

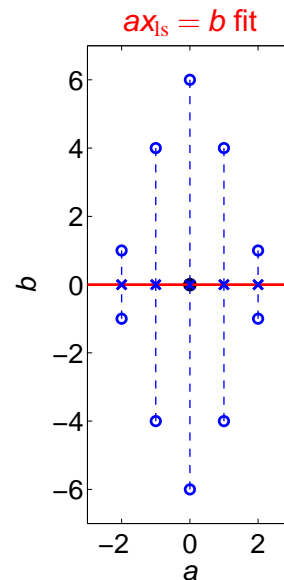
Low-rank approximation and its applications for data fitting

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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 $d_i = \text{col}(a_i, b_i)$ and solve the **least squares problem**

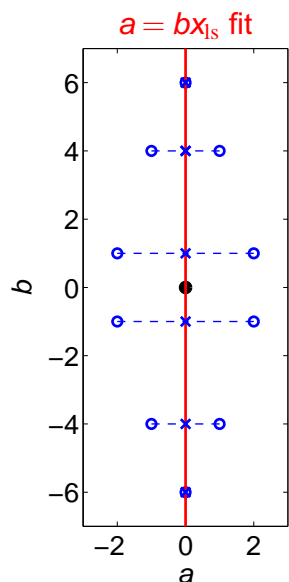
$$\text{col}(a_1, \dots, a_{10})x = \text{col}(b_1, \dots, b_{10}).$$

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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A line fitting example (cont.)



Minimizing vertical distances does not seem appropriate in this example.

Revised LS problem:

$$\text{col}(a_1, \dots, a_{10}) = \text{col}(b_1, \dots, b_{10})x$$

minimize the horizontal distances

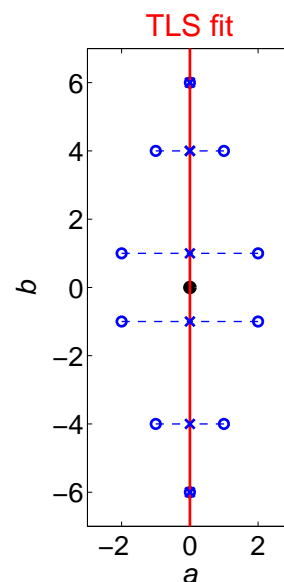
The fitting line is now given by $a = bx_{ls}$.

Total least squares fitting:

minimize the orthogonal distances

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A line fitting example (cont.)



Total least squares problem:

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

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

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

If we represent the fitting line as an

$$\text{image } d = P I \quad \text{or} \quad \text{kernel } R d = 0$$

TLS solutions do exist, e.g.,

$$P_{\text{tls}} = \text{col}(0, 1) \quad \text{and} \quad R_{\text{tls}} = \begin{bmatrix} 1 & 0 \end{bmatrix}.$$

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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.

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Outline

Low-rank approximation as data modeling

Applications

Algorithms

Related problems

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In this talk ...

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

approximate $D := [d_1 \ \cdots \ d_{10}]$ 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**

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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

$$\hat{D}^* := \arg \min_{\hat{D}} \|D - \hat{D}\| \quad \text{subject to} \quad \text{rank}(\hat{D}) \leq m.$$

Interpretation:

\hat{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

$$m := \text{rank}(D) < d := \text{row dim}(D).$$

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

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

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

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Structured low-rank approximation

Given

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

find

$$\hat{p}^* := \arg \min_{\hat{p}} \|p - \hat{p}\| \quad \text{subject to} \quad \text{rank}(\mathcal{S}(\hat{p})) \leq r.$$

Interpretation:

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

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LRA as data modeling

Given

- N , d -variable observations $[d_1 \ \dots \ d_N] := D \in \mathbb{R}^{d \times N}$
- a matrix norm $\|\cdot\|$, and
- model complexity m , $0 < m < d$,

find

$$\hat{\mathcal{B}}^* := \arg \min_{\hat{\mathcal{B}}, \hat{D}} \|D - \hat{D}\| \quad \text{subject to} \quad \begin{aligned} &\text{colspan}(\hat{D}) \subseteq \hat{\mathcal{B}} \\ &\dim(\hat{\mathcal{B}}) \leq m \end{aligned}$$

Interpretation:

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

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Why structured low-rank approximation?

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

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

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

we have a vector difference equation for w_d with 1 lags

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

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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 $(m, 1)$, $0 \leq m < w$,

find

$$\hat{\mathcal{B}}^* := \arg \min_{\mathcal{B}, \hat{w}} \|w_d - \hat{w}\| \quad \text{s.t.} \quad \begin{array}{l} \hat{w} \in \mathcal{B}, \\ \dim(\mathcal{B}) \leq Tm + 1(w - m) \end{array} \quad (*)$$

Interpretation:

$\hat{\mathcal{B}}^*$ 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.)

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Links among the parameters R , P , and X

Define the partitionings

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

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

$$\begin{array}{ccc} \mathcal{B} = \ker(R) & \xleftrightarrow{RP=0} & \mathcal{B} = \text{colspan}(P) \\ \swarrow \begin{array}{l} X^T = -R_o^{-1} R_i \\ R = [X^T \ -I] \end{array} & & \searrow \begin{array}{l} X^T = P_o P_i^{-1} \\ P^T = [I \ X] \end{array} \\ & \mathcal{B} = \mathcal{B}_{i/o}(X) & \end{array}$$

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Kernel, image, and input/output representations

A **static model** \mathcal{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:** $\mathcal{B} = \ker(R), \quad R \in \mathbb{R}^{p \times d}$
- **image:** $\mathcal{B} = \text{colspan}(P), \quad P \in \mathbb{R}^{d \times m}$
- **input/output:** $\mathcal{B}_{i/o} = \mathcal{B}(X), \quad X \in \mathbb{R}^{m \times p}$

$$\mathcal{B}_{i/o}(X) := \{d := \text{col}(d_i, d_o) \in \mathbb{R}^d \mid d_i \in \mathbb{R}^m, d_o = X^T d_i\}$$

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

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

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LTI models of bounded complexity

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

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

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

$$\dim(\mathcal{B}|_{[0, T]}) = mT + n \leq mT + p1, \quad \text{for } T \geq 1.$$

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

\Rightarrow The complexity of \mathcal{B} is specified by (m, n) or $(m, 1)$.

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

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LTI model representations

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

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

- **Impulse response represent** (parameter $H: \mathbb{Z} \rightarrow \mathbb{R}^{p \times m}$)

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

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

$$w = \text{col}(u, y), \quad \begin{aligned} x(t+1) &= Ax(t) + Bu(t) \\ y(t) &= Cx(t) + Du(t) \end{aligned}$$

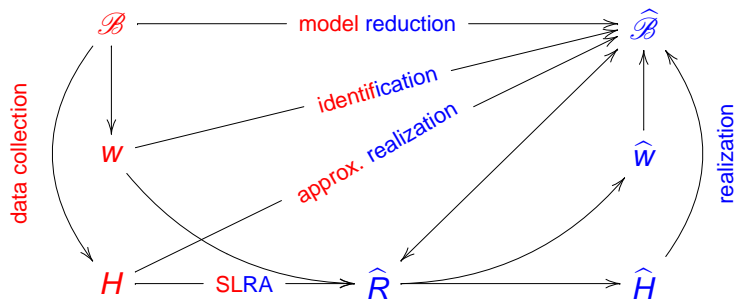
Transitions among $R, H, (A, B, C, D)$ are classic problems, e.g.,

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

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System theory applications

- | | | | |
|---------------------|-------------------------------|-----------|--------------------------------------|
| \mathcal{B} | “true” (high order) model | w | observed response |
| $\hat{\mathcal{B}}$ | approximate (low order) model | H | observed impulse resp. |
| | | \hat{w} | response of $\hat{\mathcal{B}}$ |
| | | \hat{H} | impulse resp. of $\hat{\mathcal{B}}$ |



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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)

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Generic problem: structured LRA

The applications are special cases of the SLRA problem:

$$\hat{p}^* := \arg \min_{\hat{p}} \|p - \hat{p}\| \quad \text{subject to} \quad \text{rank}(\mathcal{S}(\hat{p})) \leq r$$

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

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

Notes:

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

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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

$$\hat{\mathcal{B}}^* := \operatorname{argmin}_{\hat{\mathcal{B}}, \hat{w}} \|w_d - \hat{w}\|_{\ell_2} \quad \text{subject to} \quad \hat{w} \in \hat{\mathcal{B}} \in \mathcal{L}_{m,1}.$$

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

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

\bar{w} — true data, $\bar{\mathcal{B}}$ — true model, \tilde{w} — measurement noise

$\hat{\mathcal{B}}^*$ is a maximum likelihood estimate of $\bar{\mathcal{B}}$, in the EIV model

consistent and assympt. normal \Rightarrow confidence regions

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System theory \leftrightarrow Signal proc. \leftrightarrow Computer algebra

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

$$(u, y) \in \mathcal{B}(H) \quad \Leftrightarrow \quad y = H \star u \quad \Leftrightarrow \quad y(z) = H(z)u(z)$$

FIR sys. traj. convolution polyn. multipl.

Multivariable case: block Toeplitz structure

$$\begin{array}{ccc} \text{multivariable} & \Leftrightarrow & \text{matrix valued} \\ \text{systems} & & \text{time series} \end{array} \quad \Leftrightarrow \quad \begin{array}{c} \text{matrix valued} \\ \text{polynomials} \end{array}$$

2D case: block Toeplitz–Toeplitz block structure

$$\begin{array}{ccc} \text{multidim.} & \Leftrightarrow & \text{function of several} \\ \text{system} & & \text{indep. variables} \end{array} \quad \Leftrightarrow \quad \begin{array}{c} \text{polyn. of} \\ \text{several var.} \end{array}$$

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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.

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

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

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

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

\Rightarrow With “rough data $w_d = (u_d, y_d)$ ”, there is **no exact solution**.

\rightsquigarrow 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.

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Outline

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SISTA

Structured low-rank approximation

No closed form solution is known for the general SLRA problem

$$\hat{p}^* := \arg \min_{\hat{p}} \|p - \hat{p}\| \quad \text{subject to} \quad \text{rank}(\mathcal{S}(\hat{p})) \leq r.$$

NP-hard, consider solution methods based on local optimization

Representing the constraint in a kernel form, the problem is

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

Note: Double minimization with bilinear equality constraint.

There is a matrix $G(R)$, such that $R\mathcal{S}(\hat{p}) = 0 \iff G(R)p = 0$.

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Unstructured low-rank approximation

$$\hat{D}^* := \arg \min_{\hat{D}} \|D - \hat{D}\|_F \quad \text{subject to} \quad \text{rank}(\hat{D}) \leq m$$

Theorem (closed form solution)

Let $D = U\Sigma V^T$ be the SVD of D and define

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

An optimal LRA solution is

$$\hat{D}^* = U_1 \Sigma_1 V_1^T, \quad \hat{\mathcal{B}}^* = \ker(U_2^T) = \text{colspan}(U_1).$$

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

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Variable projection vs. alternating projections

Two ways to approach the double minimization:

- **Variable projections (VARPRO):**
solve the inner minimization analytically

$$\min_{R, RR^T = I_{m-r}} \text{vec}^T(R\mathcal{S}(\hat{p})) \left(G(R)G^T(R) \right)^{-1} \text{vec}(R\mathcal{S}(\hat{p}))$$

\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.

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Software implementation

The structure of \mathcal{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**.

Weighted low-rank approximation

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

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

$$\min_{\hat{D}} \text{vec}^\top(D - \hat{D})W \text{vec}(D - \hat{D}) \quad \text{subject to} \quad \text{rank}(\hat{D}) \leq m$$

Known in **chemometrics** as **maximum likelihood PCA**.

NP-hard problem, alternating projections is effective heuristic

Variations on low-rank approximation

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

Nonnegative low-rank approximation

Constrained LRA arise in Markov chains and image mining

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

Using an image representation, an **equivalent problem** is

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

Alternating projections algorithm:

- Choose an initial approximation $P^{(0)} \in \mathbb{R}^{d \times m}$ and set $k := 0$.
- Solve: $L^{(k)} = \arg \min_L \|D - P^{(k)}L\|$ subject to $L \geq 0$.
- Solve: $P^{(k+1)} = \arg \min_P \|D - PL^{(k)}\|$ subject to $P \geq 0$.
- Repeat until convergence.

Data fitting by a second order model

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

Consider first **exact data**:

$$\begin{aligned} d \in \mathcal{B}(A, b, c) &\iff d^\top A d + b^\top d + c = 0 \\ &\iff \underbrace{\langle \text{col}(d \otimes_s d, d, 1), \text{col}(\text{vec}_s(A), b, c) \rangle}_{\substack{d_{\text{ext}} \\ \theta}} = 0 \end{aligned}$$

$$\begin{aligned} \{d_1, \dots, d_N\} \in \mathcal{B}(\theta) &\iff \theta \in \text{left ker} \underbrace{\begin{bmatrix} d_{\text{ext},1} & \dots & d_{\text{ext},N} \end{bmatrix}}_{D_{\text{ext}}}, \quad \theta \neq 0 \\ &\iff \text{rank}(D_{\text{ext}}) \leq d - 1 \end{aligned}$$

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

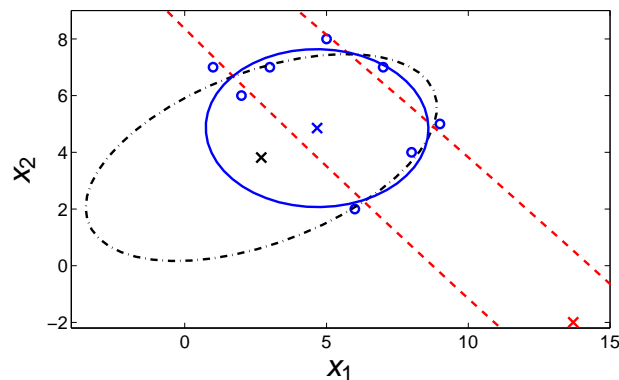
Notes:

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

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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)

○ — data points × — centers

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Consistency in the errors-in-variables setting

Assume that the data is collected according to the EIV model

$$d_i = \bar{d}_i + \tilde{d}_i, \quad \text{where } \bar{d}_i \in \mathcal{B}(\bar{\theta}), \quad \tilde{d}_i \sim \mathcal{N}(0, \sigma^2 I).$$

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

$$\tilde{d}_{\text{ext},i} := \text{col}(\tilde{d}_i \otimes_s \tilde{d}_i, \tilde{d}_i, 0) \text{ is not Gaussian}$$

proposed method — incorporate bias correction in the LRA

Notes:

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

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Summary

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

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