1} \in \mathbb{R} \\ & \qquad \operatorname{trace}\Big(\big([p\ q] - [\widehat{p}\ \widehat{q}]\big)^{\top}\big([p\ q] - [\widehat{p}\ \widehat{q}]\big)\Big) \\ \text{subject to} & [\widehat{p}\ \widehat{q}] = \mathscr{T}_{n-\mathtt{d}+1}^{\top}(c)\,[u\ v]. \end{array}$$

Substituting $[\widehat{p}\ \widehat{q}]$ in the cost function and minimizing with respect to $[u\ v]$ by solving a least squares problem gives the equivalent problem (AGCD').

Proof of Theorem 5.17

First, we show that the sequence $\widehat{D}^{(1)}, \widehat{D}^{(1)}, \ldots, \widehat{D}^{(k)}, \ldots$ converges monotonically in the Σ-weighted norm $\|\cdot\|_{\Sigma}$. On each iteration, Algorithm 6 solves two optimization problems (steps 1 and 2), which cost functions and constraints coincide with the ones of problem (C$_0$–C$_5$). Therefore, the cost function $\|D - \widehat{D}^{(k)}\|_{\Sigma}^2$ is monotonically nonincreasing. The cost function is bounded from below, so that the sequence

$$\|D - \widehat{D}^{(1)}\|_{\Sigma}^2, \quad \|D - \widehat{D}^{(2)}\|_{\Sigma}^2, \quad \ldots$$

is convergent. This proves $(f(k) \to f^*)$.

Although, $\widehat{D}^{(k)}$ converges in norm, it may not converge element-wise. A sufficient condition for element-wise convergence is that the underlying optimization problem has a solution and this solution is unique, see (Kiers, 2002, Theorem 5). The element-wise convergence of $\widehat{D}^{(k)}$ and the uniqueness (due to the normalization condition (A$_1$)) of the factors $P^{(k)}$ and $L^{(k)}$, implies element-wise convergence of the factor sequences $P^{(k)}$ and $L^{(k)}$ as well. This proves $(D^{(k)} \to D^*)$.

In order to show that the algorithm convergence to a minimum point of (C$_0$–C$_5$), we need to verify that the first order optimality conditions for (C$_0$–C$_5$) are satisfied at a cluster point of the algorithm. The algorithm converges to a cluster point if and only if the union of the first order optimality conditions for the problems on steps 1 and 2 are satisfied. Then

$$P'^{(k-1)} = P'^{(k)} =: P'^{*} \qquad \text{and} \qquad L'^{(k-1)} = L'^{(k)} =: L'^{*}.$$

From the above conditions for a stationary point and the Lagrangians of the problems of steps 1 and 2 and (C$_0$–C$_5$), it is easy to see that the union of the first order optimality conditions for the problems on steps 1 and 2 coincides with the first order optimality conditions of (C$_0$–C$_5$).

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Appendix P
Problems

P.1 (Least squares data fitting). Verify that the least squares fits, shown in Figure 1.1 on page 4, minimize the sums of squares of horizontal and vertical distances. The data points are:

$$d_1 = \begin{bmatrix} -2 \\ 1 \end{bmatrix}, \quad d_2 = \begin{bmatrix} -1 \\ 4 \end{bmatrix}, \quad d_3 = \begin{bmatrix} 0 \\ 6 \end{bmatrix}, \quad d_4 = \begin{bmatrix} 1 \\ 4 \end{bmatrix}, \quad d_5 = \begin{bmatrix} 2 \\ 1 \end{bmatrix},$$
$$d_6 = \begin{bmatrix} 2 \\ -1 \end{bmatrix}, \quad d_7 = \begin{bmatrix} 1 \\ -4 \end{bmatrix}, \quad d_8 = \begin{bmatrix} 0 \\ -6 \end{bmatrix}, \quad d_9 = \begin{bmatrix} -1 \\ -4 \end{bmatrix}, \quad d_{10} = \begin{bmatrix} -2 \\ -1 \end{bmatrix}.$$

P.2 (Distance from a data point to a linear model). The 2-norm distance from a point $d \in \mathbb{R}^{\mathtt{q}}$ to a linear static model $\mathscr{B} \subset \mathbb{R}^{\mathtt{q}}$ is defined as

$$\operatorname{dist}(d, \mathscr{B}) := \min_{\widehat{d} \in \mathscr{B}} \|d - \widehat{d}\|_2, \qquad \text{(dist)}$$

i.e., $\operatorname{dist}(d, \mathscr{B})$ is the shortest distance from d to a point $\widehat{d}$ in $\mathscr{B}$. A vector $\widehat{d}^*$ that achieves the minimum of (dist) is a point in $\mathscr{B}$ that is closest to d.

Next we consider the special case when $\mathscr{B}$ is a linear static model.

1. Let
$$\mathscr{B} = \operatorname{image}(a) = \{\, \alpha a \mid \alpha \in \mathbb{R} \,\}.$$
Explain how to find $\operatorname{dist}\big(d, \operatorname{image}(a)\big)$. Find
$$\operatorname{dist}\big(\operatorname{col}(1,0), \operatorname{image}\big(\operatorname{col}(1,1)\big)\big).$$
Note that the best approximation $\widehat{d}^*$ of d in $\operatorname{image}(a)$ is the orthogonal projection of d onto $\operatorname{image}(a)$.
2. Let $\mathscr{B} = \operatorname{image}(P)$, where P is a given full column rank matrix. Explain how to find $\operatorname{dist}(d, \mathscr{B})$.
3. Let $\mathscr{B} = \ker(R)$, where R is a given full row rank matrix. Explain how to find $\operatorname{dist}(d, \mathscr{B})$.
4. Prove that in the linear static case, a solution $\widehat{d}^*$ of (dist) is always unique?

5. Prove that in the linear static case, the approximation error $\Delta d^* := d - \widehat{d}^*$ is orthogonal to $\mathscr{B}$. Is the converse true, *i.e.*, is it true that if for some $\widehat{d}$, $d - \widehat{d}$ is orthogonal to $\mathscr{B}$, then $\widehat{d} = \widehat{d}^*$?

P.3 (Distance from a data point to an affine model). Consider again the distance $\operatorname{dist}(d, \mathscr{B})$ defined in (dist). In this problem, $\mathscr{B}$ is an affine static model, *i.e.*,

$$\mathscr{B} = \mathscr{B}' + a,$$

where $\mathscr{B}'$ is a linear static model and a is a fixed vector.

1. Explain how to reduce the problem of computing the distance from a point to an affine static model to an equivalent problem of computing the distance from a point to a linear static model (Problem P.2).
2. Find
$$\operatorname{dist}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \ker\big(\begin{bmatrix} 1 & 1 \end{bmatrix}\big) + \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right).$$

P.4 (Geometric interpretation of the total least squares problem). Show that the total least squares problem

$$\begin{aligned} &\text{minimize} \quad \text{over } x \in \mathbb{R},\ \widehat{a} \in \mathbb{R}^N, \text{ and } \widehat{b} \in \mathbb{R}^N \quad \sum_{j=1}^{N} \left\| d_j - \begin{bmatrix} \widehat{a}_j \\ \widehat{b}_j \end{bmatrix} \right\|_2^2 \\ &\text{subject to} \quad \widehat{a}_j x = \widehat{b}_j, \quad \text{for } j = 1, \dots, N \end{aligned} \qquad \text{(tls)}$$

minimizes the sum of the squared orthogonal distances from the data points $d_1, \dots, d_N$ to the fitting line

$$\mathscr{B} = \{\, \operatorname{col}(a,b) \mid xa = b \,\}$$

over all lines passing through the origin, except for the vertical line.

P.5 (Unconstrained problem, equivalent to the total least squares problem). A total least squares approximate solution x_{tls} of the linear system of equations $Ax \approx b$ is a solution to the following optimization problem

$$\text{minimize} \quad \text{over } x, \widehat{A}, \text{ and } \widehat{b} \quad \left\| \begin{bmatrix} A & b \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{b} \end{bmatrix} \right\|_{\text{F}}^2 \quad \text{subject to} \quad \widehat{A}x = \widehat{b}. \qquad \text{(TLS)}$$

Show that (TLS) is equivalent to the unconstrained optimization problem

$$\text{minimize } f_{\text{tls}}(x), \quad \text{where} \quad f_{\text{tls}}(x) := \frac{\|Ax - b\|_2^2}{\|x\|_2^2 + 1}. \qquad \text{(TLS')}$$

Give an interpretation of the function f_{tls}.

P.6 (Lack of total least squares solution). Using the formulation (TLS'), derived in Problem P.5, show that the total least squares line fitting problem (tls) has no solution for the data in Problem P.1.

P.7 (Geometric interpretation of rank-1 approximation). Show that the rank-1 approximation problems

$$\begin{aligned} &\text{minimize} \quad \text{over } R \in \mathbb{R}^{1\times 2},\ R \neq 0, \text{ and } \widehat{D} \in \mathbb{R}^{2\times N} \quad \|D - \widehat{D}\|_{\mathrm{F}}^2 \\ &\text{subject to} \quad R\widehat{D} = 0. \end{aligned} \tag{lra$_R$}$$

and

$$\begin{aligned} &\text{minimize} \quad \text{over } P \in \mathbb{R}^{2\times 1} \text{ and } L \in \mathbb{R}^{1\times N} \quad \|D - \widehat{D}\|_{\mathrm{F}}^2 \\ &\text{subject to} \quad \widehat{D} = PL. \end{aligned} \tag{lra$_P$}$$

minimize the sum of the squared orthogonal distances from the data points $d_1, \dots, d_N$ to the fitting line $\mathscr{B} = \ker(P) = \operatorname{image}(P)$ over all lines passing through the origin. Compare and contrast with the similar statement in Problem P.4.

P.8 (Quadratically constrained problem, equivalent to rank-1 approximation). Show that (lra$_P$) is equivalent to the quadratically constrained optimization problem

$$\text{minimize} \ f_{\mathrm{lra}}(P) \quad \text{subject to} \quad P^\top P = 1, \tag{lra$'_P$}$$

where

$$f_{\mathrm{lra}}(P) = \operatorname{trace}\big(D^\top (I - PP^\top)D\big).$$

Explain how to find all solutions of (lra$_P$) from a solution of (lra$'_P$). Assuming that a solution to (lra$'_P$) exists, is it unique?

P.9 (Line fitting by rank-1 approximation). Plot the cost function $f_{\mathrm{lra}}(P)$ for the data in Problem P.1 over all P such that $P^\top P = 1$. Find from the graph of f_{lra} the minimum points. Using the link between (lra$'_P$) and (lra$_P$), established in Problem P.7, interpret the minimum points of f_{lra} in terms of the line fitting problem for the data in Problem P.1. Compare and contrast with the total least squares approach, used in Problem P.6.

P.10 (Analytic solution of a rank-1 approximation problem). Show that for the data in Problem P.1,

$$f_{\mathrm{lra}}(P) = P^\top \begin{bmatrix} 140 & 0 \\ 0 & 20 \end{bmatrix} P.$$

Using geometric or analytic arguments, conclude that the minimum of f_{lra} for a P on the unit circle is 20 and is achieved for

$$P^{*,1} = \operatorname{col}(0,1) \qquad \text{and} \qquad P^{*,2} = \operatorname{col}(0,-1).$$

Compare the results with those obtained in Problem P.9.

P.11 (Analytic solution of two-variate rank-1 approximation problem). Find an analytic solution of the Frobenius norm rank-1 approximation of a $2 \times N$ matrix.

P.12 (Analytic solution of scalar total least squares). Find an analytic expression for the total least squares solution of the system $ax \approx b$, where $a, b \in \mathbb{R}^m$.

P.13 (Alternating projections algorithm for low-rank approximation). In this problem, we consider a numerical method for rank-r approximation:

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{D} \quad \|D - \widehat{D}\|_{\mathrm{F}}^2 \\ &\text{subject to} \quad \operatorname{rank}(\widehat{D}) \leq \mathtt{m}. \end{aligned} \tag{LRA}$$

The alternating projections algorithm, outlined next, is based on an image representation $\widehat{D} = PL$, where $P \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}$ and $L \in \mathbb{R}^{\mathtt{m}\times N}$, of the rank constraint.

Algorithm 8 Alternating projections algorithm for low rank approximation

```
Input: A matrix $D \in \mathbb{R}^{\mathtt{q}\times N}$, with $\mathtt{q} \leq N$, an initial approximation $\widehat{D}^{(0)} = P^{(0)}L^{(0)}$, $P^{(0)} \in \mathbb{R}^{\mathtt{q}\times\mathtt{m}}$,
    $L^{(0)} \in \mathbb{R}^{\mathtt{m}\times N}$, with $\mathtt{m} \leq \mathtt{q}$, and a convergence tolerance $\varepsilon > 0$.
1: Set $k := 0$.
2: repeat
3:     $k := k + 1$.
4:     Solve: $P^{(k+1)} := \arg\min_P \|D - PL^{(k)}\|_{\mathrm{F}}^2$
5:     Solve: $L^{(k+1)} := \arg\min_L \|D - P^{(k+1)}L\|_{\mathrm{F}}^2$
6:     $\widehat{D}^{(k+1)} := P^{(k+1)}L^{(k+1)}$
7: until $\|\widehat{D}^{(k)} - \widehat{D}^{(k+1)}\|_{\mathrm{F}} < \varepsilon$
Output: Output the matrix $\widehat{D}^{(k+1)}$.
```

1. Implement the algorithm and test it on random data matrices D of different dimensions with different rank specifications and initial approximations. Plot the approximation errors

$$e_k := \|D - \widehat{D}^{(k)}\|_{\mathrm{F}}^2, \qquad \text{for } k = 0, 1, \dots$$

as a function of the iteration step k and comment on the results.

* 2. Give a proof or a counter example for the conjecture that the sequence of approximation errors $e := (e_0, e_1, \dots)$ is well defined, independent of the data and the initial approximation.

* 3. Assuming that e is well defined. Give a proof or a counter example for the conjecture that e converges monotonically to a limit point e_∞.

* 4. Assuming that e_∞ exists, give proofs or counter examples for the conjectures that e_∞ is a local minimum of (LRA) and e_∞ is a global minimum of (LRA).

P.14 (Two-sided weighted low rank approximation). Prove Theorem 2.29 on page 67.

P.15 (Most poweful unfalsified model for autonomous models). Given a trajectory

$$y = \big(y(1), y(2), \dots, y(T)\big)$$

of an autonomous linear time-invariant system $\mathscr{B}$ of order $\mathtt{n}$, find a state space representation $\mathscr{B}_{\text{i/s/o}}(A,C)$ of $\mathscr{B}$. Modify your procedure, so that it does not require prior knowledge of the system order $\mathtt{n}$ but only an upper bound $\mathtt{n}_{\max}$ for it.

P.16 (Algorithm for exact system identification). Develop an algorithm for exact system identification that computes a kernel representation of the model, *i.e.*, implement the mapping

$$w_{\mathrm{d}} \mapsto R(z), \qquad \text{where } \widehat{\mathscr{B}} := \ker\big(R(z)\big) \text{ is the identified model.}$$

Consider separately the cases of known and unknown model order. You can assume that the system is single input single output.

P.17 (A simple method for approximate system identification). Modify the algorithm developed in Problem P.16, so that it can be used as an approximate identification method. You can assume that the system is single input single output and the order is known.

* **P.18 (When is $\mathscr{B}_{\text{mpum}}(w_{\mathrm{d}})$ equal to the data generating system?).** Choose a (random) linear time-invariant system $\mathscr{B}_0$ (the "true data generating system") and a trajectory $w_{\mathrm{d}} = (u_{\mathrm{d}}, y_{\mathrm{d}})$ of $\mathscr{B}_0$. The aim is to recover the data generating system $\mathscr{B}_0$ back from the data w_{d}. Conjecture that this can be done by computing the most powerful unfalsified model $\mathscr{B}_{\text{mpum}}(w_{\mathrm{d}})$. Verify whether and when in simulation $\mathscr{B}_{\text{mpum}}(w_{\mathrm{d}})$ coincides with $\mathscr{B}_0$. Find counter examples when the conjecture is not true and based on this experience revise the conjecture. Find sufficient conditions for $\mathscr{B}_{\text{mpum}}(w_{\mathrm{d}}) = \mathscr{B}_0$.

P.19 (Algorithms for approximate system identification).

1. Download the file `flutter.dat` from a Database for System Identification (Moor et al, 1997).
2. Apply the function developed in Problem **??** on the flutter data using model order $\mathtt{n} = 3$.
3. Compute the misfit between the flutter data and the model obtained in step 1.
4. Compute a locally optimal model of order $\mathtt{n} = 3$ and compare the misfit with the one obtained in step 3.
5. Repeat steps 2–4 for different partitions of the data into identification and validation parts (*e.g.*, first 60% for identification and remaining 40% for validation). More specifically, use only the identification part of the data to find the models and compute the misfit on the unused validation part of the data.

P.20 (Computing approximate common divisor with `slra`). Given polynomials p and q of degree n or less and an integer $\mathtt{d} < \mathtt{n}$, use `slra` to solve the Sylvester structured low rank approximation problem

$$\begin{aligned} &\text{minimize} \quad \text{over } \widehat{p},\widehat{q} \in \mathbb{R}^{n+1} \quad \big\| \begin{bmatrix} p & q \end{bmatrix} - \begin{bmatrix} \widehat{p} & \widehat{q} \end{bmatrix} \big\|_{\mathrm{F}} \\ &\text{subject to} \quad \operatorname{rank}\big(\mathscr{R}_{\mathtt{d}}(\widehat{p},\widehat{q})\big) \leq 2n - 2\mathtt{d} + 1 \end{aligned}$$

in order to compute an approximate common divisor c of p and q with degree at least $\mathtt{d}$. Verify the answer with the alternative approach developed in Section 3.2.

P.21 (Matrix centering). Prove Proposition 5.5.

P.22 (Mean computation as an optimal modeling). Prove Proposition 5.6.

P.23 (Nonnegative low rank approximation). Implement and test the algorithm for nonnegative low rank approximation (Algorithm 7 on page 178).

P.24 ((Luenberger, 1979, Page 53)). A thermometer reading 21°C, which has been inside a house for a long time, is taken outside. After one minute the thermometer reads 15°C; after two minutes it reads 11°C. What is the outside temperature? (According to Newton's law of cooling, an object of higher temperature than its environment cools at a rate that is proportional to the difference in temperature.)

P.25. Solve first Problem P.24. Consider the system of equations

$$\begin{bmatrix} \mathbf{1}_{T-\mathtt{n}} \otimes G & \mathscr{H}_{T-\mathtt{n}}(\Delta y) \end{bmatrix} \begin{bmatrix} \bar{u} \\ \ell \end{bmatrix} = \operatorname{col}\Big(y\big((\mathtt{n}+1)t_s\big), \cdots, y\big(Tt_s\big)\Big), \qquad \text{(SYS DD)}$$

(the data-driven algorithm for input estimation on page 212) in the case of a first order single input single output system and three data points. Show that the solution of the system (SYS DD) coincides with the one obtained in Problem P.24.

P.26. Consider the system of equations (SYS DD) in the case of a first order single input single output system and N data points. Derive an explicit formula for the least squares approximate solution of (SYS DD). Propose a recursive algorithm that updates the current solution when new data point is obtained.

P.27. Solve first Problem P.26. Implement the solution obtained in Problem P.26 and validate it against the function `stepid_dd`.

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Moor BD, Gersem PD, Schutter BD, Favoreel W (1997) DAISY: A database for identification of systems. Journal A 38(3):4–5, available from `http://homes.esat.kuleuven.be/~smc/daisy/`

Appendix S
Solutions

P.1 (Least squares data fitting). Minimization of the vertical distances (lse) for the data in the example is

$$\underbrace{\operatorname{col}(-2,-1,0,1,2,2,1,0,-1,-2)}_{\mathbf{a}}\, x = \underbrace{\operatorname{col}(1,4,6,4,1,-1,-4,-6,-4,-1)}_{\mathbf{b}}.$$

The least squares approximate solution is given by

$$x_{\text{ls}} = (\mathbf{a}^\top \mathbf{a})^{-1}\mathbf{a}^\top \mathbf{b} = \frac{-2-4+0+4+2-2-4+0+4+2}{\mathbf{a}^\top \mathbf{a}} = 0,$$

so that the corresponding fitting line is

$$\mathscr{B}_{\text{ls}} = \{\, d = \operatorname{col}(a,0) \mid a \in \mathbb{R} \,\}$$

the horizontal line passing through the origin.

Minimization of the horizontal distances (lse′), is $\mathbf{a} = \mathbf{b}x'$, with the $\mathbf{a}$ and $\mathbf{b}$ defined above. The least squares approximate solution in this case is

$$x'_{\text{ls}} = (\mathbf{b}^\top \mathbf{b})^{-1}\mathbf{b}^\top \mathbf{a} = 0,$$

so that the corresponding fitting line is

$$\mathscr{B}'_{\text{ls}} = \{\, d = \operatorname{col}(0,b) \mid b \in \mathbb{R} \,\}$$

the vertical line passing through the origin.

P.2 (Distance from a data point to a linear model).

1. Using the image representation image(P) of the model $\mathscr{B}$, the distance computation problem (tls″) is equivalent to the standard least squares problem

$$\operatorname{dist}(d,\mathscr{B}) := \min \|d - \widehat{d}\|_2 \quad \text{subject to} \quad \widehat{d} = P\ell.$$

Therefore, assuming that P is full column rank, the best approximation is

$$\widehat{d}^* = P(P^\top P)^{-1}P^\top d =: \Pi_P d \tag{d^*}$$

and the distance of d to $\mathscr{B}$ is

$$\operatorname{dist}(d,\mathscr{B}) = \|d - \widehat{d}^*\|_2 = \sqrt{d^\top (I - \Pi_P)d}. \tag{dist$_P$}$$

The assumption that "P is full column rank" can be done without loss of generality because there are aways full column rank P's such that image$(P) = \mathscr{B}$ (choose any basis for $\mathscr{B}$).

2. Using the kernel representation ker(R) of the model $\mathscr{B}$, the distance computation problem (tls″) is equivalent to the problem

$$\operatorname{dist}(d,\mathscr{B}) := \min_{\widehat{d}} \|d - \widehat{d}\|_2 \quad \text{subject to} \quad R\widehat{d} = 0.$$

As written, this problem is not a standard least squares problem, however, with the change of variables $\Delta d := d - \widehat{d}$ it can be rewritten as an equivalent ordinary least norm problem

$$\operatorname{dist}(d,\mathscr{B}) := \min_{\widehat{d}} \|\Delta d\|_2 \quad \text{subject to} \quad R\Delta d = Rd.$$

Therefore, assuming that R is full row rank,

$$\Delta d^* = R^\top (RR^\top)^{-1}Rd = \Pi_{R^\top} d$$

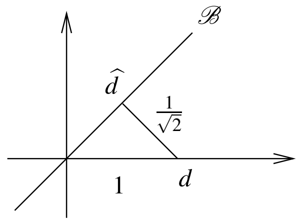
and

$$\operatorname{dist}(d,\mathscr{B}) = \|\Delta d^*\|_2 = \sqrt{d^\top \Pi_{R^\top} d}. \tag{dist$_R$}$$

Again, the assumption that R is full row rank is done without loss of generality because there are full row rank matrices R, such that ker$(R) = \mathscr{B}$.

3. Substituting $d = \left[\begin{smallmatrix}1\\0\end{smallmatrix}\right]$ and $P = \left[\begin{smallmatrix}1\\1\end{smallmatrix}\right]$ in (dist$_P$), we have

$$\begin{aligned}\operatorname{dist}\left(\begin{bmatrix}1\\0\end{bmatrix}, \operatorname{image}\left(\begin{bmatrix}1\\1\end{bmatrix}\right)\right) &= \sqrt{\begin{bmatrix}1 & 0\end{bmatrix}\left(\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} - \begin{bmatrix}1\\1\end{bmatrix}\left(\begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}1\\1\end{bmatrix}\right)^{-1}\begin{bmatrix}1 & 1\end{bmatrix}\right)\begin{bmatrix}1\\0\end{bmatrix}} \\ &= \sqrt{\begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}1/2 & -1/2\\-1/2 & 1/2\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix}} = 1/\sqrt{2}\end{aligned}$$



4. As shown in part 1, $\widehat{d}^*$ is unique (and can be computed by, *e.g.*, (d^*) and (dist$_R$)).
5. A vector Δd is orthogonal to the model $\mathscr{B}$ if and only if Δd is orthogonal to all vectors in $\mathscr{B}$. Using (d^*) and the basis P for $\mathscr{B}$, we have

$$\Delta d^{*\top} P = (d - \widehat{d}^*)^\top P = d^\top (I - \Pi_P) P = 0,$$

which shows that is Δd^* is orthogonal to $\mathscr{B}$.
The converse statement "$\Delta d = d - \widehat{d}$ being orthogonal to $\mathscr{B}$ implies that $\widehat{d}$ is the closest point in $\mathscr{B}$ to d" is also true. It completes the proof of what is known as the *orthogonality principle*—$\widehat{d}$ is an optimal approximation of a point d in a model $\mathscr{B}$ if and only if the approximation error $d - \widehat{d}$ is orthogonal to $\mathscr{B}$.

P.3 (Distance from a data point to an affine model).

- The problem of computing $\operatorname{dist}(d, \mathscr{B})$ reduces to an equivalent problem of computing the distance of a point to a subspace by the change of variables

$$d' := d - a.$$

We have

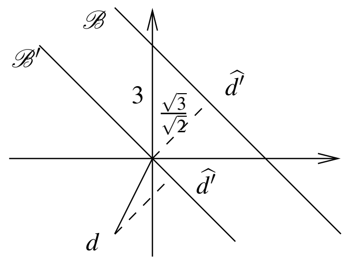
$$\operatorname{dist}(d, \mathscr{B}) = \min_{\widehat{d} \in \mathscr{B}} \|d - \widehat{d}\|_2 = \min_{\widehat{d}' \in \mathscr{B}'} \|d' - \widehat{d}'\|_2 = \operatorname{dist}(d', \mathscr{B}').$$

- Using the change of variables argument we have

$$\operatorname{dist}\left(\begin{bmatrix}0\\0\end{bmatrix}, \ker([1\ 1]) + \begin{bmatrix}1\\2\end{bmatrix}\right) = \operatorname{dist}\left(-\begin{bmatrix}1\\2\end{bmatrix}, \ker([1\ 1])\right).$$

Then using (dist$_R$) we have

$$\operatorname{dist}\left(-\begin{bmatrix}1\\2\end{bmatrix}, \ker([1\ 1])\right) = \sqrt{[1\ 2]\begin{bmatrix}1\\1\end{bmatrix}\left([1\ 1]\begin{bmatrix}1\\1\end{bmatrix}\right)^{-1}[1\ 1]\begin{bmatrix}1\\2\end{bmatrix}} = \sqrt{9/2}.$$



P.4 (Geometric interpretation of the total least squares problem). The constraint of (tls),

$$\widehat{a}_j x = \widehat{b}_j, \quad \text{for } j = 1, \dots, N$$

is equivalent to the constraint that

$$\widehat{d}_1 := (\widehat{a}_1, \widehat{b}_1), \quad \dots, \quad \widehat{d}_N := (\widehat{a}_N, \widehat{b}_N)$$

lie on the line

$$\mathscr{B}_{\text{i/o}}(x) := \{\, d = \operatorname{col}(a, b) \in \mathbb{R}^2 \mid ax = b \,\},$$

i.e., (tls) can be written as

$$\begin{array}{ll} \text{minimize} & \text{over } x \text{ and } \widehat{d}_1, \dots, \widehat{d}_N \quad \sum_{j=1}^N \|d_j - \widehat{d}_j\|_2^2 \\ \text{subject to} & \widehat{d}_j \in \mathscr{B}_{\text{i/o}}(x), \quad \text{for } j = 1, \dots, N. \end{array} \tag{tls'}$$

In turn, problem (tls') is equivalent to minimization of the function $f_{\text{tls}} : \mathbb{R} \to \mathbb{R}$ defined by

$$\begin{aligned} f_{\text{tls}}(x) := \min_{\widehat{d}_1, \dots, \widehat{d}_N} \sum_{j=1}^N \|d_j - \widehat{d}_j\|_2^2 \\ \text{subject to} \quad \widehat{d}_j \in \mathscr{B}_{\text{i/o}}(x), \quad \text{for } j = 1, \dots, N. \end{aligned} \tag{tls''}$$

The minimization in (tls'') is separable in the variables $\widehat{d}_1, \dots, \widehat{d}_N$, *i.e.*, (tls'') decouples into N independent problems

$$f_{\text{tls},i}(x) = \min_{\widehat{d}_j} \|d_j - \widehat{d}_j\|_2^2 \quad \text{subject to} \quad \widehat{d}_j \in \mathscr{B}_{\text{i/o}}(x).$$

By the orthogonality principle, $f_{\text{tls},j}(x)$ is the squared orthogonal distance from d_j to the line $\mathscr{B}_{\text{i/o}}(x)$. Subsequently,

$$f_{\text{tls}}(x) = \sum_{j=1}^N f_{\text{tls},j}(x)$$

is the sum of squared orthogonal distances from the data points to the line $\mathscr{B}_{\text{i/o}}(x)$.

For any $x \in \mathbb{R}$, $\mathscr{B}_{\mathrm{i/o}}(x)$ is a line passing through the origin and any line passing through the origin, except for the vertical line, corresponds to a set $\mathscr{B}_{\mathrm{i/o}}(x)$, for some $x \in \mathbb{R}$. Therefore, the total least squares problem $\min_{x\in\mathbb{R}} f_{\mathrm{tls}}(x)$ minimizes the sum of squared orthogonal distances from the data points to a line, over all lines passing through the origin, except for the vertical line.

P.5 (Unconstrained problem, equivalent to the total least squares problem). The total least squares approximation problem (TLS) is $\min_x f_{\mathrm{tls}}(x)$, where

$$f_{\mathrm{tls}}(x) = \min_{\widehat{A},\widehat{b}} \left\| \begin{bmatrix} A & b \end{bmatrix} - \begin{bmatrix} \widehat{A} & \widehat{b} \end{bmatrix} \right\|_{\mathrm{F}}^2 \quad \text{subject to} \quad \widehat{A}x = \widehat{b} \qquad (f_{\mathrm{tls}})$$

or with the change of variables $\Delta A := A - \widehat{A}$ and $\Delta b := b - \widehat{b}$,

$$f_{\mathrm{tls}}(x) = \min_{\Delta A,\Delta b} \left\| \begin{bmatrix} \Delta A & \Delta b \end{bmatrix} \right\|_{\mathrm{F}}^2 \quad \text{subject to} \quad Ax - b = \Delta A x - \Delta b. \qquad (f'_{\mathrm{tls}})$$

Define

$$\Delta b := Ax - b, \qquad \Delta D := \begin{bmatrix} \Delta A & \Delta b \end{bmatrix}^\top, \quad \text{and} \quad r = \begin{bmatrix} x^\top & -1 \end{bmatrix}$$

in order to write (f'_{tls}) as a standard linear least norm problem

$$\min_{\Delta D} \|\Delta D\|_{\mathrm{F}}^2 \quad \text{subject to} \quad r\Delta D = \Delta b^\top.$$

The least norm solution for ΔD is

$$\Delta D^* = \frac{r^\top \Delta b}{rr^\top},$$

so that, we have

$$f_{\mathrm{tls}}(x) = \|\Delta D^*\|_{\mathrm{F}}^2 = \operatorname{trace}\big((\Delta D^*)^\top D^*\big) = \frac{\Delta b^\top \Delta b}{rr^\top} = \frac{\|Ax-b\|^2}{\|x\|^2+1}.$$

From Problem P.4 and the derivation of f_{tls}, we see that $f_{\mathrm{tls}}(x)$ is the sum of squared orthogonal distances from the data points to the model $\mathscr{B}_{\mathrm{i/o}}(x)$, defined by x.

P.6 (Lack of total least squares solution). The total least squares line fitting method, applied to the data in Problem P.1 leads to the overdetermined system of equations

$$\underbrace{\operatorname{col}(-2,-1,0,1,2,2,1,0,-1,-2)}_{\mathbf{a}}\, x = \underbrace{\operatorname{col}(1,4,6,4,1,-1,-4,-6,-4,-1)}_{\mathbf{b}}.$$

Therefore, using the (TLS') formulation, the problem is to minimize the function

$$f_{\mathrm{tls}}(x) = \frac{(\mathbf{a}x-\mathbf{b})^\top(\mathbf{a}x-\mathbf{b})}{x^2+1} = \cdots \begin{array}{c}\text{substituting } \mathbf{a} \text{ and } \mathbf{b} \text{ with} \\ \text{their numerical values}\end{array} \cdots = 20\frac{x^2+7}{x^2+1}.$$

The first derivative of f_{tls} is

$$\frac{\mathrm{d}}{\mathrm{d}x} f_{\mathrm{tls}}(x) = -\frac{240x}{(x^2+1)^2},$$

so that f_{tls} has a unique stationary point at $x = 0$. The second derivative of f_{tls} at $x = 0$ is negative, so that the stationary point is a maximum. This proves that the function f_{tls} has no minimum and therefore the total least squares problem has no solution.

Figure S.1 shows the plot of f_{tls} over the interval $[-6.3, 6.3]$. It can be verified that the infimum of f_{tls} is 20 and f_{tls} has asymptotes

$$f_{\mathrm{tls}}(x) \to 20 \qquad \text{for} \quad x \to \pm\infty,$$

i.e., the infimum is achieved asymptotically as x tends to infinity and to minus infinity.

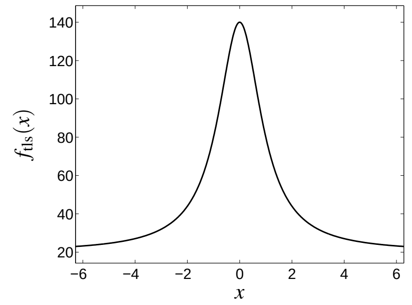


Fig. S.1 Cost function of the total least squares problem (TLS') in Problem P.6.

P.7 (Geometric interpretation of rank-1 approximation). In both problems (lra_R) and (lra_P) the cost function is

$$\|D - \widehat{D}\|_{\mathrm{F}}^2 = \sum_{j=1}^{N} \|d_j - \widehat{d}_j\|_2^2,$$

i.e., the sum of the squared distances from the data points d_j to their approximations $\widehat{d}_j$. The rank-1 constraint of

$$\widehat{D} = \begin{bmatrix} \widehat{d}_1 & \cdots & \widehat{d}_N \end{bmatrix},$$

however, is equivalent to the constraint that the approximations $\widehat{d}_j$ lie on a line $\mathscr{B}$ passing through the origin. In (lra_R), $\mathscr{B} = \ker(R)$ and, in (lra_P), $\mathscr{B} = \operatorname{image}(P)$. By the orthogonality principle, $\widehat{d}_j$ must be the orthogonal projection of d_j on $\mathscr{B}$, so that $\|d - \widehat{d}_j\|_2^2$ is the squared orthogonal distance from d_j to $\mathscr{B}$. Therefore, the rank-1 approximation problems (lra_R) and (lra_P) minimize the sum of the squared orthogonal distances from the data points to the fitting line $\mathscr{B} = \ker(P) = \text{image}(P)$ over all lines passing through the origin.

Comparing the geometric interpretations of the low rank approximation problems (lra_R) and (lra_P) and the total least squares problem (tls), we see that in both cases the same data fitting criterion is minimized, however, the minimization is over different sets of candidate solutions—in the low rank approximation problems *all* lines passing through the origin are considered, while in the total least squares problem all lines passing through the origin *except for* the vertical line are considered.

P.8 (Quadratically constrained problem, equivalent to rank-1 approximation). Consider the rank-1 approximation problem (lra_P) and observe that for a fixed parameter $P \in \mathbb{R}^{2\times 1}$, problem ($\text{lra}_P$) becomes a least squares problem in the parameter $L \in \mathbb{R}^{1\times N}$

$$\text{minimize} \quad \text{over } L \quad \|D - PL\|_\text{F}^2$$

Assuming that P is full column rank (*i.e.*, $P \neq 0$), the solution is unique and is given by

$$L^* = (P^\top P)^{-1} P^\top D.$$

Then the minimum $f_\text{lra}(P) = \|D - PL^*\|_\text{F}^2$ is given by

$$f_\text{lra}(P) = \text{trace}\Big(D^\top \big(I - P(P^\top P)^{-1}P^\top\big)D\Big).$$

The function f_lra, however, depends only on the direction of P, *i.e.*,

$$f_\text{lra}(P) = f_\text{lra}(\alpha P), \quad \text{for all } \alpha \neq 0.$$

Therefore, without loss of generality we can assume that $\|P\|_2 = 1$. This argument and the derivation of f_lra show that problem (lra'_P) is equivalent to problem (lra_P). All solutions of (lra_P) are obtained from a solution P'^* of (lra'_P) by multiplication with a nonzero scalar and vice verse a solution P^* of (lra_P) is reduced to a solution of (lra'_P) by normalization $P^*/\|P^*\|$. A solution to (lra'_P), however, is still not unique because if P'^* is a solution so is $-P'^*$.

P.9 (Line fitting by rank-1 approximation). The set of vectors $P \in \mathbb{R}^2$, such that $P^\top P = 1$, is parametrized by

$$P(\theta) = \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix},$$

where $\theta \in [0, 2\pi)$. The plot of $f_\text{lra}\big(P(\theta)\big)$ over θ is shown in Figure S.2. The global minimum points are

$$\theta^{*,1} = \pi/2 \qquad \text{and} \qquad \theta^{*,2} = 3\pi/2$$

(indicated with dots on the figure) and the global minimum is

$$f_\text{lra}\big(P(\theta^{*,1})\big) = f_\text{lra}\big(P(\theta^{*,2})\big) = 20.$$

The minimum points

$$\theta^{*,1} = \pi/2 \qquad \text{and} \qquad \theta^{*,2} = 3\pi/2$$

correspond to optimal parameters

$$P^{*,1} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \text{and} \qquad P^{*,2} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \tag{$*$}$$

which in the context of the line fitting problem correspond to the vertical line passing through the origin. The link between the low rank approximation (lra_P) and total least squares (tls) problems allow us to compare their respective cost functions f_lra and f_tls. In particular, we see that f_lra achieves the infimum of f_tls.

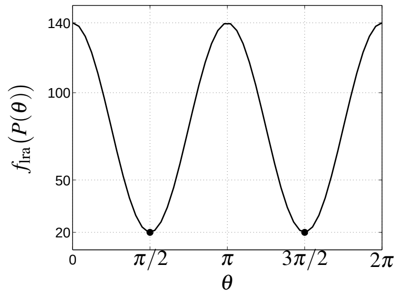


Fig. S.2 Cost function of the rank-1 approximation problem (lra'_P) in Problem P.9.

P.10 (Analytic solution of a rank-1 approximation problem). We have

$$\begin{aligned} f_\text{lra}(P) &= \text{trace}\big(D^\top (I - PP^\top) D\big) \\ &= \text{trace}\big((I - PP^\top) DD^\top\big) \\ &= \cdots \text{ substituting the data and using } P^\top P = p_1^2 + p_2^2 = 1 \;\cdots \\ &= \text{trace}\left(\begin{bmatrix} p_2^2 & -p_1p_2 \\ -p_1p_2 & p_1^2 \end{bmatrix}\begin{bmatrix} 20 & 0 \\ 0 & 140 \end{bmatrix}\right) \\ &= 140p_1^2 + 20p_2^2 = 140\sin^2(\theta) + 20\cos^2(\theta). \end{aligned}$$

From the analytic expression of f_lra it is easy to see that

$$20 \leq f_\text{lra}\big(P(\theta)\big) \leq 140$$

and the minimum is achieved for ($*$), which is the result established in Problem P.9 by less rigorous methods.

P.14 (Two-sided weighted low rank approximation). Define

$$D_{\mathrm{m}} := \sqrt{W_{\mathrm{l}}}D\sqrt{W_{\mathrm{r}}} \qquad \text{and} \qquad \widehat{D}_{\mathrm{m}} := \sqrt{W_{\mathrm{l}}}\widehat{D}\sqrt{W_{\mathrm{r}}}.$$

Since W_{l} and W_{r} are nonsingular,

$$\operatorname{rank}(\widehat{D}) = \operatorname{rank}(\widehat{D}_{\mathrm{m}}).$$

Then, from (WLRA2), we obtain the equivalent problem

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D}_{\mathrm{m}} \quad \|D_{\mathrm{m}} - \widehat{D}_{\mathrm{m}}\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank}(\widehat{D}_{\mathrm{m}}) \leq \mathtt{m}, \end{array} \qquad \text{(WLRA2')}$$

which is an unweighted low rank approximation.

P.11 (Analytic solution of two-variate rank-1 approximation problem). A solution is given by the eigenvalue decomposition of the 2×2 matrix

$$S := DD^{\top} = \begin{bmatrix} s_1 & s_{12} \\ s_{21} & s_2 \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^N d_{1j}^2 & \sum_{j=1}^N d_{1j}d_{2j} \\ \sum_{j=1}^N d_{1j}d_{2j} & \sum_{j=1}^N d_{2j}^2 \end{bmatrix}.$$

Let λ_1 and λ_2 be the eigenvalues of S. We have

$$\begin{array}{ccc} \lambda_1 + \lambda_2 = s_1 + s_2 & \Longrightarrow & \lambda_2 = s_1 + s_2 - \lambda_1 \\ \lambda_1\lambda_2 = s_1s_2 - s_{12}^2 & & \end{array}$$

Substituting the expression for λ_2 in the second equation, we have

$$\lambda_1^2 - (s_1 + s_2)\lambda_1 + (s_1s_2 - s_{12}^2) = 0,$$

so that

$$\lambda_{1,2} = \frac{1}{2}\left(s_1 + s_2 \pm \sqrt{(s_1 - s_2)^2 + 4s_{12}^2}\right).$$

Let $\lambda_{\min}$ be the smaller eigenvalue. (It corresponds to the minus sign.)

Next, we solve for an eigenvector v, corresponding to $\lambda_{\min}$:

$$(s - \lambda_{\min}I)v = 0$$
$$\Updownarrow$$
$$\begin{bmatrix} s_1 - s_2 + \sqrt{(s_1 - s_2)^2 + 4s_{12}^2} & 2s_{12} \\ 2s_{12} & s_2 - s_1 + \sqrt{(s_1 - s_2)^2 + 4s_{12}^2} \end{bmatrix} v = 0.$$

Provided, $s_{12} \neq 0$, *i.e.*, the rows of D are not perpendicular,

$$v = \alpha \begin{bmatrix} x \\ -1 \end{bmatrix}, \qquad \text{where} \quad x := \frac{s_2 - s_1 + \sqrt{(s_1 - s_2)^2 + 4s_{12}^2}}{2s_{12}}, \qquad (*)$$

and α is an arbitrary nonzero constants.

In this case, parameters of kernel and image representations of the optimal model are

$$R = \begin{bmatrix} x & -1 \end{bmatrix}, \qquad \text{and} \qquad P = \begin{bmatrix} 1 \\ x \end{bmatrix}.$$

(We fixed $\alpha = 1$.) Finally, the optimal approximation $\widehat{D}$ of D is

$$\widehat{D} = P(P^{\top}P)^{-1}P^{\top}D = \frac{x}{1 + x^2}\begin{bmatrix} \frac{1}{x}d_{11} + d_{21} & \cdots & \frac{1}{x}d_{1N} + xd_{2N} \\ d_{11} + xd_{21} & \cdots & d_{1N} + xd_{2N} \end{bmatrix}.$$

Note that in the case $s_{12} \neq 0$, alternative formulas for the eigenvector v, corresponding to $\lambda_{\min}$ can be derived.

P.12 (Analytic solution of scalar total least squares). In the case when a is not perpendicular to b, the total least squares solution exists and is unique. In this case, it is given by $(*)$ (derived in Problem P.11). In the case when $a \perp b$, but $\|a\| > \|b\|$, the total least squares solution is $x = 0$. Otherwise, a total least squares solution does not exists.

P.13 (Alternating projections algorithm for low-rank approximation).

a) MATLAB code for the alternating least squares algorithm:

256a ⟨*Alternating least squares algorithm for low rank approximation* 256a⟩≡
```
function [dh, e] = lra_als(d, p, l, tol, maxiter)
dh = p*l;
e(1) = norm(d - dh, 'fro') ^ 2;
for i = 2:maxiter
    p = d * l' / (l * l'); l = (p' * p) \ p' * d;
    dh_old = dh; dh = p * l; e(i) = norm(d - dh, 'fro') ^ 2;
    if norm(dh_old - dh, 'fro') ^ 2 < tol, break, end
end
```
Defines:
`lra_als`, used in chunk 256b.

A typical error convergence plot (for a 10×10 matrix with rank specification $r = 5$) is shown on Figure S.3.

256b ⟨*test* `lra_als` 256b⟩≡
```
q = 10; N = 10; r = 5;
d = rand(q, N); p = rand(q, r); l = rand(r, N);
[dh, e] = lra_als(d, p, l, 0.0, 25); plot(e)
print_fig('als-conv')
```
Uses `lra_als` 256a.

The convergence is monotonic. The approximation error drops significantly in the first few iteration steps and after that decreases slowly.

b) The sequence e is well defined when $P^{(k)}$ and $L^{(k)}$ are full rank for all $k = 0, 1, \ldots$, however, it may not be well defined when $P^{(k)}$ or $L^{(k)}$ become rank deficient at certain iteration step k. Indeed, rank efficiently of $P^{(k)}$ or $L^{(k)}$ implies that a solution for, respectively, $L^{(k)}$ or $P^{(k+1)}$ is not unique. Then, depending on the choice of the solution different values of e_{k+1} may be obtained.

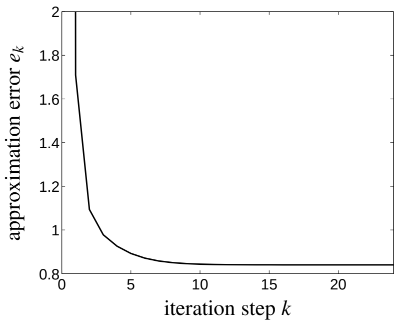


Fig. S.3 Error convergence plot for the alternating least squares algorithm in Problem P.13 (random 10×10 matrix, rank specification $r = 5$, and random initial approximation).

For example, the data Problem P.1 with the initial approximation $L^{(0)} = \mathbf{1}_{10}^{\top}$, results in $P^{(1)} = 0$, which implies that $L^{(1)}$ is arbitrary. Choosing $L^{(1)} = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}$, leads to the error sequence

$$e_1 = 160,\ e_2 = 20,\ e_3 = 20,\ \ldots$$

while $L^{(1)} = \begin{bmatrix} 0 & \cdots & 0 & 1 \end{bmatrix}$, leads to the error sequence

$$e_1 = 160,\ e_2 = 116,\ e_3 = 29,\ e_4 = 20.1996,\ e_5 = 20.0041,\ e_6 = 20.0001,\ \ldots$$

c) See, the proof of Theorem 5.17 on page 240.
d) See, the proof of Theorem 5.17 on page 240.

P.15 (Most poweful unfalsified model for autonomous models). Realization of $H : \mathbb{Z}_+ \to \mathbb{R}^{\mathtt{p}\times\mathtt{m}}$ is equivalent to exact modeling of the time series

$$w_{\mathrm{d},1} = (u_{\mathrm{d},1}, y_{\mathrm{d},1}) := (\delta e_1, h_1), \quad \ldots \quad , w_{\mathrm{d},\mathtt{m}} = (u_{\mathrm{d},\mathtt{m}}, y_{\mathrm{d},\mathtt{m}}) := (\delta e_{\mathtt{m}}, h_{\mathtt{m}}).$$

Consider the impulse response H of the system

$$\mathscr{B}_{\mathrm{i/s/o}}\left(A, \begin{bmatrix} b_1 & \cdots & b_{\mathtt{m}} \end{bmatrix}, C, \bullet\right)$$

and the responses $y_1, \ldots, y_{\mathtt{m}}$ of the autonomous system $\mathscr{B}_{\mathrm{i/s/o}}(A, C)$ due to the initial conditions $b_1, \ldots, b_{\mathtt{m}}$. It is easy to verify that

$$\sigma H = \begin{bmatrix} y_1 & \cdots & y_{\mathtt{m}} \end{bmatrix}.$$

Thus, with the obvious substitution

$$B = \begin{bmatrix} x_0^1 & \cdots & x_0^{\mathtt{m}} \end{bmatrix},$$

where $x_0^1, \ldots, x_0^{\mathtt{m}}$ are the initial conditions generating the responses $h_1, \ldots, h_{\mathtt{m}}$, realization algorithms can be used for exact identification of an autonomous system and

vice verse; algorithms for identification of an autonomous systems can be used for realization.

P.16 (Algorithm for exact system identification). If the order n of the system is known, the exact identification problem reduces to the computation of a basis for the left kernel of the Hankel matrix $\mathscr{H}_{n+1}(w_{\mathrm{d}})$.

258a ⟨*wn2r* 258a⟩≡
```
function R = wn2r(w, n), R = null(blkhank(w, n + 1)')';
```

With unknown order, one can proceed iteratively by attempting to find an exact model of order $n = 1, 2, \ldots$, till such a model exists. This approach moreover guarantees that the result is the most powerful unfalsified model for the data in the model class of linear time-invariant systems.

258b ⟨*w2r* 258b⟩≡
```
function R = w2r(w)
⟨reshape w and define q, T (never defined)⟩
nmax = floor((T - ttw) / (ttw + 1));
for n = 1:nmax
  R = wn2r(w, n); if ~isempty(R), break, end
end
```

P.17 (Algorithm for approximate system identification). A trivial modification in `wn2r`—replacement of exact by approximate computation of left kernel—makes `wn2r` an approximate identification method. The modification based on replacment of `null` by `lra` in `wn2r` is used as initial approximation in the optimization based method `ident_siso` and in Problem P.19. In the single input single output case, the resulting function is

258c ⟨`wn2r_approx` 258c⟩≡
```
function R = wn2r_approx_siso(w, n)
R = lra(blkhank(w, n + 1), 2 * n + 1);
```

P.18 (When is $\mathscr{B}_{\mathrm{mpum}}(w_{\mathrm{d}})$ equal to the data generating system?). Sufficeint conditions are given in Willems et al (2005).

P.19 (Algorithms for approximate system identification).

258d ⟨`test_flutter` 258d⟩≡
```
load flutter.dat; u = flutter(:, 1); y = flutter(:, 2); w = [u'; y']; n = 3
R = wn2r(w, n); ⟨R ↦ P (never defined)⟩
[M1, wh1] = misfit_siso(w, P)
[sysh2, wh2, info] = ident_siso(w, n); M2 = info.M;

figure(1), plot(w(1, :), 'k-'), hold on, plot(wh1(1, :), 'b-'), plot(wh2(1,
figure(2), plot(w(2, :), 'k-'), hold on, plot(wh1(2, :), 'b-'), plot(wh2(2,
```

P.20 (Computing approximate common divisor with `slra`).

258e ⟨*Sylvester matrix constructor* 258e⟩≡
```
function S = sylvester(R, q, n)
[g, nc] = size(R); S = zeros(n * g, nc + (n - 1) * q);
for i = 1:n
  S((1:g) + (i - 1) * g, (1:nc) + (i - 1) * q) = R;
end
```

259 ⟨*Approximate common divisor* 259⟩≡
```
  function c = agcd(R, q, n)
  g = size(R, 1); l = size(R, 2) / q - 1;
  S = sylvester(R, q, n);
  w = lra(S', size(S, 2) - n)'; T = size(w, 1);
  c = lra(blkhank(reshape(w', q, n, T), n + 1), n);
```

P.21 (Matrix centering).

$$\begin{aligned}\mathbf{E}\big(\mathbf{C}(D)\big) &= \mathbf{E}\big(D-\mathbf{E}(D)\mathbf{1}_N^\top\big)\\ &= \frac{1}{N}\big(D-\frac{1}{N}D\mathbf{1}_N\mathbf{1}_N^\top\big)\mathbf{1}_N\\ &= \frac{1}{N}D\mathbf{1}_N-\frac{1}{N^2}D\mathbf{1}_N\underbrace{\mathbf{1}_N^\top\mathbf{1}_N}_{N}=0.\end{aligned}$$

P.22 (Mean computation as an optimal modeling). The optimization problem is a linear least squares problem and its solution is

$$\widehat{c}=D\mathbf{1}_N(\mathbf{1}_N^\top\mathbf{1}_N)^{-1}=\frac{1}{N}D\mathbf{1}_N=\mathbf{E}(D).$$

P.23 (Nonnegative low rank approximation).

P.24 ((Luenberger, 1979, Page 53)). Let $y(t)$ be the reading of the thermometer at time t and let $\bar{u}$ be the environmental temperature. From Newton's law of cooling, we have that

$$\frac{\mathrm{d}}{\mathrm{d}t}y=a\big(\bar{u}s-y\big)$$

for some unknown constant $a\in\mathbb{R}$, $a>0$, which describes the cooling process. Integrating the differential equation, we obtain an explicit formula for y in terms of the constant a, the environmental temperature $\bar{u}$, and the initial condition $y(0)$

$$y(t)=e^{-at}y(0)+(1-e^{-at})\bar{u},\qquad \text{for } t\geq 0 \tag{$*$}$$

The problem is to find $\bar{u}$ from ($*$) given that

$$y(0)=21,\qquad y(1)=15,\qquad \text{and}\qquad y(2)=11.$$

Substituting the data in ($*$), we obtain a nonlinear system of two equations in the unknowns $\bar{u}$ and $f:=e^{-a}$

$$\begin{cases} y(1)=fy(0)+(1-f)\bar{u}\\ y(2)=f^2y(0)+(1-f^2)\bar{u}\end{cases} \tag{$**$}$$

We may stop here and declare that the solution can be computed by a method for solving numerically a general nonlinear system of equations. (Such methods and software are available, see, *e.g.*, (Dennis and Schnabel, 1987).)

System ($**$), however, can be solved without using "nonlinear" methods. Define Δy to be the temperature increment from one measurement to the next, *i.e.*,

$$\Delta y(t):=y(t)-y(t-1),\qquad \text{for all } t.$$

The increments satisfy the homogeneous differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\Delta y(t)=a\Delta y(t),$$

so that

$$\Delta y(t+1)=e^{-a}\Delta y(t)\qquad \text{for } t=0,1,\ldots \tag{$***$}$$

From the given data we evaluate

$$\Delta y(0)=y(1)-y(0)=15-21=-6,\qquad \Delta y(1)=y(2)-y(1)=11-15=-4.$$

Substituting in ($***$), we find the constant

$$f=e^{-a}=2/3.$$

With f known, the problem of solving ($**$) in $\bar{u}$ is linear, and the solution is found to be $\bar{u}=3°\mathrm{C}$.

P.25 The system (SYS DD) is

$$\begin{bmatrix} g & \Delta y(2)\\ g & \Delta y(3)\end{bmatrix}\begin{bmatrix}\bar{u}\\ \ell\end{bmatrix}=\begin{bmatrix}y(2)\\ y(3)\end{bmatrix},$$

and has the unique solution

$$\begin{bmatrix}\bar{u}\\ \ell\end{bmatrix}=\frac{1}{g\big(y(1)-2y(2)+y(3)\big)}\begin{bmatrix}y(1)y(3)-y^2(2)\\ g\big(y(3)-y(2)\big)\end{bmatrix}.$$

It can be shown that in this case

$$e^{-a}=f=\frac{\ell}{\ell-1}\qquad \text{and}\qquad \ell=\frac{f}{f-1}.$$

P.26 The system (SYS DD) is

$$\begin{bmatrix} g & \Delta y(2)\\ \vdots & \vdots\\ g & \Delta y(T)\end{bmatrix}\begin{bmatrix}\bar{u}\\ \ell\end{bmatrix}=\begin{bmatrix}y(2)\\ \vdots\\ y(T)\end{bmatrix},$$

and the corresponding normal equations are

$$\begin{bmatrix}(T-1)g^2 & g\sum_{t=2}^T\Delta y(t)\\ g\sum_{t=2}^T\Delta y(t) & \sum_{t=2}^T\Delta y^2(t)\end{bmatrix}\begin{bmatrix}\bar{u}\\ \ell\end{bmatrix}=\begin{bmatrix}g\sum_{t=2}^T y(t)\\ \sum_{t=2}^T\Delta y(t)y(t)\end{bmatrix}.$$

The least squares approximation of $\bar{u}$ is

$$\widehat{u}(T) = \frac{1}{g\Big((T-1)\sum_{t=2}^{T}\Delta y^2(t) - \big(\sum_{t=2}^{T}\Delta y(t)\big)^2\Big)} \Big(\sum_{t=2}^{T}\Delta y^2(t)\sum_{t=2}^{T}y(t) - \sum_{t=2}^{T}\Delta y(t)\sum_{t=2}^{T}\Delta y(t)y(t)\Big)$$

A recursive algorithm for computing $\widehat{u}$ in real time requires only the four running sums

$$\sum_{\tau=2}^{t}\Delta y^2(\tau), \qquad \sum_{\tau=2}^{t}\Delta y(\tau), \qquad \sum_{\tau=2}^{t}y(\tau), \quad \text{and} \quad \sum_{\tau=2}^{t}\Delta y(\tau)y(\tau).$$

P.27

References

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Notation

Symbolism can serve three purposes. It can communicate ideas effectively; it can conceal ideas; and it can conceal the absence of ideas.

M. Kline, Why Johnny Can't Add: The Failure of the New Math

Sets of numbers

$\mathbb{R}$	the set of real numbers
$\mathbb{Z}$, $\mathbb{Z}_+$	the sets of integers and positive integers (natural numbers)

Norms and extreme eigen/singular values

$\|x\| = \|x\|_2,\ x \in \mathbb{R}^n$	vector 2-norm
$\|w\|,\ w \in (\mathbb{R}^{\mathtt{q}})^T$	signal 2-norm
$\|A\|,\ A \in \mathbb{R}^{m\times n}$	matrix induced 2-norm
$\|A\|_{\mathrm{F}},\ A \in \mathbb{R}^{m\times n}$	matrix Frobenius norm
$\|A\|_W,\ W \geq 0$	matrix weighted norm
$\|A\|_*$	nuclear norm
$\lambda(A),\ A \in \mathbb{R}^{m\times m}$	spectrum (set of eigenvalues)
$\lambda_{\min}(A)$, $\lambda_{\max}(A)$	minimum, maximum eigenvalue of a symmetric matrix
$\sigma_{\min}(A)$, $\sigma_{\max}(A)$	minimum, maximum singular value of a matrix

Matrix operations

A^+, $A^\top$	pseudoinverse, transpose
$\mathrm{vec}(A)$	column-wise vectorization
vec^{-1}	operator reconstructing the matrix A back from $\mathrm{vec}(A)$
$\mathrm{col}(a,b)$	the column vector $\left[\begin{smallmatrix} a \\ b \end{smallmatrix}\right]$
$\mathrm{col\,dim}(A)$	the number of block columns of A
$\mathrm{row\,dim}(A)$	the number of block rows of A
$\mathrm{image}(A)$	the span of the columns of A (the image or range of A)
$\ker(A)$	the null space of A (kernel of the function defined by A)
$\mathrm{diag}(v),\ v \in \mathbb{R}^n$	the diagonal matrix $\mathrm{diag}(v_1,\dots,v_n)$
$\otimes$	Kronecker product $A \otimes B := [a_{ij}B]$
$\odot$	element-wise (Hadamard) product $A \odot B := [a_{ij}b_{ij}]$

Expectation, covariance, and normal distribution

$\mathbf{E}$, cov	expectation, covariance operator
$x \sim \mathrm{N}(m,V)$	x is normally distributed with mean m and covariance V

Fixed symbols

$\mathscr{B}$, $\mathscr{M}$	model, model class
$\mathscr{S}$	structure specification
$\mathscr{H}_i(w)$	Hankel matrix with i *block* rows, see ($\mathscr{H}_i$) on page 10
$\mathscr{T}_i(c)$	upper triangular Toeplitz matrix with i *block* rows, see ($\mathscr{T}$) on page 88
$\mathscr{R}(p,q)$	Sylvester matrix for the pair of polynomials p and q, see ($\mathscr{R}$) on page 11
$\mathscr{O}_i(A,C)$	extended observability matrix with i block-rows, see ($\mathscr{O}$) on page 52
$\mathscr{C}_i(A,B)$	extended controllability matrix with i block-columns, see ($\mathscr{C}$) on page 52

Linear time-invariant model class

$\mathtt{m}(\mathscr{B})$, $\mathtt{p}(\mathscr{B})$	number of inputs, outputs of $\mathscr{B}$
$\mathtt{l}(\mathscr{B})$, $\mathtt{n}(\mathscr{B})$	lag, order of $\mathscr{B}$
$w\|_{[1,T]}$, $\mathscr{B}\|_{[1,T]}$	restriction of w, $\mathscr{B}$ to the interval $[1,T]$, see ($\mathscr{B}\|_{[1,T]}$) on page 53

$$\mathscr{L}^{\mathtt{q},\mathtt{n}}_{\mathtt{m},\mathtt{l}} := \{\, \mathscr{B} \subset (\mathbb{R}^{\mathtt{q}})^{\mathbb{Z}} \mid \mathscr{B} \text{ is linear time-invariant with } \mathtt{m}(\mathscr{B}) \leq \mathtt{m},\ \mathtt{l}(\mathscr{B}) \leq \mathtt{l}, \text{ and } \mathtt{n}(\mathscr{B}) \leq \mathtt{n} \,\}$$

If $\mathtt{m}$, $\mathtt{l}$, or $\mathtt{n}$ are not specified, the corresponding invariants are not bounded.

Miscellaneous

$:= / =:$	left (right) hand side is defined by the right (left) hand side
$:\Longleftrightarrow$	left-hand side is defined by the right-hand side
$\Longleftrightarrow:$	right-hand side is defined by the left-hand side
σ^τ	the shift operator $(\sigma^\tau f)(t) = f(t+\tau)$
$\mathbf{i}$	imaginary unit
δ	Kronecker delta, $\delta_0 = 1$ and $\delta_t = 0$ for all $t \neq 0$
$\mathbf{1}_n = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$	vector with n elements that are all ones
$W \succ 0$	W is positive definite
$\lceil a \rceil$	rounding to the nearest integer greater than or equal to a

With some abuse of notation, the discrete-time signal, vector, and polynomial

$$\big(w(1),\dots,w(T)\big) \quad \leftrightarrow \quad \mathrm{col}\big(w(1),\dots,w(T)\big) \quad \leftrightarrow \quad z^1 w(1) + \cdots + z^T w(T)$$

are all denoted by w. The intended meaning is understood from the context.

List of code chunks

Functions and scripts index

Here is a list of the defined functions and where they appear. Underlined entries indicate the place of definition. This index is generated automatically by `noweb`.

Index