Low-rank approximation and its applications for data fitting

Ivan Markovsky

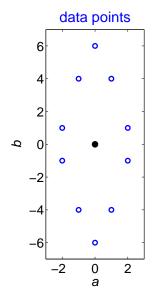
K.U.Leuven, ESAT-SISTA



Algorithms

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A line fitting example



Classical problem: Fit the points

$$d_1 = \begin{bmatrix} 0 \\ 6 \end{bmatrix}, \ d_2 = \begin{bmatrix} 1 \\ 4 \end{bmatrix}, \ \dots, \ d_{10} = \begin{bmatrix} -1 \\ 4 \end{bmatrix}$$

by a line passing through the origin.

Classical solution: Define $d_i =: col(a_i, b_i)$ and solve the least squares problem

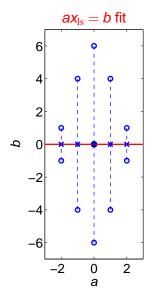
$$\operatorname{col}(a_1,\ldots,a_{10})x=\operatorname{col}(b_1,\ldots,b_{10}).$$

The LS fitting line is given by $ax_{ls} = b$.

It minimizes the vertical distances from the data points to the fitting line.

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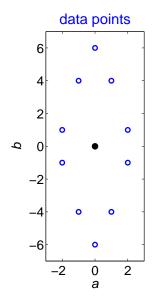
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A line fitting example (cont.)



Minimizing vertical distances does not seem appropriate in this example.

Revised LS problem:

 $\operatorname{col}(a_1,\ldots,a_{10})=\operatorname{col}(b_1,\ldots,b_{10})x$

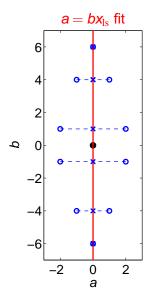
minimize the horizontal distances

The fitting line is now given by $a = bx_{ls}$.

Total least squares fitting:

minimize the orthogonal distances

A line fitting example (cont.)



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Revised LS problem:

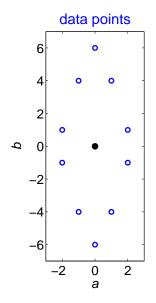
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Total least squares fitting: minimize the orthogonal distances



A line fitting example (cont.)



Total least squares problem:

$$\min_{\substack{x, \widehat{a}_i, \widehat{b}_i}} \sum_{i=1}^{10} \left((a_i - \widehat{a}_i)^2 + (b_i - \widehat{b}_i)^2 \right)$$

subject to $\widehat{a}_i x = \widehat{b}_i, \quad i = 1, \dots, 10$

However, x_{tls} does not exist! ($x_{tls} = \infty$)

If we represent the fitting line as an

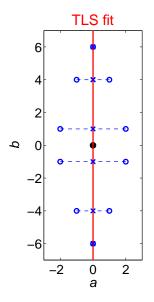
image d = PI or kernel Rd = 0

TLS solutions do exist, e.g.,

$$\label{eq:relation} \textit{P}_{tls} = \textit{col}(0,1) \quad \textit{and} \quad \textit{R}_{tls} = \begin{bmatrix} 1 & 0 \end{bmatrix}.$$

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A line fitting example (cont.)



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What are the issues?

- LS is representation dependent
- TLS is representation invariant
- TLS using I/O representation might have no solution

The representation is a matter of convenience and should not affect the solution.

Orthogonal distance minimization combined with image or kernel representation is a better concept.

Algorithms

In this talk ...

In fact, line fitting is a low-rank approximation (LRA) problem:

approximate $D := \begin{bmatrix} d_1 & \cdots & d_{10} \end{bmatrix}$ by a rank-one matrix,

... a representation free concept applying to general multivariable static and dynamic linear fitting problems.

LRA is closely related to:

- principle component analysis PCA
- latent semantic analysis LSA
- factor models

Algorithms

Related problems



Low-rank approximation as data modeling

Applications

Algorithms

Related problems



Algorithms

Related problems

Low-rank approximation

Given

- a matrix $D \in \mathbb{R}^{d \times N}$, $d \leq N$
- a matrix norm $\|\cdot\|$, and
- an integer m, 0 < m < d,

find

$$\widehat{D}^* := \operatorname*{arg\,min}_{\widehat{D}} \|D - \widehat{D}\|$$
 subject to $\operatorname{rank}(\widehat{D}) \leq \mathfrak{m}.$

Interpretation:

 \widehat{D}^* is optimal rank-m (or less) approximation of D (w.r.t. $\|\cdot\|$).

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Why low-rank approximation?

D is low-rank $\iff D$ is generated by a linear model so that LRA \iff data modeling

Suppose

$$m := \operatorname{rank}(D) < d := \operatorname{rowdim}(D).$$

Then there is a full rank $R \in \mathbb{R}^{p \times d}$, p := d - m, such that RD = 0.

The columns d_1, \ldots, d_N of *D* obey p independent linear relations $r_i d_j = 0$, given by the rows r_1, \ldots, r_p of *R*.

Rd = 0 is a kernel representation of the model $\mathscr{B} := \{ d \mid Rd = 0 \}.$

LRA as data modeling

Given

- *N*, d-variable observations $\begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix} := D \in \mathbb{R}^{d \times N}$
- a matrix norm $\|\cdot\|$, and
- model complexity m, 0 < m < d,

find

$$\widehat{\mathscr{B}}^* := \arg\min_{\widehat{\mathscr{B}},\widehat{D}} \|D - \widehat{D}\| \quad \text{subject to} \quad \begin{array}{c} \operatorname{col} \operatorname{span}(\widehat{D}) \subseteq \widehat{\mathscr{B}} \\ \dim(\widehat{\mathscr{B}}) \leq \mathfrak{m} \end{array}$$

Interpretation:

 $\widehat{\mathscr{B}}^*$ is optimal (w.r.t. $\|\cdot\|$) approximate model for *D* with bounded complexity: dim $(\widehat{\mathscr{B}}) \leq \mathfrak{m} \iff \#$ inputs $\leq \mathfrak{m}$.

Structured low-rank approximation

Given

- a vector $p \in \mathbb{R}^{n_p}$,
- a mapping $\mathscr{S} : \mathbb{R}^{n_p} \to \mathbb{R}^{m \times n}$ (structure specification)
- a vector norm || · ||, and
- an integer *r*, 0 < *r* < min(*m*,*n*),

find

$$\widehat{p}^* := \operatorname*{arg\,min}_{\widehat{p}} \|p - \widehat{p}\|$$
 subject to $\operatorname{rank} \left(\mathscr{S}(\widehat{p}) \right) \leq r.$

Interpretation:

 $\widehat{D}^* := \mathscr{S}(\widehat{\rho}^*)$ is optimal rank-*r* (or less) approx. of $D := \mathscr{S}(\rho)$, within the class of matrices with the same structure as *D*.

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Why structured low-rank approximation?

D = S(p) is low-rank and (Hankel) structured \iff p is generated by a LTI dynamic model

Example: $D = \mathscr{H}_{1+1}(w_d)$ block Hankel and rank deficient $\exists R$, such that $R\mathscr{H}_{1+1}(w_d) = 0$. Taking into account the structure

$$\begin{bmatrix} R_0 & R_1 & \cdots & R_1 \end{bmatrix} \begin{bmatrix} w_d(1) & w_d(2) & \cdots & w_d(T-1) \\ w_d(2) & w_d(3) & \cdots & w_d(T-1+1) \\ \vdots & \vdots & & \vdots \\ w_d(1+1) & w_d(1+2) & \cdots & w_d(T) \end{bmatrix} = 0$$

we have a vector difference equation for w_d with 1 lags

 $R_0 w_d(t) + R_1 w_d(t+1) + \dots + R_1 w_d(t+1) = 0$ for $t = 1, \dots, T-1$.

 \sim

SLRA as time-series modeling

Given

- *T* samples, w variables, vector time series $w_{d} \in (\mathbb{R}^{w})^{T}$,
- a signal norm $\|\cdot\|$, and
- model complexity (m, 1), $0 \leq \mathtt{m} < \mathtt{w},$

find

$$\widehat{\mathscr{B}}^* := \operatorname*{arg\,min}_{\widehat{\mathscr{B}},\widehat{w}} \| w_{\mathrm{d}} - \widehat{w} \| \quad \mathrm{s.t.} \quad \begin{array}{c} \widehat{w} \in \mathscr{B}, \\ \dim(\widehat{\mathscr{B}}) \leq T_{\mathrm{m}} + \mathbb{1}(w-\mathrm{m}) \end{array}$$
(*)

Interpretation:

 $\widehat{\mathscr{B}}^*$ is optimal (w.r.t. $\|\cdot\|$) model for the time series w_d with a bounded complexity: # inputs $\leq m$ and lag ≤ 1 .

(Go back to page 25.)

Kernel, image, and input/output representations

A static model \mathscr{B} with d variables is a subset of \mathbb{R}^d .

How to represent a linear model \mathcal{B} (a subspace) by equations?

Representations:

- kernel: $\mathscr{B} = \ker(R), \qquad R \in \mathbb{R}^{p \times d}$
- image: $\mathscr{B} = \operatorname{col}\operatorname{span}(P), \quad P \in \mathbb{R}^{d \times m}$
- input/output: $\mathscr{B}_{\mathrm{i/o}} = \mathscr{B}(X), \qquad X \in \mathbb{R}^{\mathrm{m} imes \mathrm{p}}$

 $\mathscr{B}_{\mathrm{i/o}}(\boldsymbol{X}) := \{ \, \boldsymbol{d} := \mathsf{col}(\boldsymbol{d}_{\mathrm{i}}, \boldsymbol{d}_{\mathrm{o}}) \in \mathbb{R}^{\mathrm{d}} \mid \boldsymbol{d}_{\mathrm{i}} \in \mathbb{R}^{\mathrm{m}}, \; \boldsymbol{d}_{\mathrm{o}} = \boldsymbol{X}^{\top} \boldsymbol{d}_{\mathrm{i}} \, \}$

In terms of *D*, the I/O repr. is $AX \approx B$, where $\begin{bmatrix} A & B \end{bmatrix} := D^{\top}$.

⇒ Solving $AX \approx B$ approximately by LS, TLS, ... is LRA using I/O representation

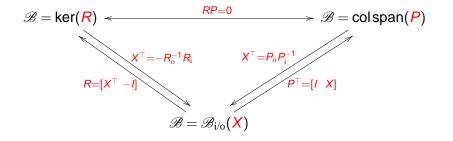
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Links among the parameters *R*, *P*, and *X*

Define the partitionings

$$R =: \begin{bmatrix} R_i & R_o \end{bmatrix}, \quad R_o \in \mathbb{R}^{p imes p} \quad \text{and} \quad P =: \begin{bmatrix} P_i \\ P_o \end{bmatrix}, \quad P_i \in \mathbb{R}^{m imes m}.$$

We have the following links among *R*, *P*, and *X*:



LTI models of bounded complexity

A dynamic model \mathscr{B} with w variables is a subset of $(\mathbb{R}^w)^{\mathbb{Z}}$.

 \mathscr{B} is LTI : $\iff \mathscr{B}$ is a shift-invariant subspace of $(\mathbb{R}^{\mathbb{W}})^{\mathbb{Z}}$.

Let \mathscr{B} be LTI with m inputs, p outputs, of order n and lag 1,

$$\dim \left(\mathscr{B}|_{[0,T]} \right) = \mathsf{m}T + \mathsf{n} \le \mathsf{m}T + \mathsf{pl}, \quad \text{for } T \ge \mathsf{l}.$$

 $dim(\mathscr{B})$ is an indication of the model complexity.

 $\implies \text{The complexity of } \mathscr{B} \text{ is specified by } (\mathtt{m},\mathtt{n}) \text{ or } (\mathtt{m},\mathtt{l}).$

Notation: $\mathscr{L}_{m,1}^{w}$ — LTI model class with bounded complexity # inputs $\leq m$ and lag ≤ 1 .

LTI model representations

• Kernel representation (parameter $R(z) := \sum_{i=0}^{1} R_i z^i$)

$$R_0 w(t) + R_1 w(t+1) + \cdots + R_1 w(t+1) = 0$$

• Impulse response represent (parameter $H : \mathbb{Z} \to \mathbb{R}^{p \times m}$)

$$w = \operatorname{col}(u, y), \qquad y(t) = \sum_{\tau = -\infty}^{t} H(\tau) u(t - \tau)$$

• Input/state/output representation (parameter (A, B, C, D))

$$w = \operatorname{col}(u, y), \qquad \begin{array}{rcl} x(t+1) &=& Ax(t) + Bu(t) \\ y(t) &=& Cx(t) + Du(t) \end{array}$$

Transitions among R, H, (A, B, C, D) are classic problems, e.g.,

R or $H \mapsto (A, B, C, D)$ are realization problems.

Algorithms

Related problems

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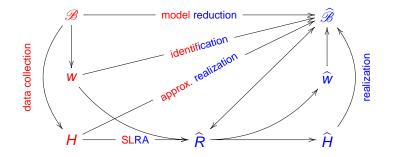
Applications

- System theory
 - 1. Approximate realization
 - 2. Model reduction
 - 3. Errors-in-variables system identification
 - 4. Output error system identification
- Signal processing
 - 5. Output only (autonomous) system identification
 - 6. Finite impulse response (FIR) system identification
 - 7. Harmonic retrieval
 - 8. Image deblurring
- Computer algebra
 - 9. Approximate greatest common divisor (GCD)

System theory applications

- *Itrue* (high order) model
- approximate (low order) model

- w observed response
- *H* observed impulse resp.
- $\widehat{\boldsymbol{w}}$ response of $\widehat{\mathscr{B}}$
- \widehat{H} impulse resp. of $\widehat{\mathscr{B}}$



Generic problem: structured LRA

The applications are special cases of the SLRA problem:

 $\widehat{p}^* := \operatorname*{arg\,min}_{\widehat{p}} \|p - \widehat{p}\|$ subject to $\operatorname{rank} \left(\mathscr{S}(\widehat{p}) \right) \leq r$

for specific choices of p, \mathcal{S} , and r.

 \implies Algorithms and software for SLRA can be readily used.

Notes:

- In many applications, S(·) is composed of blocks that are:
 (H) block Hankel, (U) Unstructured, or (F) Fixed.
- Of interest is the model $\widehat{\mathscr{B}}^*$, given, *e.g.*, by left ker $(\mathscr{S}(\widehat{p}^*))$.
- The algorithms compute \widehat{R} , such that $\widehat{R}\mathscr{S}(\widehat{p}^*) = 0$.

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Errors-in-variables identification

Statistical name for the fitting problem (*) considered before.

Given $w_d \in (\mathbb{R}^w)^T$ and complexity specification (m, 1), find $\widehat{\mathscr{B}}^* := \operatorname*{arg\,min}_{\widehat{\mathscr{B}},\widehat{w}} \|w_d - \widehat{w}\|_{\ell_2}$ subject to $\widehat{w} \in \widehat{\mathscr{B}} \in \mathscr{L}_{m,1}$.

SLRA with $\mathscr{S}(p) = \mathscr{H}_{1+1}(w_d)$, H structure, and r = p.

EIV model: $w_d = \bar{w} + \widetilde{w}, \quad \bar{w} \in \bar{\mathscr{B}} \in \mathscr{L}^w_{m,1}, \quad \widetilde{w} \sim \text{Normal}(0, \sigma^2 I)$

 \overline{w} — true data, $\overline{\mathscr{B}}$ — true model, \widetilde{w} — measurement noise $\widehat{\mathscr{B}}^*$ is a maximum likelihood estimate of $\overline{\mathscr{B}}$, in the EIV model consistent and assympt. normal \implies confidence regions

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Statistical vs. deterministic formulation

The EIV model gives a quality certificate to the method.

The method works "well" (consistency) and is optimal (efficiency) under certain specified conditions.

However, the assumption that the data is generated by a true model with additive noise is sometimes not realistic.

Model-data mismatch is often due to a restrictive (LTI) model class being used and not (only) due to measurement noise.

⇒ The approximation aspect is often more important than the stochastic estimation one.

System theory \leftrightarrow Signal proc. \leftrightarrow Computer algebra

The Toeplitz matrix–vector product $y = \mathscr{T}(H)u = \mathscr{T}(u)H$ is equivalent to (may describe):

$$(u, y) \in \mathscr{B}(H) \iff y = H \star u$$
 $\iff y(z) = H(z)u(z)$
FIR sys. traj. \iff convolution \iff polyn. multipl.
Multivariable case: block Toeplitz structure
multivariable \iff matrix valued \iff matrix valued
systems \iff time series \iff polynomials
2D case: block Toeplitz–Toeplitz block structure
multidim. \iff function of several \iff polyn. of
system \iff indep. variables \iff several var.

(F) Forward problem define $y := \mathscr{T}(u)H$

(I) Inverse problem solve $y = \mathcal{T}(u)H$ for H

| | System theory | Signal proc. | Computer algebra |
|---|-------------------------|--------------|------------------|
| F | FIR sys. simulation | convolution | polyn. multipl. |
| 1 | FIR sys. identification | deconv. | polyn. division |

Typically $y = \mathscr{T}(u)H$ is an overdetermined system of eqns

- \implies With "rough data $w_d = (u_d, y_d)$ ", there is no exact solution.
- → approximate identification, deconvolution, polyn. division.

SLRA: find the smallest modification of the data w_d that allows the modified data \hat{w} to have an exact solution.

Algorithms

Related problems



Low-rank approximation as data modeling

Applications

Algorithms

Related problems



Unstructured low-rank approximation

$$\widehat{D}^* := rgmin_{\widehat{D}} \|D - \widehat{D}\|_{\mathrm{F}}$$
 subject to $\mathrm{rank}(\widehat{D}) \leq \mathfrak{m}$

Theorem (closed form solution)

Let $D = U \Sigma V^{\top}$ be the SVD of D and define

$$U =: \begin{bmatrix} m & p \\ U_1 & U_2 \end{bmatrix} d , \quad \Sigma =: \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} m & \text{and} & V =: \begin{bmatrix} m & p \\ V_1 & V_2 \end{bmatrix} N$$

An optimal LRA solution is

 $\widehat{D}^* = U_1 \Sigma_1 V_1^\top, \qquad \widehat{\mathscr{B}}^* = \ker(U_2^\top) = \operatorname{col}\operatorname{span}(U_1).$

It is unique if and only if $\sigma_m \neq \sigma_{m+1}$.

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Structured low-rank approximation

No closed form solution is known for the general SLRA problem

$$\widehat{\boldsymbol{\rho}}^* := rg\min_{\widehat{\boldsymbol{\rho}}} \|\boldsymbol{\rho} - \widehat{\boldsymbol{\rho}}\| \quad ext{subject to} \quad ext{rank}\left(\mathscr{S}(\widehat{\boldsymbol{\rho}})
ight) \leq r.$$

NP-hard, consider solution methods based on local optimization

Representing the constraint in a kernel form, the problem is

$$\min_{R,RR^{\top}=I_{m-r}} \left(\min_{\widehat{p}} \|p - \widehat{p}\| \quad \text{subject to} \quad R\mathscr{S}(\widehat{p}) = 0 \right)$$

Note: Double minimization with bilinear equality constraint. There is a matrix G(R), such that $R\mathscr{S}(\hat{p}) = 0 \iff G(R)p = 0$.

Variable projection vs. alternating projections

Two ways to approach the double minimization:

• Variable projections (VARPRO): solve the inner minimization analytically

$$\min_{R,RR^{\top}=I_{m-r}} \operatorname{vec}^{\top} \left(R\mathscr{S}(\widehat{\rho}) \right) \left(G(R)G^{\top}(R) \right)^{-1} \operatorname{vec} \left(R\mathscr{S}(\widehat{\rho}) \right)$$

 \rightsquigarrow a nonlinear least squares problem for *R* only.

• Alternating projections (AP): alternate between solving two least squares problems

VARPRO is globally convergent with a super linear conv. rate.

AP is globally convergent with a linear convergence rate.

Algorithms

Related problems

Software implementation

The structure of \mathscr{S} can be exploited for efficient $O(\dim(p))$ cost function and first derivative evaluations.

SLICOT library includes high quality FORTRAN implementation of algorithms for block Toeplitz matrices.

SLRA C software using I/O repr. and VARPRO approach

http://www.esat.kuleuven.be/~imarkovs

Based on the Levenberg–Marquardt alg. implemented in MINPACK.

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Variations on low-rank approximation

- Cost functions
 - weighted norms $(\operatorname{vec}^{\top}(D)W\operatorname{vec}(D))$
 - information criteria (logdet(D))
- Constraints and structures
 - nonnegative
 - sparse
- Data structures
 - nonlinear models
 - tensors
- Optimization algorithms
 - convex relaxations

Weighted low-rank approximation

In the EIV model, LRA is ML assuming $cov(vec(\widetilde{D})) = I$.

Motivation: incorporate prior knowledge W about $cov(vec(\widetilde{D}))$

$$\min_{\widehat{D}} \operatorname{vec}^{\top}(D - \widehat{D}) W \operatorname{vec}(D - \widehat{D}) \quad \operatorname{subject to} \quad \operatorname{rank}(\widehat{D}) \leq \mathfrak{m}$$

Known in chemometrics as maximum likelihood PCA.

NP-hard problem, alternating projections is effective heuristic

Nonnegative low-rank approximation

Constrained LRA arise in Markov chains and image mining

$$\min_{\widehat{D}} \|D - \widehat{D}\| \quad \text{subject to} \quad \operatorname{rank}(\widehat{D}) \leq \mathfrak{m} \text{ and } \widehat{D}_{ij} \geq 0 \text{ for all } i, j.$$

Using an image representation, an equivalent problem is

 $\min_{P \in \mathbb{R}^{d \times m}, L \in \mathbb{R}^{m \times N}} \|D - PL\| \quad \text{subject to} \quad P_{ik}, L_{kj} \ge 0 \text{ for all } i, k, j.$

Alternating projections algorithm:

- Choose an initial approximation $P^{(0)} \in \mathbb{R}^{d \times m}$ and set k := 0.
- Solve: $L^{(k)} = \operatorname{arg\,min}_L \|D P^{(k)}L\|$ subject to $L \ge 0$.
- Solve: $P^{(k+1)} = \operatorname{argmin}_P \|D PL^{(k)}\|$ subject to $P \ge 0$.
- Repeat until convergence.

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Data fitting by a second order model

$$\mathscr{B}(A, b, c) := \{ d \in \mathbb{R}^{d} \mid d^{\top}Ad + b^{\top}d + c = 0 \}, \text{ with } A = A^{\top}$$

Consider first exact data:

$$d \in \mathscr{B}(A, b, c) \iff d^{\top}Ad + b^{\top}d + c = 0$$

$$\iff \langle \underbrace{\operatorname{col}(d \otimes_{s} d, d, 1)}_{d_{ext}}, \underbrace{\operatorname{col}\left(\operatorname{vec}_{s}(A), b, c\right)}_{\theta} \rangle = 0$$

$$\{d_{1}, \dots, d_{N}\} \in \mathscr{B}(\theta) \iff \theta \in \operatorname{leftker}\left[\underbrace{d_{ext,1} \cdots d_{ext,N}}_{D_{ext}}\right], \quad \theta \neq 0$$

$$\iff \operatorname{rank}(D_{ext}) \leq d - 1$$

Therefore, for measured data \rightsquigarrow LRA of D_{ext} .

Notes:

- Special case \mathscr{B} an ellipsoid (for A > 0 and $4c < b^{\top}A^{-1}b$).
- Related to kernel PCA

Consistency in the errors-in-variables setting

Assume that the data is collected according to the EIV model

$$d_i = \overline{d}_i + \widetilde{d}_i$$
, where $\overline{d}_i \in \mathscr{B}(\overline{\theta})$, $\widetilde{d}_i \sim N(0, \sigma^2 I)$.

LRA of D_{ext} (kernel PCA) \rightsquigarrow inconsistent estimator

$$\widetilde{d}_{\mathrm{ext},i} := \mathsf{col}(\widetilde{d}_i \otimes_{\mathrm{s}} \widetilde{d}_i, \widetilde{d}_i, 0)$$
 is not Gaussian

proposed method — incorporate bias correction in the LRA

Notes:

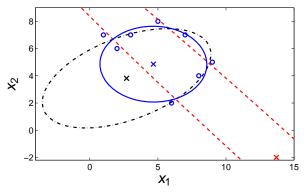
- works on the sample covariance matrix $D_{ext}D_{ext}^{\top}$
- the correction depends on the noise variance σ^2
- the core of the proposed method is the σ² estimator (possible link with methods for choosing regularization par.)

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Example: ellipsoid fitting

benchmark example of (Gander et.al. 94), called "special data"



dashed — LRA solid — proposed method

dashed-dotted — orthogonal regression (geometric fitting)

 \circ — data points \times — centers

Algorithms

Summary

- LRA \iff linear data modeling (in the behavioral setting)
- rank and behavior ~> representation-free problems
- however, different repr. are convenient for different goals
- $AX \approx B$ is LRA with fixed I/O repr. \rightarrow lack of solution
- applications in system theory, signal processing, and computer algebra
- links with rank minimization, structured pseudospectra, and positive rank

Algorithms

Related problems

Thank you

