DYSCO course on low-rank approximation and its applications

Behavioral approach

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Low-rank $\leftrightarrow$ behavioral approach

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Linear static models representations

Linear time-invariant model representations

Solution methods

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Line fitting $\overset{?}{\leftrightarrow}$ $Ax \approx b$

- classic problem: fit the points

$$\mathscr{D} := \{ d_1, \dots, d_N \} \in \mathbb{R}^2$$

by a line passing through the origin

- classic solution: find approx. solution $x \in \mathbb{R}$ of

$$\begin{bmatrix} a_1 \\ \vdots \\ a_N \end{bmatrix} x = \begin{bmatrix} b_1 \\ \vdots \\ b_N \end{bmatrix}$$

where $d_i = (a_i, b_i)$

- the fitting line is

$$\mathscr{B}(x) := \{ (a,b) \in \mathbb{R}^2 \mid ax = b \} \qquad (*)$$

Line fitting $\overset{?}{\leftrightarrow}$ $Ax \approx b$

- another solution: find approx. solution $x' \in \mathbb{R}$ of

$$\begin{bmatrix} b_1 \\ \vdots \\ b_N \end{bmatrix} x' = \begin{bmatrix} a_1 \\ \vdots \\ a_N \end{bmatrix}$$

- the fitting line is

$$\mathscr{B}(x') := \{ (a, b) \in \mathbb{R}^2 \mid a = bx' \} \qquad (**)$$

- if exact solution exists, $x' = 1/x$, unless $x = 0$

- exceptions:
  - horizontal line ($x = 0$)
  - vertical line ($x' = 0$)

Approximation criteria

- solving approximately the overdetermined systems

$$Ax = B \quad \text{and} \quad A = Bx'$$

  where

$$A := \operatorname{col}(a_1, \ldots, a_{10}) \quad \text{and} \quad B := \operatorname{col}(b_1, \ldots, b_{10})$$

  in the least squares sense $\rightsquigarrow$ different solutions

- $\Longrightarrow$ the data modeling criterion depends on the (arbitrary) choice of model representation

Input/output representation

- $Ax = b$ and $A = bx'$ define lines in $\mathbb{R}^2$

$$\mathscr{B}(x) := \{\, (a, b) \in \mathbb{R}^2 \mid ax = b \,\} \qquad (*)$$

$$\mathscr{B}(x') := \{\, (a, b) \in \mathbb{R}^2 \mid a = bx' \,\} \qquad (**)$$

- $(*)$ and $(**)$ define a line $\mathscr{B}$ by functions
  - $a \mapsto b$ in $(*)$
  - $b \mapsto a$ in $(**)$

- input/output representations
  - in $(*)$, a is input, b is output   (a causes b)
  - in $(**)$, b is input, a is output   (b causes a)

Input/output representation

- we are interested in $\mathscr{M}$ — set of lines through 0
- separately $(*)$, $(**)$ don't represent all lines through 0
- I/O representation: any $\mathscr{B} \in \mathscr{M}$ is representable as

$$\mathscr{B} = \mathscr{B}(x, \Pi) = \{ \Pi \left[\begin{smallmatrix} a \\ b \end{smallmatrix} \right] \mid ax = b \}$$

  for some $x \in \mathbb{R}$ and a permutation matrix Π

- link to system of linear equations

$$\mathscr{D} \subset \mathscr{B}(x, \left[\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix} \right]) \quad \iff \quad Ax = B$$

$$\mathscr{D} \subset \mathscr{B}(x, \left[\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix} \right]) \quad \iff \quad Bx' = A$$

Kernel representation

- any $\mathscr{B} \in \mathscr{M}$ can be represented as

$$\mathscr{B} = \ker(R) := \{\, d \in \mathbb{R}^2 \mid Rd = R_1 a + R_2 b = 0 \,\}$$

  for some nonzero vector $R \in \mathbb{R}^{1\times 2}$

- $Rd = 0$ defines a relation between a and b

- $\mathscr{D} \subset \ker(R)$ implies that

$$R \underbrace{\begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix}}_{D} = 0$$

Image representation

- any $\mathscr{B} \in \mathscr{M}$ can be represented as

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

for some vector $P \in \mathbb{R}^{2\times 1}$

- $\mathscr{D} \subset \text{image}(P)$ implies that

$$\begin{bmatrix} d_1 & \cdots & d_N \end{bmatrix} = PL$$

for some $L \in \mathbb{R}^{1\times N}$

Summary

- common feature of the representations considered

$$\left.\begin{array}{llcl} \exists\ x \in \mathbb{R} & Ax = B & \Longrightarrow \\ \exists\ x' \in \mathbb{R} & Bx' = A & \Longrightarrow \\ \exists\ x \in \mathbb{R}, \Pi \text{ permut.} & \begin{bmatrix} x & -1 \end{bmatrix} \Pi D = 0 & \Longleftrightarrow \\ \exists\ R \in \mathbb{R}^{1\times 2}, R \neq 0 & RD = 0 & \Longleftrightarrow \\ \exists\ P \in \mathbb{R}^{2\times 1}, L \in \mathbb{R}^{1\times N} & D = PL & \Longleftrightarrow \end{array}\right\} \text{rank}(D) = 1$$

- representation free characterization of the exact data

$$\mathscr{D} \subset \mathscr{B} \text{ and}$$

$$\mathscr{B} \text{ is a line through } 0$$

$$\Updownarrow$$

$$\text{rank}(D) = 1$$

Low-rank approximation

- representation free formulation

- exact modeling problem:

$$\exists \text{ exact model for } \mathscr{D} \iff D \text{ is rank deficient}$$

- approximate modeling problem:

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{\mathscr{D}} \quad \text{error}(\mathscr{D}, \widehat{\mathscr{D}}) \\ \text{subject to} & \exists \text{ exact model for } \widehat{\mathscr{D}} \end{array}$$

$$\Updownarrow$$

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D} \quad \text{error}(D, \widehat{D}) \\ \text{subject to} & \widehat{D} \text{ is rank deficient} \end{array}$$

Generalizations

1. multivariable data fitting $\mathscr{U} = \mathbb{R}^q$
   - linear static model $\leftrightarrow$ subspace
   - model complexity $\leftrightarrow$ subspace dimension
   - rank(D) $\leftrightarrow$ upper bound on the model complexity

2. nonlinear static modeling
   - $\mathscr{D} \mapsto D$ — nonlinear function
   - nonlinearly structured low-rank approximation

3. linear time-invariant dynamical models
   - $\mathscr{D} \mapsto$ Hankel matrix D
   - Hankel structured low-rank approximation

4. nonlinear dynamic (2. + 3.)

Structure $\mathscr{S} \leftrightarrow$ Model class $\mathscr{M}$

unstructured	linear static
Hankel	scalar LTI
$q \times 1$ Hankel	q-variate LTI
$q \times N$ Hankel	N equal length traj.
mosaic Hankel	N general traj.
$\begin{bmatrix}\text{Hankel} & \text{unstructured}\end{bmatrix}$	finite impulse response
block-Hankel Hankel-block	2D linear shift-invariant

Related frameworks

- behavioral approach in systems and control theory
  - representation free: model $=$ set (the behavior)
  - no a priori separation of inputs and outputs
- errors-in-variables modeling
  - all variables are perturbed by noise
  - maximum likelihood estimation $\leftrightarrow$ LRA
- principal component analysis
  - another statistical setting for LRA
- factor analysis
  - factors $\leftrightarrow$ latent variables in image repr.

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Behavioral approach

- Jan C. Willems (1939–2013)

Outline

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Linear static model

"Good definition should formalize sensible intuition."
Jan Willems

- linear static model with q variables $=$ subspace of $\mathbb{R}^q$
- model complexity $\quad\leftrightarrow\quad$ subspace dimension
  (the more the model can fit, the less useful it is)
- linear static models with complexity at most $\mathtt{m}$ — $\mathscr{L}^q_{\mathtt{m},0}$
- any $\mathscr{B} \in \mathscr{L}^q_{\mathtt{m},0}$ admits kernel, image, and input/output representations

Representations

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

$$\ker(R) := \{\, d \mid Rd = 0 \,\}$$

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

$$\operatorname{image}(P) := \{\, d = P\ell \mid \ell \in \mathbb{R}^{\mathtt{m}} \,\}$$

- input/output representation

$$\mathscr{B}_{\mathrm{i/o}}(X, \Pi) := \{\, d = \Pi \begin{bmatrix} u \\ y \end{bmatrix} \mid u \in \mathbb{R}^{\mathtt{m}},\ y = X^\top u \,\}$$

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

Nonuniqueness of the parameters

- columns of P are generators of the model $\mathscr{B}$
- rows of R are annihilators of $\mathscr{B}$
- the parameters R and P are not unique due to
  - addition of linearly dependent generators/annihilators
  - change of basis transformation

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

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

- the smallest number of generators $\mathrm{m} := \dim(\mathscr{B})$
- max. number of annihilators $\mathrm{p} := q - \dim(\mathscr{B})$

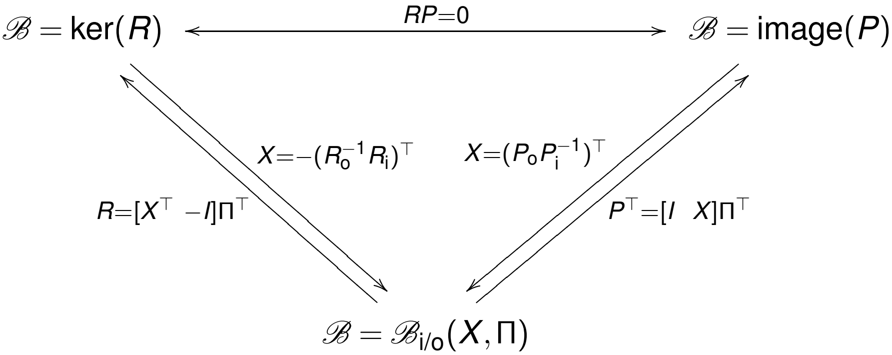
Inputs and outputs

- input is a "free" variable

$$\Pi\,\mathrm{col}(u,y) \in \mathscr{B} \text{ and } u \text{ input} \quad \Longleftrightarrow \quad u \in \mathbb{R}^{\mathtt{m}}$$

- output is bound by input and model
- fact: $\mathtt{m} := \dim(\mathscr{B})$ — number of inputs
- $\mathtt{p} := q - \mathtt{m}$ — number of outputs
- generically any I/O partition is possible
- choosing a partition amounts to choosing full rank $\mathtt{p} \times \mathtt{p}$ submatrix of R or full rank $\mathtt{m} \times \mathtt{m}$ submatrix of P

Transition among representations



$$\Pi^\top P =: \begin{bmatrix} P_i \\ P_o \end{bmatrix} \begin{matrix} \mathtt{m} \\ \mathtt{p} \end{matrix} \quad \text{and} \quad R\Pi =: \begin{matrix} \mathtt{m} & \mathtt{p} \\ [R_i & R_o] \end{matrix}$$

(for details, see Section 2.1)

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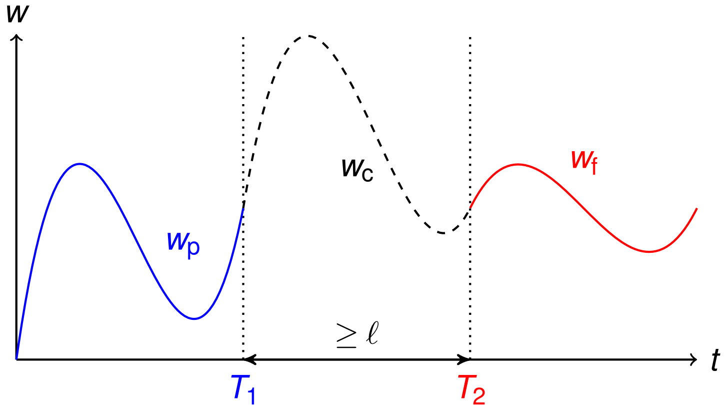
Dynamical models

- observations are trajectories: functions $\mathscr{T} \mapsto \mathbb{R}^q$
- universal set: $(\mathbb{R}^q)^{\mathscr{T}}$ — set of functions
- the time axis $\mathscr{T}$ is $\mathbb{Z}$ (discrete) or $\mathbb{R}$ (continuous)
- dynamic model $\mathscr{B}$ is a subset of $(\mathbb{R}^q)^{\mathscr{T}}$
- linearity: $w, v \in \mathscr{B} \implies \alpha w + \beta v \in \mathscr{B}, \; \forall\, \alpha, \beta$
- shift operator: $(\sigma^\tau w)(t) := w(t+\tau)$, for all $t \in \mathscr{T}$
- time-invariance: $\sigma^\tau \mathscr{B} = \mathscr{B}$, for all $\tau \in \mathscr{T}$

Controllability



for all w_p, $w_f \in \mathscr{B}$, $\exists$ w_c, such that $w_p \wedge w_c \wedge w_f \in \mathscr{B}$

Complexity of an LTI model

- static model $\mathscr{B} \in \mathscr{L}^q_{\mathtt{m},0}$ — complexity $= \mathtt{m}$
  (increasing $\mathtt{m}$ requires increasing # of var. q)

- LTI dynamic model has two aspects:
  - multivariable — number of inputs $\mathtt{m}$
  - dynamics — time memory span ℓ

- complexity of an LTI model is ordered pair $(\mathtt{m}, \ell)$

- notation:
  - $\mathscr{L}^q$ — all LTI models with q variables
  - $\mathscr{L}^q_{\mathtt{m}}$ — at most $\mathtt{m}$ inputs
  - $\mathscr{L}^q_{\mathtt{m},\ell}$ — complexity bounded by $(\mathtt{m}, \ell)$

Restriction of the behavior on an interval

- $w_{\rm p} \wedge w_{\rm f}$ — concatenation of $w_{\rm p}$ and $w_{\rm f}$

$$\mathscr{B}|_T := \{\, w \in (\mathbb{R}^q)^T \mid \exists\, w_{\rm p},\ w_{\rm f},\ \text{such that } w_{\rm p} \wedge w \wedge w_{\rm f} \in \mathscr{B} \,\}$$

- for $\mathscr{B} \in \mathscr{L}^q$ and $T > 0$, $\mathscr{B}|_T$ is a subspace

$$\dim(\mathscr{B}|_T) \;\leq\; T\mathtt{m} + \mathtt{p}\ell$$

- complexity of $\mathscr{B} \sim \dim(\mathscr{B}|_T)$
- therefore, $(\mathtt{m}, \ell)$ specifies the complexity

Representations

- kernel representation with par. $R(z) \in \mathbb{R}^{g \times q}[z]$

$$\ker(R) = \{\, w \mid R(\sigma)w = R_0 w + R_1 \sigma w + \cdots + R_\ell \sigma^\ell w = 0 \,\}$$

- image representation with par. $P(z) \in \mathbb{R}^{q \times g}[z]$

$$\operatorname{image}(P) = \{\, w = P(\sigma)v \mid \text{for some } v \,\}$$

- input/state/output representation

$$\begin{aligned}\mathscr{B}(A,B,C,D,\Pi) := \{\, & w = \Pi \operatorname{col}(u,y) \mid \\ & \exists\, x,\ \text{such that } \sigma x = Ax + Bu \text{ and } y = Cx + Du \,\}\end{aligned}$$

(default $\Pi = I$, in which case it is skipped)

- any $\mathscr{B} \in \mathscr{L}^q$ admits kernel and I/S/O representations
- any controllable $\mathscr{B} \in \mathscr{L}^q$ admits image representation
- lag of $\mathscr{B}$ — minimal ℓ, for which kernel repr. exists
- minimal $\text{row dim}(R) =$ number of outputs
- minimal $\text{col dim}(P) =$ number of inputs

(for details, see Section 2.2)

Nonuniqueness of I/S/O representation

- choice of an input/output partition
- redundant states (nonminimality of representation)
- change of state space basis

$$\mathscr{B}(A, B, C, D) = \mathscr{B}(T^{-1}AT, T^{-1}B, CT, D),$$

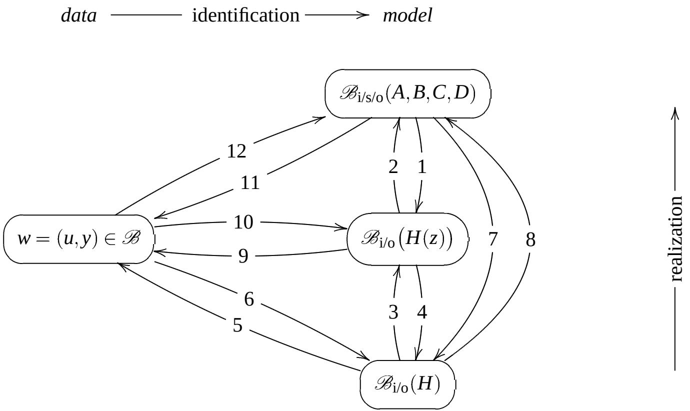
for any nonsingular matrix $T \in \mathbb{R}^{\mathrm{n} \times \mathrm{n}}$

- minimal representation $\implies$ smallest n = order of $\mathscr{B}$

Transition among representations

- using different representations is a powerful idea
- problems are trivial, given suitable representations
- *cf.*, matrix factorizations in numerical linear algebra
- the problem becomes to transform representations

Links among I/O model representations



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 $y_{\text{d}}=H\star u_{\text{d}}$
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 $x(0)=x_{\text{ini}}$
12. exact identification

Outline

Problems with analytic solutions

- unstructured, unweighted $\qquad (\|\cdot\|_F := \|\mathrm{vec}(\cdot)\|_2)$

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D} \quad \|D - \widehat{D}\|_F \\ \text{subject to} & \operatorname{rank}(\widehat{D}) \leq r \end{array} \qquad \text{(LRA)}$$

- unstructured, with left/right weighting matrices

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D} \quad \|W_l(D - \widehat{D})W_r\|_F \\ \text{subject to} & \operatorname{rank}(\widehat{D}) \leq r \end{array}$$

- circulant structure

Truncated SVD

Theorem

Let $D = U\Sigma V^\top$ be the (thin) SVD of $D \in \mathbb{R}^{q\times N}$ and define

$$U =: \begin{matrix} & r & q-r & \\ & [U_1 & U_2] & q \end{matrix}, \quad \Sigma =: \begin{matrix} & r & q-r & \\ & \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} & \begin{matrix} r \\ q-r \end{matrix} \end{matrix}, \quad V =: \begin{matrix} & r & q-r & \\ & [V_1 & V_2] & N \end{matrix}$$

An optimal low-rank approximation (a solution of (LRA)) is

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

It is unique if and only if $\sigma_r \neq \sigma_{r+1}$.

- $\widehat{\mathscr{B}}^*$ depends only on the left singular vectors

- in general
  - structures other than circular
  - norms other than 2-norm
  - weights other than "left/right" multiplication of $D - \widehat{D}$

  lead to hard non-convex optimization problems

- there are many (heuristic) solution methods

Overview of algorithms

- global solution methods
  - SDP relaxations of rational function min. problem
  - systems of polynomial equations (computer algebra)
  - branch-and-bound, simulating annealing, ...
- local optimization methods
  - variable projections
  - alternating projections
  - variations (parameterization $+$ optimization method)
- convex relaxations / multistage methods
  - subspace methods
  - nuclear norm heuristic

Summary

- linear static model $=$ subspace
- model representations
  - input/output (a function, system $AX = B$)
  - kernel (implicit function, relation)
  - image (introduces latent variables)
- representation invariant problem formulation $\rightsquigarrow$ LRA
- different representations $\rightsquigarrow$ different solution methods

". . . most linear resistors let us treat current as a function of voltage or voltage as a function of current, since R is neither zero nor infinite. But in the two limiting cases - the short circuit and the open circuit - that's not true. To fit these cases neatly in a unified framework, we shouldn't think of the relation between current and voltage as defining a function. It's just a relation!"

John Baez