DYSCO course on low-rank approximation and its applications

Computational tools

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Weighted and regularized least squares problems

Exercise

Total least squares problems

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Orthonormal set of vectors

- consider a finite set of vectors $\mathscr{Q} := \{ q_1, \ldots, q_k \} \subset \mathbb{R}^n$
- $\mathscr{Q}$ is orthogonal $:\iff \langle q_i, q_j \rangle := q_i^\top q_j = 0$, for all $i \neq j$
- $\mathscr{Q}$ is normalized $:\iff \|q_i\|_2^2 := \langle q_i, q_i \rangle = 1$, $i = 1, \ldots, k$
- $\mathscr{Q}$ is orthonormal $:\iff \mathscr{Q}$ is orthogonal $+$ normalized
- $Q := \begin{bmatrix} q_1 & \cdots & q_k \end{bmatrix}$ orthonormal $\iff Q^\top Q = I_k$
- properties:
  - orthonormal vectors are independent
  - multiplication preserves inner product and norm

$$\langle Qz, Qy \rangle = z^\top Q^\top Q y = z^\top y = \langle z, y \rangle$$

Orthogonal projectors

- consider an orthonormal set $\mathscr{Q} := \{ q_1, \ldots, q_k \}$
- $\mathscr{Q}$ is an orthonormal basis for $\mathscr{L} := \mathrm{span}(\mathscr{Q}) \subseteq \mathbb{R}^n$
- $Q^\top Q = I_k$, however, for $k < n$, $QQ^\top \neq I_n$
- $\Pi_{\mathrm{span}(\mathscr{Q})} := QQ^\top$ is orthogonal projector on span($\mathscr{Q}$)

$$\Pi_{\mathscr{L}} x = \arg\min_y \|x - y\|_2 \quad \text{subject to} \quad y \in \mathscr{L}$$

- Properties:
  - $\Pi = \Pi^2$, $\Pi = \Pi^\top$ (necessary and sufficient conditions)
  - $\Pi^\perp := (I - \Pi)$ is orthogonal projector on

$$(\mathrm{span}(\Pi))^\perp \subseteq \mathbb{R}^n \text{— orth. complement of span}(\Pi)$$

Orthonormal basis for $\mathbb{R}^n$

- orthonormal set $\mathscr{Q} := \{ q_1, \ldots, q_n \} \subset \mathbb{R}^n$ of n vectors
- $Q := \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix}$ is orthogonal and $Q^\top Q = I_n$
- it follows that $Q^{-1} = Q^\top$ and

$$QQ^\top = \sum_{i=1}^{n} q_i q_i^\top = I_n$$

- expansion in orthonormal basis $x = QQ^\top x$
  - $\widetilde{x} := Q^\top x$ coordinates of x in the basis $\mathscr{Q}$
  - $x = Q\widetilde{x}$ reconstruct x from the coordinates a
- geometrically multiplication by Q (and $Q^\top$) is rotation

Gram-Schmidt (G-S) procedure

- given independent set $\{ a_1, \ldots, a_k \} \subset \mathbb{R}^n$
- G-S produces orthonormal set $\{ q_1, \ldots, q_k \} \subset \mathbb{R}^n$

$$\operatorname{span}(a_1, \ldots, a_r) = \operatorname{span}(q_1, \ldots, q_r), \quad \text{for all } r \leq k$$

- G-S procedure: Let $q_1 := a_1 / \|a_1\|_2$. For $i = 2, \ldots, k$
  1. orthogonalized a_i w.r.t. $q_1, \ldots, q_{i-1}$:

$$v_i := \underbrace{(I - \Pi_{\operatorname{span}(q_1, \ldots, q_{i-1})}) a_i}_{\text{projection of } a_i \text{ on } (\operatorname{span}(q_1, \ldots, q_{i-1}))^{\perp}}$$

  2. normalize the result: $q_i := v_i / \|v_i\|_2$

QR decomposition

G-S gives as a byproduct scalars r_{ji}, $j \le i$, $i = 1, \dots, k$

$$\begin{aligned} a_i &= (q_1^\top a_i) q_1 + \dots + (q_{i-1}^\top a_i) q_{i-1} + \|v_i\|_2 q_i \\ &= r_{1i} q_1 + \dots + r_{ii} q_i \end{aligned}$$

in a matrix form G-S produces the matrix decomposition

$$\underbrace{\begin{bmatrix} a_1 & a_2 & \cdots & a_k \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} q_1 & q_1 & \cdots & q_k \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1k} \\ 0 & r_{22} & \cdots & r_{2k} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & r_{kk} \end{bmatrix}}_{R}$$

with orthonormal $Q \in \mathbb{R}^{n \times k}$ and upper triangular $R \in \mathbb{R}^{k \times k}$

- If $\{ a_1, \ldots, a_k \}$ are dependent

$$v_i := (I - \Pi_{\mathrm{span}(q_1,\ldots,q_{i-1})}) a_i = 0 \quad \text{for some } i$$

- conversely, if $v_i = 0$ for some i, a_i is linearly dependent on $\{ a_1, \ldots, a_{i-1} \}$

- Modified G-S procedure: when $v_i = 0$, skip to a_{i+1} $\implies$ *R is in upper staircase form,* *e.g.*,

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times & \times \\ & \times & \times & \times & \times & \times & \times \\ & & & \times & \times & \times & \times \\ & & & & & & \times \\ & & & & & & \end{bmatrix}$$

(empty elements are zeros)

Full QR

$$A = \underbrace{\begin{bmatrix} Q_1 & Q_2 \end{bmatrix}}_{\text{orthogonal}} \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \qquad \begin{array}{rcl} \operatorname{colspan}(A) & = & \operatorname{colspan}(Q_1) \\ \left(\operatorname{colspan}(A)\right)^{\perp} & = & \operatorname{colspan}(Q_2) \end{array}$$

- procedure for finding Q_2

  complete A to full rank matrix, e.g.,
  $A_m := \begin{bmatrix} A & I \end{bmatrix}$, *and apply G-S on* A_m

- application:
  complete an orthonormal matrix $Q_1 \in \mathbb{R}^{n \times k}$
  to an orthogonal matrix $Q = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \in \mathbb{R}^{n \times n}$
  (by computing the full QR of $\begin{bmatrix} Q_1 & I \end{bmatrix}$)

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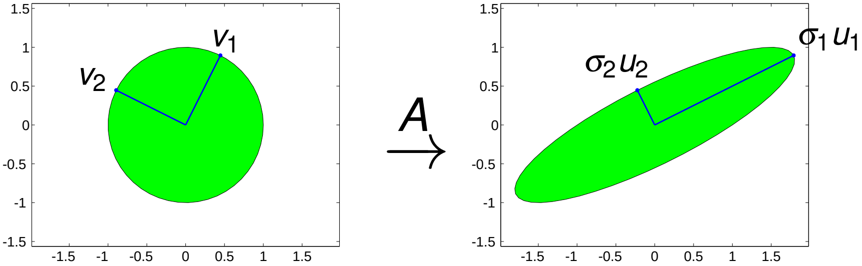
Geometric fact motivating the SVD

The image of a unit ball under linear map is a hyperellips.

$$\underbrace{\begin{bmatrix} 1.00 & 1.50 \\ 0 & 1.00 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 0.89 & -0.45 \\ 0.45 & 0.89 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 2.00 & 0 \\ 0 & 0.50 \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} 0.45 & -0.89 \\ 0.89 & 0.45 \end{bmatrix}}_{V^\top}$$



Singular value decomposition

any $m \times n$ matrix A of rank r has a reduced SVD

$$A = \underbrace{\begin{bmatrix} u_1 & \cdots & u_r \end{bmatrix}}_{U_1} \underbrace{\begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{bmatrix}}_{\Sigma_1} \underbrace{\begin{bmatrix} v_1 & \cdots & v_r \end{bmatrix}^\top}_{V_1^\top}$$

with U_1 and V_1 orthonormal

- $\sigma_1 \geq \cdots \geq \sigma_r$ are called singular values
- $u_1, \ldots, u_r$ are called left singular vectors
- $v_1, \ldots, v_r$ are called right singular vectors

The SVD is both computational and analytical tool

Full SVD $\quad A = U\Sigma V^\top$

where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal and

$$\Sigma = \begin{array}{cc} \begin{array}{cc} r & n-r \end{array} & \\ \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} & \begin{array}{c} r \\ m-r \end{array} \end{array} \qquad \text{where} \qquad \Sigma_1 = \operatorname{diag}(\sigma_1, \ldots, \sigma_r)$$

the singular values of A are

$$\sigma(A) := \left(\sigma_1, \ldots, \sigma_r, \quad \underbrace{0, \ldots, 0}_{\min(n-r, m-r)} \quad\right)$$

- $\sigma_{\min}(A)$ — smallest singular value of A
- $\sigma_{\max}(A)$ — largest singular value of A

Proof of existence of an SVD

- constructive, based on induction, assume $m \geq n$
- end of induction: vector $A \in \mathbb{R}^{m \times 1}$ has reduced SVD

$$A = U \Sigma V^\top, \quad \text{with} \quad U := A / \|A\|_2, \quad \Sigma := \|A\|_2, \quad V := 1$$

- inductive step: let $\sigma_i := \|A_i\|_2$, $\exists\ u_i \in \mathbb{R}^m$ and $v_i \in \mathbb{R}^n$

$$A_i v_i =: \sigma_i u_i, \quad \text{where} \quad \|u_i\|_2 = 1, \quad \text{with} \quad \|v_i\|_2 = 1$$

- complete u_i and v_i to orthogonal matrices (QR)

$$U_i := \begin{bmatrix} u_i & \star \end{bmatrix} \qquad \text{and} \qquad V_i := \begin{bmatrix} v_i & \star \end{bmatrix}$$

- for certain $w \in \mathbb{R}^{n-1}$ and $A_{i+1} \in \mathbb{R}^{(n-1)\times(n-1)}$

$$U_i^\top A_i V_i = \begin{bmatrix} \sigma_i & w^\top \\ 0 & A_{i+1} \end{bmatrix}$$

- next we show that $w = 0$

$$\sigma_i^2 = \|A_i\|_2^2 = \max_v \frac{\|A_i v\|_2^2}{\|v\|_2^2} \geq \frac{\|A_i \left[\begin{smallmatrix} \sigma_i \\ w \end{smallmatrix}\right]\|_2^2}{\|\left[\begin{smallmatrix} \sigma_i \\ w \end{smallmatrix}\right]\|_2^2}$$

$$= \frac{1}{\sigma_i^2 + w^\top w} \left\| \begin{bmatrix} \sigma_i^2 + w^\top w \\ A_{i+1} w \end{bmatrix} \right\|_2^2$$

$$\geq \frac{1}{\sigma_i^2 + w^\top w} (\sigma_i^2 + w^\top w)^2 = \sigma_i^2 + w^\top w$$

- $\sigma_i^2 \geq \sigma_i^2 + w^\top w \implies w = 0$

Low-rank approximation

given

- a matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$, and
- an integer r, $0 < r < n$,

find

$$\widehat{A} := \arg\min_{\widehat{A}} \|A - \widehat{A}\| \quad \text{subject to} \quad \operatorname{rank}(\widehat{A}) \leq r$$

- Interpretation: $\widehat{A}^*$ is optimal rank-r approx. of A w.r.t.

$$\|A\|_{\mathrm{F}}^2 := \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2 \qquad \text{or} \qquad \|A\|_2 := \max_x \frac{\|Ax\|_2}{\|x\|_2}$$

- $\widehat{A}^*$ is optimal in any unitarily invariant norm

Solution via truncated SVD

$$\widehat{A}^* := \arg\min_{\widehat{A}} \|A - \widehat{A}\|_F \quad \text{subject to} \quad \operatorname{rank}(\widehat{A}) \leq r \quad \text{(LRA)}$$

Theorem Let $A = U\Sigma V^\top$ be the SVD of A and define

$$U =: \begin{array}{cc} r & r-n \\ \left[U_1 \right. & \left. U_2 \right] \end{array} \; n\,, \quad \Sigma =: \begin{array}{cc} \begin{array}{cc} r & r-n \end{array} & \\ \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} & \begin{array}{c} r \\ r-n \end{array} \end{array}, \quad V =: \begin{array}{cc} r & r-n \\ \left[V_1 \right. & \left. V_2 \right] \end{array} \; n$$

A solution to (LRA) is

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

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

Numerical rank

- distance of A to the manifold of rank-r matrices

$$\sqrt{\textstyle\sum_{i=r+1}^{n} \sigma_i^2} = \min_{\widehat{A}} \|A - \widehat{A}\|_{\mathsf{F}} \quad \text{subject to} \quad \operatorname{rank}(\widehat{A}) \le r$$

$$\sigma_{r+1} = \min_{\widehat{A}} \|A - \widehat{A}\|_2 \quad \text{subject to} \quad \operatorname{rank}(\widehat{A}) \le r$$

- $\sigma_{\min}(A)$ is the distance of A to rank deficiency

- numerical rank: $\operatorname{rank}(A, \varepsilon) :=$ # of singular values $> \varepsilon$

- $\operatorname{rank}(A, \varepsilon)$ depends on an a priori given tolerance ε

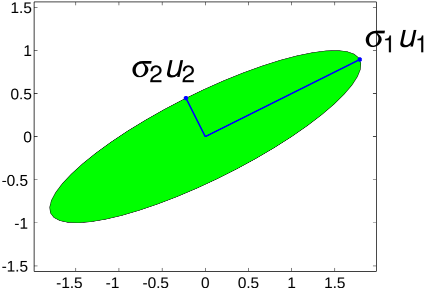
Pseudo-inverse $A^+ := V_1 \Sigma_1^{-1} U_1^\top \in \mathbb{R}^{n \times m}$

$$\begin{aligned}
\mathrm{rank}(A) = n = m \quad &\Longrightarrow \quad A^+ = A^{-1} \\
\mathrm{rank}(A) = n \quad &\Longrightarrow \quad A^+ = (A^\top A)^{-1} A^\top \\
\mathrm{rank}(A) = m \quad &\Longrightarrow \quad A^+ = A^\top (A A^\top)^{-1}
\end{aligned}$$

- $A^+ y$ is least squares-least norm solution of $Ax = y$
- the pseudo-inverse depends on the rank of A
- in practice, the numerical rank $\mathrm{rank}(A, \varepsilon)$ is used
- the SVD, gives reliable way of solving $Ax = y$

Condition number $\kappa(A) := \sigma_{\max}(A)/\sigma_{\min}(A)$

- $\kappa(A)$ is eccentricity of hyperellipsoid $A\{\, x \mid \|x\|_2 = 1 \,\}$



- $\kappa(A)$ — sensitivity of $A^+ y$ to perturbations in y, A
- for large $\kappa(A)$ (≥ 1000) A is called ill-conditioned

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Least squares

- overdetermined system of linear equations $Ax = b$
- given $A \in \mathbb{R}^{m \times n}$, $m > n$ and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$
- for "most" A and b, there is no solution x
- Least squares approximation:

  choose x that minimizes 2-norm of the residual

$$e(x) := b - Ax$$

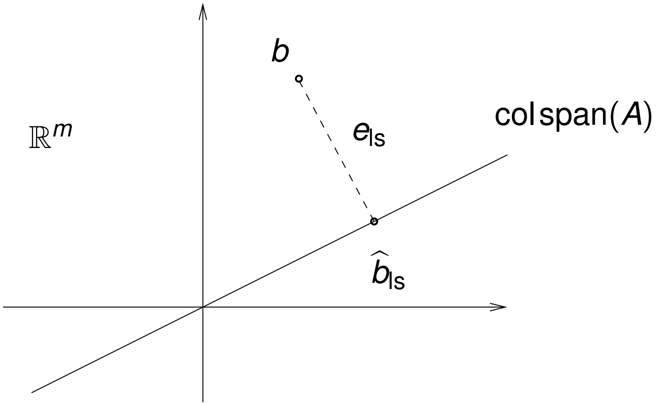
- least squares approximate solution

$$\widehat{x}_{\mathrm{ls}} := \arg\min_x \| \underbrace{b - Ax}_{e(x)} \|_2$$

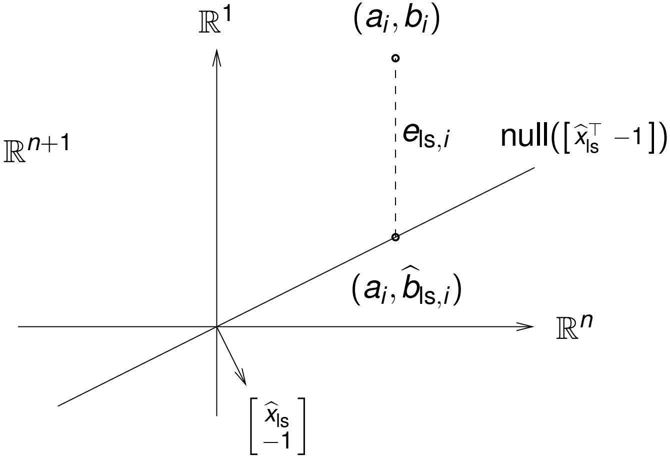
Geometric interpretation: project b onto the image of A

($\widehat{b}_{\text{ls}} := A\widehat{x}_{\text{ls}}$ is the projection)

$$e_{\text{ls}} := \widehat{b}_{\text{ls}} - A\widehat{x}_{\text{ls}}$$



Another geometric interpretation of the LS approximation:



$$
\begin{aligned}
A\widehat{x}_{\mathrm{ls}} = \widehat{b}_{\mathrm{ls}} \quad &\iff \quad \begin{bmatrix} A & \widehat{b}_{\mathrm{ls}} \end{bmatrix} \begin{bmatrix} \widehat{x}_{\mathrm{ls}} \\ -1 \end{bmatrix} = 0 \\
&\iff \quad \begin{bmatrix} a_i & \widehat{b}_{\mathrm{ls},i} \end{bmatrix} \begin{bmatrix} \widehat{x}_{\mathrm{ls}} \\ -1 \end{bmatrix} = 0, \quad \text{for } i = 1, \ldots, m
\end{aligned}
$$

(a_i is the ith row of A)

- $\begin{bmatrix} a_i \\ \widehat{b}_{\mathrm{ls},i} \end{bmatrix}$ lies on subspace perpendicular to span$\left(\begin{bmatrix} \widehat{x}_{\mathrm{ls}} \\ -1 \end{bmatrix}\right)$
- "data point" $\begin{bmatrix} a_i \\ b_i \end{bmatrix} = \begin{bmatrix} a_i \\ \widehat{b}_{\mathrm{ls},i} \end{bmatrix} + \begin{bmatrix} 0 \\ e_{\mathrm{ls},i} \end{bmatrix}$
- approx. error $\begin{bmatrix} 0 \\ e_{\mathrm{ls},i} \end{bmatrix}$ is the vertical distance

Notes

- assuming $m \geq n = \text{rank}(A)$, *i.e.*, A is full column rank,

$$\widehat{x}_{\text{ls}} = (A^\top A)^{-1} A^\top b$$

  is the unique least squares approximate solution

- $\widehat{x}_{\text{ls}}$ is a linear function of b
- if A is square, $\widehat{x}_{\text{ls}} = A^{-1} b$
- $\widehat{x}_{\text{ls}}$ is an exact solution if $Ax = b$ has an exact solution
- $\widehat{b}_{\text{ls}} := A\widehat{x}_{\text{ls}} = A(A^\top A)^{-1} A^\top b$ is LS approx. of b

Projector onto the span of A

- the $m \times m$ matrix

$$\Pi_{\mathrm{col\,span}(A)} := A(A^\top A)^{-1}A^\top$$

  is the orthogonal projector onto $\mathscr{L} := \mathrm{col\,span}(A)$

- the columns of A are an arbitrary basis for $\mathscr{L}$
- if the columns of Q form an orthonormal basis for $\mathscr{L}$

$$\Pi_{\mathrm{col\,span}(Q)} := QQ^\top$$

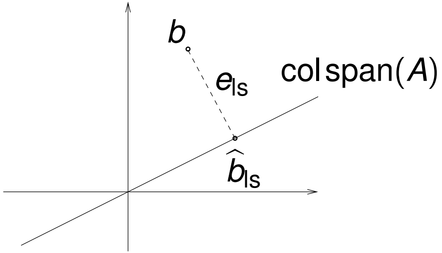
Orthogonality principle

the least squares residual vector

$$e_{\text{ls}} := b - A\widehat{x}_{\text{ls}} = \underbrace{\left(I_m - A(A^\top A)^{-1}A^\top\right)}_{\Pi_{(\text{col span}(A))^\perp}} b$$

is orthogonal to col span(A)

$$\langle e_{\text{ls}}, A\widehat{x}_{\text{ls}}\rangle = b^\top\left(I_m - A(A^\top A)^{-1}A^\top\right)A\widehat{x}_{\text{ls}} = 0, \quad \text{for all } b \in \mathbb{R}^m$$



Least squares via QR decomposition

Let $A = QR$ be the reduced QR decomposition of A.

$$
\begin{aligned}
(A^\top A)^{-1} A^\top &= (R^\top Q^\top Q R)^{-1} R^\top Q^\top \\
&= (R^\top Q^\top Q R)^{-1} R^\top Q^\top = R^{-1} Q^\top
\end{aligned}
$$

$$\widehat{x}_{\mathrm{ls}} = R^{-1} Q^\top b \quad \text{and} \quad \widehat{b}_{\mathrm{ls}} := A x_{\mathrm{ls}} = Q Q^\top b$$

we have a sequence of LS problems ($A =: \begin{bmatrix} a_1 & \cdots & a_n \end{bmatrix}$)

$$A^i x^i = b, \quad \text{where } A^i := \begin{bmatrix} a_1 & \cdots & a_i \end{bmatrix}, \quad \text{for } i = 1, \dots, n$$

R_i — leading $i \times i$ submatrix of R and $Q_i := \begin{bmatrix} q_1 & \cdots & q_i \end{bmatrix}$

$$\widehat{x}_{\mathrm{ls}}^i = R_i^{-1} Q_i^\top b$$

Least norm solution

underdetermined system $Ax = b$, with full rank $A \in \mathbb{R}^{m \times n}$

The set of solutions is

$$\{\, x \in \mathbb{R}^n \mid Ax = b \,\} = \{\, x_{\mathrm{p}} + z \mid z \in \mathrm{null}(A) \,\}$$

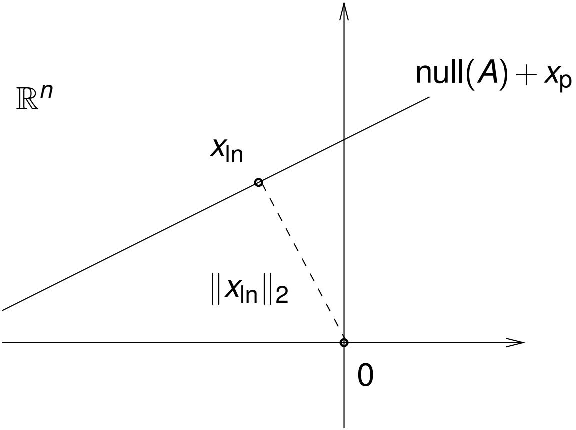
where x_{p} is a particular solution, *i.e.*, $Ax_{\mathrm{p}} = b$.

Least norm problem

$$x_{\mathrm{ln}} := \arg\min_{x} \|x\|_2 \quad \text{subject to} \quad Ax = b$$

Geometric interpretation:

- x_{ln} is the projection of 0 onto the solution set
- orthogonality principle $x_{\text{ln}} \perp \text{null}(A)$



Derivation via Lagrange multipliers

consider the least norm problem with A full rank

$$\min_x \|x\|_2^2 \quad \text{subject to} \quad Ax = b$$

introduce Lagrange multipliers $\lambda \in \mathbb{R}^m$

$$L(x, \lambda) = xx^\top + \lambda^\top (Ax - b)$$

the optimality conditions are

$$\nabla_x L(x, \lambda) = 2x + A^\top \lambda = 0$$
$$\nabla_\lambda L(x, \lambda) = Ax - b = 0$$

substituting $x = -A^\top \lambda / 2$ into the second eqn.

$$\lambda = -2(AA^\top)^{-1} b \quad \Longrightarrow \quad x_{\text{ln}} = A^\top (AA^\top)^{-1} b$$

Solution via QR decomposition

Let $A^\top = QR$ be the reduced QR decomposition of $A^\top$.

$$A^\top (AA^\top)^{-1} = QR(R^\top Q^\top QR)^{-1} = Q(R^\top)^{-1}$$

is a right inverse of A. Then

$$x_{\text{ln}} = Q(R^\top)^{-1} b$$

Outline

Weighted least squares

- weighted 2-norm, defined by $W \in \mathbb{R}^{m \times m}$, $W > 0$

$$\|e\|_W^2 := e^\top W e$$

- weighted least squares approximation problem

$$\widehat{x}_{W,\text{ls}} := \arg\min_x \|b - Ax\|_W$$

- orthogonality principle holds with inner product

$$\langle e, b \rangle_W := e^\top W b$$

- solution

$$\widehat{x}_{W,\text{ls}} = (A^\top W A)^{-1} A^\top W b$$

Recursive least squares

- let $a_i^\top$ be the ith row of A

$$A = \begin{bmatrix} — & a_1^\top & — \\ & \vdots & \\ — & a_m^\top & — \end{bmatrix}$$

$$\|b - Ax\|_2^2 = \sum_{i=1}^{m} (b_i - a_i^\top x)^2$$

$$\hat{x}_{\text{ls}} = \hat{x}_{\text{ls}}(m) := \left(\sum_{i=1}^{m} a_i a_i^\top \right)^{-1} \left(\sum_{i=1}^{m} a_i b_i \right)$$

- (a_i, b_i) correspond to a measurement
- often the (a_i, b_i)'s come sequentially (*e.g.*, in time)

Recursive comput. of $\widehat{x}_{\text{ls}}(m) = \left(\sum_{i=1}^{m} a_i a_i^\top\right)^{-1} \left(\sum_{i=1}^{m} a_i b_i\right)$

- $P(0) = 0 \in \mathbb{R}^{n \times n}$, $q(0) = 0 \in \mathbb{R}^n$

- For $m = 0, 1, \ldots$
  - $P(m+1) := P(m) + a_{m+1} a_{m+1}^\top$
    $q(m+1) := q(m) + a_{m+1} b_{m+1}$
  - $x_{\text{ls}}(m) = P^{-1}(m) q(m)$

Notes:

- the algorithm requires inversion of an $n \times n$ matrix

- $P(m)$ invertible $\implies$ $P(m')$ invertible, for all $m' > m$

Rank-1 update formula:

$$(P + aa^\top)^{-1} = P^{-1} - \frac{1}{1 + a^\top P^{-1} a}(P^{-1}a)(P^{-1}a)^\top$$

Notes:

- $O(n^2)$ method for computing $P^{-1}(m+1)$ from $P^{-1}(m)$
- standard methods based on dense LU, QR, or SVD for computing $P^{-1}(m+1)$ require $O(n^3)$ operations

Multiobjective least squares

- least squares minimizes $J_1(x) := \|b - Ax\|_2^2$
- consider second cost function $J_2(x) := \|z - Bx\|_2^2$
- usually $\min_x J_1(x)$ and $\min_x J_2(x)$ are competing
- common example: $J_2(x) := \|x\|_2^2$ — small x
- feasible objectives:

  $$\{\, (\alpha, \beta) \in \mathbb{R}^2 \mid \exists\, x \in \mathbb{R}^n \text{ subject to } J_1(x) = \alpha,\ J_2(x) = \beta \,\}$$

- trade-off curve: boundary of the feasible objectives
- the corresponding x is called Pareto optimal

Set of Pareto optimal solutions

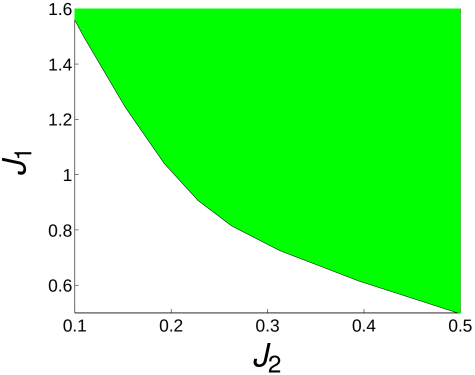
Example:

green area — feasible

white area — infeasible

black line — marginally feasible

Pareto optimal solutions $\leftrightarrow$ points on the line



$\widehat{x}(\mu) = \arg\min_x J_1(x) + \mu J_2(x)$ is Pareto optimal.

varying $\mu \in [0, \infty)$, $\widehat{x}(\mu)$ sweeps the Pareto solutions

Regularized least squares

- Tychonov regularization

$$\widehat{x}_{\text{tych}}(\mu) = \arg\min_x \|b - Ax\|_2^2 + \mu \|x\|_2^2$$

- solution

$$\widehat{x}_{\text{tych}}(\mu) = (A^\top A + \mu I_n)^{-1} A^\top b$$

- exists for any $\mu > 0$, independent of size / rank of A

- trade-off between
  - fitting accuracy $J_1(x) = \|b - Ax\|_2$, and
  - solution size $J_2(x) = \|x\|_2$

Quadratically constrained least squares

- consider biobjective LS problem $\min_x J_1(x)$ and $J_2(x)$
- scalarization approach:

$$\widehat{x}_{\text{tych}}(\mu) = \operatorname*{arg\,min}_x \; J_1(x) + \mu J_2(x)$$

where μ is trade-off parameter

- constrained optimization approach:

$$\widehat{x}_{\text{constr}}(\gamma) = \operatorname*{arg\,min}_x \; J_1(x) \quad \text{subject to} \quad J_2(x) \leq \gamma$$

where γ is upper bound on the J_2 objective

Regularized least squares

- Tychonov regularization is scalarization with
  - fitting accuracy $J_1(x) = \|b - Ax\|_2$, and
  - solution size $J_2(x) = \|x\|_2$
- the constrained optimization approach leads to

$$\widehat{x}_{\text{constr}}(\gamma) = \arg\min_x \|b - Ax\|_2^2 \quad \text{subject to} \quad \|x\|_2^2 \leq \gamma^2$$

- least squares minimization over the ball*

$$\mathscr{U}_{\gamma^2} := \{\, x \mid \|x\|_2^2 \leq \gamma^2 \,\}$$

- solution involves scalar nonlinear equation

Secular equation

- if $\|A^+ b\|_2^2 \leq \gamma^2$, then $\widehat{x}_{\text{constr}}(\gamma) = \|A^+ b\|_2^2$
- if $\|A^+ b\|_2^2 > \gamma^2$, then $\widehat{x}_{\text{constr}}(\gamma) \in \mathscr{U}_{\gamma^2}$
- the Lagrangian of

$$\text{minimize}_x \quad \|b - Ax\|_2^2 \quad \text{subject to} \quad \|x\|_2^2 = \gamma^2$$

  is $\|b - Ax\|_2^2 + \mu(\|x\|_2^2 - \gamma^2)$, μ — Lagrange multiplier

- necessary and sufficient optimality condition

$$x_{\text{tych}}^\top(\mu) x_{\text{tych}}(\mu) = \gamma^2, \quad \text{where} \quad x_{\text{tych}}(\mu) := (A^\top A + \mu I)^{-1} b$$

- secular equation (nonlinear equation in μ)

$$b^\top (A^\top A + \mu I)^{-2} b = \gamma^2$$

- has unique positive solution because
  - $\|x_{\text{tych}}(\mu)\|$ is monotonically decreasing on $\mu \in [0, \infty)$ (by assumption $\|x_{\text{tych}}(0)\|_2^2 > \gamma^2$)
  - $\|x_{\text{tych}}(\infty)\|_2^2 = 0$

Outline

Outline

Total least squares (TLS)

- LS minimizes 2-norm of the eqn. error $e(x) := b - Ax$

$$\min_{x,e} \|e\|_2 \quad \text{subject to} \quad Ax = b - e$$

- alternatively, e can be viewed as a correction on b

- the TLS method is motivated by the asymmetry

  both A and b are given data, but only b is corrected

- TLS problem:

$$\min_{x,\Delta A,\Delta b} \left\| \begin{bmatrix} \Delta A & \Delta b \end{bmatrix} \right\|_F \quad \text{subject to} \quad (A + \Delta A)x = b + \Delta b$$

  - ΔA — correction on A, Δb — correction on b
  - Frobenius matrix norm: $\|C\|_F := \sqrt{\sum_{i=1}^m \sum_{j=1}^n c_{ij}^2}$

Geometric interpretation of the TLS criterion

- with $n = 1$, $x \in \mathbb{R}$, $a = \begin{bmatrix} a_1 \\ \vdots \\ a_m \end{bmatrix}$, $b = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$

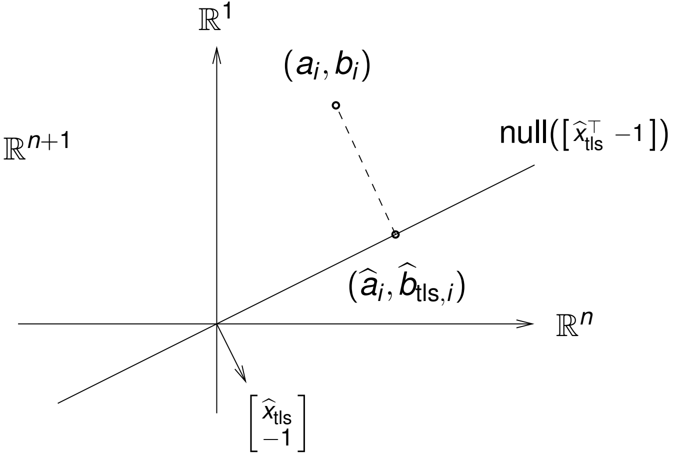
Geometric interpretation:

fit a line $\mathscr{L}(x)$ passing through 0 to the points

$$\begin{bmatrix} a_1 \\ b_1 \end{bmatrix}, \ldots, \begin{bmatrix} a_m \\ b_m \end{bmatrix}$$

- LS minimizes $\sum$ vertical distances^2 from $\begin{bmatrix} a_i \\ b_i \end{bmatrix}$ to $\mathscr{L}(x)$
- TLS minimizes $\sum$ orth. distances^2 from $\begin{bmatrix} a_i \\ b_i \end{bmatrix}$ to $\mathscr{L}(x)$

Geometric interpretation of the TLS criterion



Solution of the TLS problem

Let $\begin{bmatrix} A & b \end{bmatrix} = U\Sigma V^\top$ be the reduced SVD of $\begin{bmatrix} A & b \end{bmatrix}$ and

$$\Sigma = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{n+1} \end{bmatrix}, \quad U = \begin{bmatrix} u_1 & \cdots & u_{n+1} \end{bmatrix}, \quad V = \begin{bmatrix} v_1 & \cdots & v_{n+1} \end{bmatrix}$$

TLS solution of $Ax = b$ exists iff $v_{n+1,n+1} \neq 0$ and is unique iff $\sigma_n \neq \sigma_{n+1}$.

In the case when unique TLS solution exists, it is given by

$$\widehat{x}_{\text{tls}} = -\frac{1}{v_{n+1,n+1}} v_{n+1}(1:n)$$

The TLS correction is
$$\begin{bmatrix} \Delta A_{\text{tls}} & \Delta b_{\text{tls}} \end{bmatrix} = -\sigma_{n+1} u_{n+1} v_{n+1}^\top = \begin{bmatrix} A & b \end{bmatrix} v_{n+1} v_{n+1}^\top .$$

Link to low-rank approximation

- TLS approx. $\begin{bmatrix}\widehat{A}_{\text{tls}} & \widehat{b}_{\text{tls}}\end{bmatrix} := \begin{bmatrix}A & b\end{bmatrix} - \begin{bmatrix}\Delta A_{\text{tls}} & \Delta b_{\text{tls}}\end{bmatrix}$ is optimal (in the Frobenius norm) LRA of $\begin{bmatrix}A & b\end{bmatrix}$
- TLS approx. solution of $Ax = b$, $x \in \mathbb{R}^n$ is equivalent to LRA of $D := \begin{bmatrix}A & b\end{bmatrix}$ by rank-n matrix $\widehat{D}$ with

$$\begin{bmatrix}0 & \cdots & 0 & 1\end{bmatrix} \notin \text{kernel}(\widehat{D}) \qquad (*)$$

- generically, the condition $(*)$ is satisfied
- in nongeneric cases, the TLS solution does not exist
- note that the LRA always exists

Statistical properties of TLS

- errors-in-variables (EIV) model

$$A = \overline{A} + \widetilde{A} \quad \text{and} \quad b = \overline{b} + \widetilde{b}$$

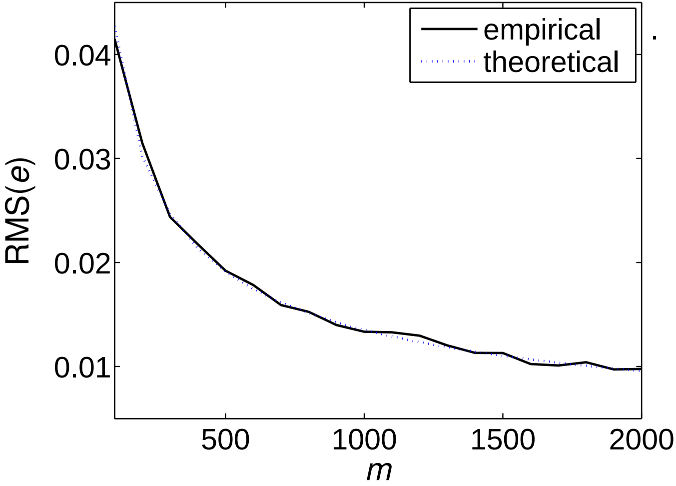
- true values $\overline{A}$, $\overline{b}$ satisfy $\overline{A}\overline{x} = \overline{b}$, for some $\overline{x} \in \mathbb{R}^n$

- perturbations $\widetilde{A}$, $\widetilde{b}$ are zero mean element-wise i.i.d.

- under additional mild assumptions the TLS approx. solution $\widehat{x}$ is a consistent estimator of the true value $\overline{x}$

- measurement errors model
  - A, b — measured data
  - $\overline{x}$ / $\widehat{x}$ — true/estimated model parameters

Estimation error $e = \overline{x} - \widehat{x}$



empirical — solid line, theoretical — dotted line

Notes

- TLS problem vs EIV model
  - TLS approx. can be used without EIV model
  - EIV model shows the correct testbed TLS approx.

- distinguish
  - corrections ΔA, Δb in the TLS problem, and
  - noise/perturbations $\widetilde{A}$, $\widetilde{b}$ in the EIV model

Confidence bounds

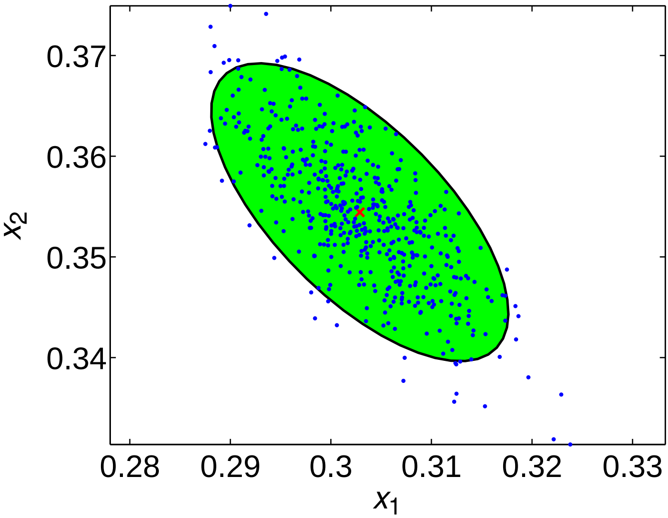
- assume that $\widetilde{A}$, $\widetilde{b}$ are i.i.d. normal with variance ξ^2
- the estimation error e is asymptorically normal
  $\rightsquigarrow$ confidence bounds for $\widehat{x}$
- the asymptotic error $e := \overline{x} - \widehat{x}$ covariance matrix is

$$V_e = \xi^2(1 + \widehat{x}^\top \widehat{x})(A^\top A - m\xi^2 I)^{-1}$$

- the noise variance ξ^2 can be estimated from the data

$$\widehat{\xi}^2 = \frac{1}{m}\sigma_{n+1}^2$$

95% confidence ellipsoid



Weighted total least squares problem

- replace the Frobenius norm by the weighted 2-norm

$$\|D\|_W := \sqrt{\operatorname{vec}^\top(D) W \operatorname{vec}(D)}$$

- $W =$ inverse noise $(\operatorname{vec}([\widetilde{A} \ \ \widetilde{b}]))$ covariance matrix
- in general, WTLS doesn't have analytic solution
- special cases $\rightsquigarrow$ structure of W
  - column/row-wise weighting
  - element-wise weighting
  - generalized TLS
  - restricted TLS

Hierarchy of WTLS problems

1. fully weighted $W \geq 0$

2. column-wise weighted

$$W = \operatorname{diag}(W_1, \ldots, W_m), \quad W_i \in \mathbb{R}_+^{(n+1)\times(n+1)}$$

3. element-wise weighted

$$W = \operatorname{diag}(w), \quad w \in \mathbb{R}_+^{m(n+1)}$$

4. column-wise GTLS: case 2, with W_i's equal

5. column-wise scaled: case 3, with W_i — diagonal

Relative error TLS

- consider the element-wise weighted case

$$\|D\|_w = \|D\|_\Sigma := \|\Sigma \odot D\|_\mathrm{F}$$

($\odot$ — element-wise product)

- $\Sigma_{ij} = 1/d_{ij} \rightsquigarrow$ approximation in relative error sense

$$e_{ij} = \frac{d_{ij} - \widehat{d}_{ij}}{d_{ij}}$$

GTLS problem

- TLS approximation with criterion

$$\|D\|_{\Sigma_l,\Sigma_r} := \|\Sigma_l D \Sigma_r\|_F$$

- link to WTLS

$$\begin{aligned}\|\Sigma_l(D-\widehat{D})\Sigma_r\|_F^2 &= \left\|\operatorname{vec}(\Sigma_l(D-\widehat{D})\Sigma_r)\right\|^2 \\ &= \left\|(\Sigma_r \otimes \Sigma_l)\operatorname{vec}(D-\widehat{D})\right\|^2 \\ &= \operatorname{vec}^\top(D-\widehat{D})\big(W_r \otimes W_l\big)\operatorname{vec}(D-\widehat{D})\end{aligned}$$

where $\sqrt{W_r} = \Sigma_r$ and $\sqrt{W_l} = \Sigma_l$

- WTLS problem with weight matrix $W = W_r \otimes W_l$

Element-wise GTLS

- element-wise weighted total least squares

$$\|D\|_w = \|D\|_\Sigma := \|\Sigma \odot D\|_\mathrm{F}$$

- element-wise generalized total least squares

$$W_\mathrm{r} = \mathrm{diag}(w_\mathrm{r}) \quad \text{and} \quad W_\mathrm{l} = \mathrm{diag}(w_\mathrm{l})$$

- $\rightsquigarrow$ rank-1 matrix $\Sigma = w_\mathrm{l} w_\mathrm{r}^\top$

GTLS solution

- $\sqrt{W_\text{r}} = \Sigma_\text{r}$, w.l.o.g. we can choose Σ_r upper triangular, *e.g.*, the Cholesky factor of W_r

- modified data matrix: $D_\text{m} := \Sigma_\text{l} D \Sigma_\text{r}$

- TLS approximation of D_m: $\widehat{D}_\text{m,tls}$ and $\widehat{x}_\text{m,tls}$

- partition Σ_r as $\begin{bmatrix} \Sigma_\text{r,11} & \Sigma_\text{r,12} \\ 0 & \Sigma_\text{r,22} \end{bmatrix}$, with $\Sigma_\text{r,11} \in \mathbb{R}^{n \times n}$

- GTLS solution

$$\widehat{x}_\text{gtls} = \frac{\Sigma_\text{r,11} \widehat{x}_\text{tls} - \Sigma_\text{r,11}}{\Sigma_\text{r,22}}, \quad \widehat{D}_\text{gtls} = (\Sigma_\text{l})^{-1} \widehat{D}_\text{m,tls} (\Sigma_\text{r})^{-1}$$

Singular weight matrix

- consider the element-wise weighted case

$$\|D\|_w = \|D\|_\Sigma := \|\Sigma \odot D\|_\mathrm{F}$$

- Σ is a matrix of element-wise nonnegative weights
- $\sigma_{ij} = 0 \implies$ the solution doesn't depend on d_{ij}
- zero weights allow us to consider missing data

Restricted total least squares problem

- impose structured correction ΔD

$$\begin{array}{rl} \text{minimize} & \|E\|_{\mathsf{F}} \\ \text{subject to} & (A+\Delta b)x = b+\Delta b \\ \text{and} & \begin{bmatrix}\Delta A & \Delta b\end{bmatrix} = LER \end{array}$$

- link to WTLS: RTLS is a GTLS problem with

$$W_{\mathrm{l}} = (LL^{\top})^{+} \quad \text{and} \quad W_{\mathrm{r}} = (RR^{\top})^{+}$$

(A^{+} is the pseudo-inverse of A)

Structured total least squares

- T. Abatzoglou, J. Mendel, and G. Harada. The constrained total least squares technique and its application to harmonic superresolution. *IEEE Trans. Signal Proc.*, 39:1070–1087, 1991

$$\begin{aligned} &\text{minimize} \quad \text{over } x, \Delta A, \Delta b \quad \left\| \begin{bmatrix} \Delta A & \Delta b \end{bmatrix} \right\|_{\mathrm{F}} \\ &\text{subject to} \quad (A + \Delta A)x = b + \Delta b \text{ and} \\ &\begin{bmatrix} \Delta A & \Delta b \end{bmatrix} \text{ has the same structure as } \begin{bmatrix} A & b \end{bmatrix} \end{aligned}$$

- types of structures
  - linear: Hankel/Toeplitz, Sylvester
  - nonlinear: Vandermonde

Link to structured low-rank approximation

- STLS is equivalent to structured low-rank approx.

$$\begin{array}{ll} \text{minimize} & \text{over } \Delta D \quad \|\Delta D\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank}(D + \Delta D) \leq r \text{ and} \\ & \color{red}{\Delta D \text{ has the same structure as } D} \end{array}$$

with $D := \begin{bmatrix} A & b \end{bmatrix}$, $r = n$, and

$$\begin{bmatrix} 0 & \cdots & 0 & 1 \end{bmatrix} \notin \operatorname{kernel}(\widehat{D}) \qquad (*)$$

- generically, the condition $(*)$ is satisfied
- in nongeneric cases, the STLS solution does not exist

History of the problem

- Errors-in-variables system identification

  M. Aoki and P. Yue. On a priori error estimates of some identification methods. *IEEE Trans. Automat. Control*, 15(5):541–548, 1970

- Sum-of-exponetials estimation

  Y. Bresler and A. Macovski. Exact maximum likelihood parameter estimation of superimposed exponential signals in noise. *IEEE Trans. Acust., Speech, Signal Proc.*, 34:1081–1089, 1986

  J. Cadzow. Signal enhancement—A composite property mapping algorithm. *IEEE Trans. Signal Proc.*, 36:49–62, 1988

- Rimmanian SVD algorithm

  B. De Moor. Structured total least squares and L_2 approximation problems. *Linear Algebra Appl.*, 188–189:163–207, 1993

- Structured total least norm algorithm

  J. Rosen, H. Park, and J. Glick. Total least norm formulation and solution of structured problems. *SIAM J. Matrix Anal. Appl.*, 17:110–126, 1996

- Variable projection algorithm

  I. Markovsky, S. Van Huffel, and R. Pintelon. Block-Toeplitz/Hankel structured total least squares. *SIAM J. Matrix Anal. Appl.*, 26(4):1083–1099, 2005