Least squares and the singular value decomposition

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Outline

- QR and SVD decompositions
- Least squares and least norm problems
- Extensions of the least squares problem
  - Recursive
  - Multiobjective
  - Regularized
  - Constrained

QR and SVD decompositions

Orthonormal set of vectors

Consider a finite set of vectors $\mathscr{Q} := \{ q_1, \dots, q_k \} \subset \mathbb{R}^n$

- $\mathscr{Q}$ is orthogonal $:\iff \langle q_i, q_j \rangle := q_i^\top q_j$, for all $i \neq j$
- $\mathscr{Q}$ is normalized $:\iff \|q_i\|_2^2 := \langle q_i, q_i \rangle = 1$, $i = 1, \dots, k$
- $\mathscr{Q}$ is orthonormal $:\iff \mathscr{Q}$ is orthogonal and normalized

with $Q := \begin{bmatrix} q_1 & \cdots & q_k \end{bmatrix}$, $\quad \mathscr{Q}$ orthonormal $\iff Q^\top Q = I_k$

Properties:

- orthonormal vectors are independent
- multiplication with Q 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 orthonormal set $\mathscr{Q} := \{q_1, \dots, q_k\}$ and $\mathscr{L} := \operatorname{span}(\mathscr{Q}) \subseteq \mathbb{R}^n$.

$\mathscr{Q}$ is an orthonormal basis for $\mathscr{L}$.

With $Q := \begin{bmatrix} q_1 & \cdots & q_k \end{bmatrix}$, $Q^\top Q = I_k$, however, for $k < n$, $QQ^\top \neq I_n$.

$\Pi_{\operatorname{span}(\mathscr{Q})} := QQ^\top$ is an orthogonal projector on span$(\mathscr{Q})$, *i.e.*,

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

Properties: $\Pi = \Pi^2$, $\Pi = \Pi^\top$ (necessary and sufficient for Π orth. proj.)

$\Pi^\perp := (I - \Pi)$ is also orthogonal projector, it projects on

$\big(\operatorname{col}\operatorname{span}(\Pi)\big)^\perp \subseteq \mathbb{R}^n$ — orth. complement of the column span of Π

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

orthonormal set $\mathcal{Q} := \{ q_1, \dots, q_k \} \subset \mathbb{R}^n$ of $k = n$ vectors

then $Q := \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix}$ is called orthogonal and satisfies $Q^\top Q = I_n$

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 $\mathcal{Q}$
- $x = Q\widetilde{x}$ 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 $\{q_1, \ldots, q_k\} \subset \mathbb{R}^n$ such that

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

G-S procedure: Let $q_1 := a_1 / \|a_1\|_2$. At the ith step $i = 2, \ldots, k$

- orthogonalized a_i w.r.t. $q_1, \ldots, q_{i-1}$:

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

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

QR decomposition

G-S procedure gives as a byproduct scalars r_{ji}, $j \leq i$, $i = 1, \ldots, k$, s.t.

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

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, $v_i := (I - \Pi_{\text{span}(q_1,\ldots,q_{i-1})})a_i = 0$ 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 the next input vector 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

$$A = \underbrace{\begin{bmatrix} Q_1 & Q_2 \end{bmatrix}}_{\text{orthogonal}} \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$

$$\begin{aligned} \operatorname{col span}(A) &= \operatorname{col span}(Q_1) \\ \big(\operatorname{col span}(A)\big)^\perp &= \operatorname{col span}(Q_2) \end{aligned}$$

Procedure for finding Q_2:

complete A to full rank matrix, *e.g.*, $A_\mathrm{m} := \begin{bmatrix} A & I \end{bmatrix}$, 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 $\begin{bmatrix} Q_1 & I \end{bmatrix}$)

Singular value decomposition (SVD)

The SVD is used as both computational and analytical tool.

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

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

where U_1 and V_1 are 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

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

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

Note that the singular values of A are

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

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

Proof of existence of an SVD

The proof is constructive and uses induction. W.l.o.g. assume $m \geq n$.

- End of induction: vector $A \in \mathbb{R}^{m \times 1}$ has (unique) SVD

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

- Inductive step: choose $v_i \in \mathbb{R}^n$ with $\|v_i\|_2 = 1$ and let

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

Complete v_i and u_i to orthogonal matrices (QR decomp.)

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

We have that 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 $w = 0$.

Proof of existence of an SVD

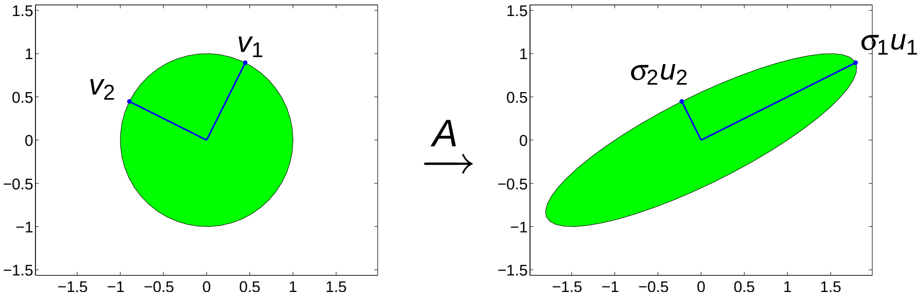
$$
\begin{aligned}
\sigma_i^2 = \|A_i\|_2^2 = \|U_i^\top A_i V_i\|_2^2 \\
&= \max_v \frac{\|A_i v\|_2^2}{\|v\|_2^2} \\
&\geq \frac{\|A_i \left[\begin{smallmatrix}\sigma_i \\ w\end{smallmatrix}\right]\|_2^2}{\|\left[\begin{smallmatrix}\sigma_i \\ w\end{smallmatrix}\right]\|_2^2} \\
&= \frac{1}{\sigma_i^2 + w^\top w}\left\|\begin{bmatrix}\sigma_i^2 + w^\top w \\ A_{i+1} w\end{bmatrix}\right\|_2^2 \\
&\geq \frac{1}{\sigma_i^2 + w^\top w}(\sigma_i^2 + w^\top w)^2 = \sigma_i^2 + w^\top w
\end{aligned}
$$

The inequality $\sigma_i^2 \geq \sigma_i^2 + w^\top w$ can be true only when $w = 0$.

Geometric fact motivating the SVD

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

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



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 approximation of A w.r.t. the norm $\|\cdot\|$, *e.g.*,

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

Solution via SVD

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

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

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

A solution to (LRA) is

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

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

Proof of the low-rank approximation theorem

Let $\widehat{A}^*$ be solution to (LRA) and let $\widehat{A}^* := U^*\Sigma^*(V^*)^\top$ be an SVD of $\widehat{A}^*$.

$$\|A - \widehat{A}^*\|_{\mathrm{F}} = \|\underbrace{(U^*)^\top A V^*}_{B} - \Sigma^*\|_{\mathrm{F}} \quad \Longrightarrow \quad \Sigma^* \text{ is an opt. approx. of } B$$

Partition $B =: \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$ conformably with $\Sigma^* =: \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix}$ and observe that

$$\operatorname{rank}\left(\begin{bmatrix} \Sigma_1^* & B_{12} \\ 0 & 0 \end{bmatrix}\right) \leq r \quad \text{and} \quad B_{12} \neq 0 \implies \left\| B - \begin{bmatrix} \Sigma_1^* & B_{12} \\ 0 & 0 \end{bmatrix} \right\|_{\mathrm{F}} < \left\| B - \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix} \right\|_{\mathrm{F}}$$

so that $B_{12} = 0$. Similarly $B_{21} = 0$. Observe also that

$$\operatorname{rank}\left(\begin{bmatrix} B_{11} & 0 \\ 0 & 0 \end{bmatrix}\right) \leq r \quad \text{and} \quad B_{11} \neq \Sigma_1^* \implies \left\| B - \begin{bmatrix} B_{11} & 0 \\ 0 & 0 \end{bmatrix} \right\|_{\mathrm{F}} < \left\| B - \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix} \right\|_{\mathrm{F}}$$

so that $B_{11} = \Sigma_1^*$. Therefore, $B = \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & B_{22} \end{bmatrix}$.

Proof of the low-rank approximation theorem

Let $B_{22} = U_{22}\Sigma_{22}V_{22}^\top$ be the SVD of B_{22}. Then the matrix

$$\begin{bmatrix} I & 0 \\ 0 & U_{22}^\top \end{bmatrix} B \begin{bmatrix} I & 0 \\ 0 & U_{22} \end{bmatrix} = \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & \Sigma_{22} \end{bmatrix}$$

has optimal rank-r approximation $\Sigma^* = \left[\begin{smallmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{smallmatrix}\right]$, so that

$$\min(\text{diag}(\Sigma_1^*)) > \max(\text{diag}(U_{22}))$$

Therefore

$$A = U^* \begin{bmatrix} I & 0 \\ 0 & U_{22} \end{bmatrix} \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & \Sigma_{22} \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & U_{22}^\top \end{bmatrix} (V^*)^\top$$

is an SVD of A.

Proof of the low-rank approximation theorem

SVD of A:

$$A = U^* \begin{bmatrix} I & 0 \\ 0 & U_{22} \end{bmatrix} \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & \Sigma_{22} \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & U_{22}^\top \end{bmatrix} (V^*)^\top$$

Then, if $\sigma_r > \sigma_{r+1}$, the rank-r SVD truncation

$$\widehat{A}^* = U^* \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix} (V^*)^\top = U^* \begin{bmatrix} I & 0 \\ 0 & U_{22} \end{bmatrix} \begin{bmatrix} \Sigma_1^* & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & U_{22}{}^\top \end{bmatrix} (V^*)^\top$$

is unique and $\widehat{A}^*$ is the unique solution of (LRA).

Note that $\widehat{A}^*$ is simultaneously optimal in any unitarily invariant norm.

Numerical rank

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

and

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

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

In particular, $\sigma_{\min}(A)$ is the distance of A to rank deficiency.

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

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

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

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

In general, $A^+ y$ is the least squares, least norm solution of $Ax = y$

Note that the pseudo-inverse depends on the rank of A.
In practice the numerical rank $\operatorname{rank}(A, \varepsilon)$ is used.

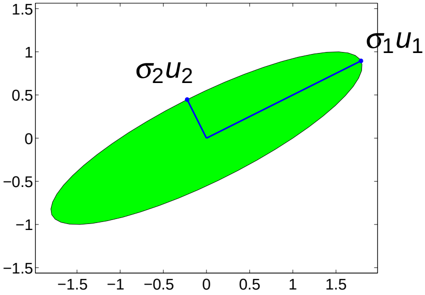
The SVD, using numerical rank and pseudo-inverse, is the most reliable way of solving $Ax = y$.

It should be used in cases when A is ill-conditioned.

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

Geometrically $\kappa(A)$ is the eccentricity of the hyperellipsoid

$$A\{x \mid \|x\|_2 = 1\}$$



$\kappa(A)$ measures the sensitivity of A^+y to perturbations in y and A

For large $\kappa(A)$ (above a few 1000) A is called ill-conditioned.

Least squares and least norm

Least squares

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

  choose x that minimizes 2-norm of the residual (eqn. error)

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

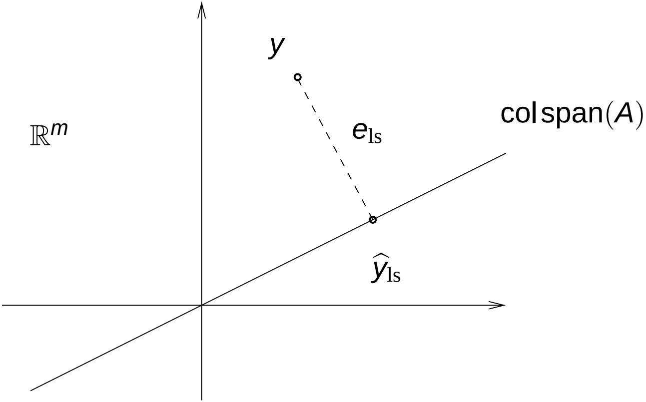
- a minimizing x is called a least squares approximate solution

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

Geometric interpretation: project y onto the image of A

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

$$e_{\mathrm{ls}} := \widehat{y}_{\mathrm{ls}} - A\widehat{x}_{\mathrm{ls}}$$

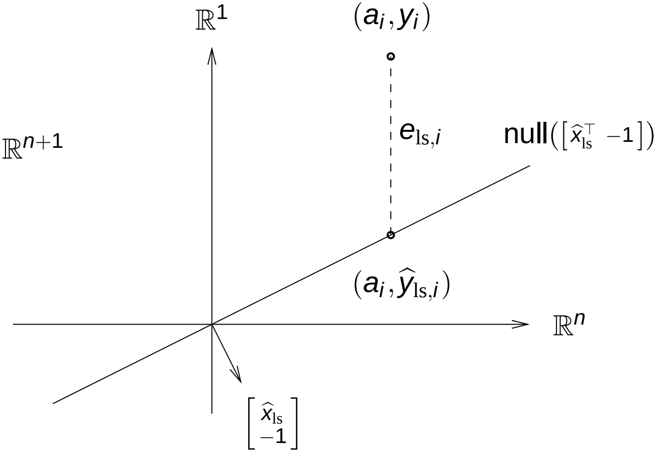


$$\begin{aligned} A\widehat{x}_{\mathrm{ls}} = \widehat{y}_{\mathrm{ls}} \quad &\iff \quad \begin{bmatrix} A & \widehat{y}_{\mathrm{ls}} \end{bmatrix} \begin{bmatrix} \widehat{x}_{\mathrm{ls}} \\ -1 \end{bmatrix} = 0 \\ &\iff \quad \begin{bmatrix} a_i & \widehat{y}_{\mathrm{ls},i} \end{bmatrix} \begin{bmatrix}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

(a_i is the ith row of A)

- $(a_i, \widehat{y}_{\mathrm{ls},i})$, for all i, lies on the subspace perpendicular to $(\widehat{x}_{\mathrm{ls}}, -1)$
- "data point" $(a_i, y_i) = (a_i, \widehat{y}_{\mathrm{ls},i}) + (0, e_{\mathrm{ls},i})$
- the approximation error $(0, e_{\mathrm{ls},i})$ is the vertical distance from (a_i, y_i) to the subspace

Another geometric interpretation of the LS approximation:



Notes

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

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

is the unique least squares approximate solution.

- $\widehat{x}_{\text{ls}}$ is a linear function of y
- If A is square $\widehat{x}_{\text{ls}} = A^{-1} y$
- $\widehat{x}_{\text{ls}}$ is an exact solution if $Ax = y$ has an exact solution
- $\widehat{y}_{\text{ls}} := A\widehat{x}_{\text{ls}} = A(A^\top A)^{-1} A^\top y$ is a least squares approximation of y

Projector onto the span of A

The $m \times m$ matrix

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

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

The columns of A are an arbitrary basis for $\mathscr{L}$.

If the columns of Q form an orthonormal basis for $\mathscr{L}$

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

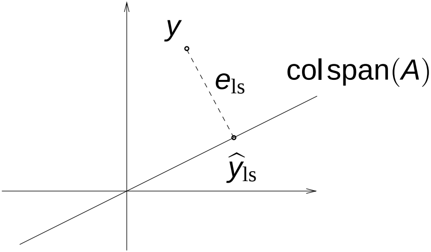
Orthogonality principle

The least squares residual vector

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

is orthogonal to $\text{col span}(A)$

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



Least squares via QR decomposition

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

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

so that

$$\widehat{x}_{\text{ls}} = R^{-1}Q^\top y \quad \text{and} \quad \widehat{y}_{\text{ls}} := Ax_{\text{ls}} = QQ^\top y$$

Let $A =: \begin{bmatrix} a_1 & \cdots & a_n \end{bmatrix}$ and consider the sequence of LS problems

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

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

$$\widehat{x}^i_{\text{ls}} = R_i^{-1}Q_i^\top y$$

Least norm solution

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

The set of solutions is

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

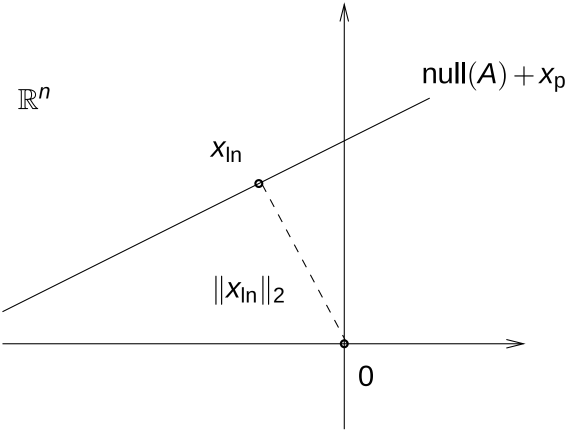
where x_{p} is a particular solution, *i.e.*, $Ax_{\mathrm{p}} = y$.

Least norm problem

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

Geometric interpretation:

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



Derivation of the solution: Lagrange multipliers

Consider the least norm problem with A full rank

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

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

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

the optimality conditions are

$$\begin{aligned} \nabla_x L(x, \lambda) &= 2x + A^\top \lambda = 0 \\ \nabla_\lambda L(x, \lambda) &= Ax - y = 0 \end{aligned}$$

from the first condition $x = -A^\top \lambda / 2$, substituting into the second

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

Solution via QR decomposition

Let $A^\top = QR$ be the 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

$$x_{\mathrm{ln}} = Q(R^\top)^{-1}y$$

Extensions

Weighted least squares

Given a positive definite matrix $W \in \mathbb{R}^{m \times m}$, define wighted 2-norm

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

Weighted least squares approximation problem

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

The orthogonality principle holds by defining the inner product as

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

and

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

Recursive least squares

Let $a_i^\top$ be the ith row of A

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

with this notation, $\|y - Ax\|_2^2 = \sum_{i=1}^m (y_i - a_i^\top x)^2$ and

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

- (a_i, y_i) correspond to a measurement
- often the measurements (a_i, y_i) come sequentially (*e.g.*, in time)

Recursive computation of $\widehat{x}_{\mathrm{ls}}(m) = \left(\sum_{i=1}^{m} a_i a_i^\top\right)^{-1} \sum_{i=1}^{m} a_i y_i$

- $P(0) = 0 \in \mathbb{R}^{n\times n}$, $q(0) = 0 \in \mathbb{R}^n$
- For $m = 0, 1, \ldots$
- $P(m+1) := P(m) + a_{m+1}a_{m+1}^\top$, $q(m+1) := q(m) + a_{m+1}y_{m+1}$.
- If $P(m)$ is invertible, $x_{\mathrm{ls}}(m) = P^{-1}(m)q(m)$.

Notes:

- In each step, 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:

- gives an $O(n^2)$ 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 the cost function $J_1(x) := \|y - Ax\|_2^2$.

Consider a second cost function $J_2(x) := \|z - Bx\|_2^2$,

which we want to minimize together with J_1.

Usually the criteria $\min_x J_1(x)$ and $\min_x J_2(x)$ are competing.

Common example: $J_2(x) := \|x\|_2^2$ — minimize J_1 with small x

- feasible objectives:

  $\{ (\alpha, \beta) \in \mathbb{R}^2 \mid \exists\, x \in \mathbb{R}^n \text{ subject to } J_1(x) = \alpha,\ J_2(x) = \beta \}$
- optimal trade-off curve: boundary of the feasible objectives
- the corresponding x is called Pareto optimal

Set of Pareto optimal solutions

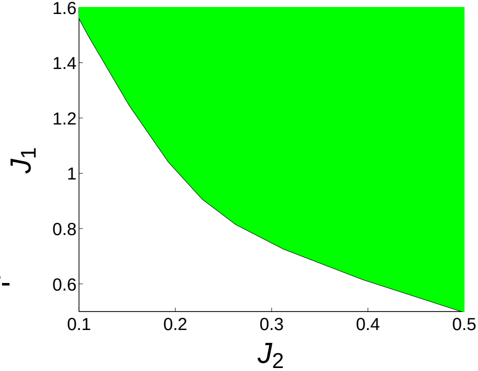
Example:

green area — feasible

white area — infeasible

black line — marginally feasible

Pareto optimal solutions correspond to points on the line



For any $\mu \geq 0$, $\widehat{x}(\mu) = \arg\min_x J_1(x) + \mu J_2(x)$ is Pareto optimal.

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

Regularized least squares

Tychonov regularization

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

the solution

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

exists for any $\mu > 0$, independent on size and rank of A.

Trade-off between

- fitting accuracy $J_1(x) = \|y - Ax\|_2$, and
- solution size $J_2(x) = \|x\|_2$.

Quadratically constrained least squares

Consider again the biobjective LS problem $\min_x J_1(x)$ and $J_2(x)$

Scalarization approach:

$$\widehat{x}_{\text{tych}}(\mu) = \arg\min_x \; J_1(x) + \mu J_2(x)$$

where μ is trade-off parameter

Constrained optimization approach:

$$\widehat{x}_{\text{constr}}(\gamma) = \arg\min_x \; J_1(x) \quad \text{subject to} \quad J_2(x) \leq \gamma$$

where γ is upper bound on the J_2 objective

Regularized least squares

Tychonov regularization corresponds to the scalarization approach for

- fitting accuracy $J_1(x) = \|y - Ax\|_2$, and
- solution size $J_2(x) = \|x\|_2$.

The constrained optimization approach leads in this case to

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

least squares minimization over the ball $\mathscr{U}_{\gamma^2} := \{\, x \mid \|x\|_2^2 \leq \gamma^2 \,\}$.

The solution to the latter problem involves scalar nonlinear equation.

Secular equation

If $\|A^+y\|_2^2 \leq \gamma^2$, then $\widehat{x}_{\text{constr}}(\gamma) = \|A^+y\|_2^2$.

If $\|A^+y\|_2^2 > \gamma^2$, then it can be shown that $\widehat{x}_{\text{constr}}(\gamma) \in \mathscr{U}_{\gamma^2}$.

The Lagrangian of

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

is $\|y - Ax\|_2^2 + \mu(\|x\|_2^2 - \gamma^2)$, where μ is a Lagrange multiplier.

Necessary and sufficient optimality condition is

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

The nonlinear equation in μ

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

is called secular equation. It has unique positive solution because $\|x_{\text{tych}}(\mu)\|$ is monotonically decreasing on the interval $\mu \in [0, \infty)$ and by assumption $\|x_{\text{tych}}(0)\|_2^2 > \gamma^2$.

Total least squares (TLS)

The LS method minimizes 2-norm of the equation error $e(x) := y - Ax$.

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

alternatively the equation error e can be viewed as a correction on y.

The TLS method is motivated by the asymmetry of the LS method:

both A and y are given data, but only y is corrected.

TLS problem: $\displaystyle \min_{x,\Delta A,\Delta y} \left\| \begin{bmatrix} \Delta A & \Delta y \end{bmatrix} \right\|_{\mathrm{F}} \quad \text{subject to} \quad (A + \Delta A)x = y + \Delta y$

- ΔA — correction on A, Δy — correction on y
- Frobenius matrix norm: $\|C\|_{\mathrm{F}} := \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} c_{ij}^2}$, where $C \in \mathbb{R}^{m \times n}$

Geometric interpretation of the TLS criterion

In the case $n = 1$, the problem of solving approximately $Ax = y$ is

$$\begin{bmatrix} a_1 \\ \vdots \\ a_m \end{bmatrix} x = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}, \qquad x \in \mathbb{R}$$

Geometric interpretation:

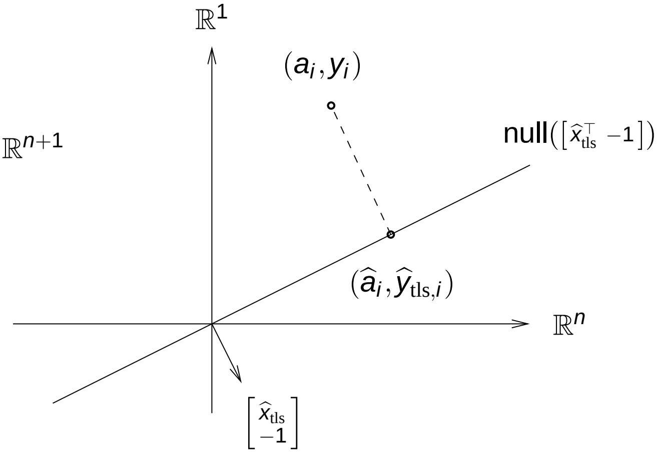
fit a line $\mathscr{L}(x)$ passing through 0 to the points $(a_1, y_1), \dots, (a_m, y_m)$

- LS minimizes

  sum of squared vertical distances from (a_i, y_i) to $\mathscr{L}(x)$

- TLS minimizes

  sum of squared orthogonal distances from (a_i, y_i) to $\mathscr{L}(x)$


$\mathbb{R}^1$
(a_i, y_i)
$\mathbb{R}^{n+1}$
$\mathrm{null}([\widehat{x}_{\mathrm{tls}}^\top \; -1])$
$(\widehat{a}_i, \widehat{y}_{\mathrm{tls},i})$
$\mathbb{R}^n$
$\begin{bmatrix} \widehat{x}_{\mathrm{tls}} \\ -1 \end{bmatrix}$

Solution of the TLS problem

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

$$\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_{n+1}), \quad U = \begin{bmatrix} u_1 & \cdots & u_{n+1} \end{bmatrix}, \quad V = \begin{bmatrix} v_1 & \cdots & v_{n+1} \end{bmatrix}.$$

A TLS solution of $Ax = y$ exists iff $v_{n+1,n+1} \neq 0$ (last element of v_{n+1}) and is unique iff $\sigma_n \neq \sigma_{n+1}$.

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

$$\widehat{x}_{\mathrm{tls}} = -\frac{1}{v_{n+1,n+1}} \begin{bmatrix} v_{1,n+1} \\ \vdots \\ v_{n,n+1} \end{bmatrix}$$

and the corresponding TLS corrections are $\begin{bmatrix} \Delta A_{\mathrm{tls}} & \Delta y_{\mathrm{tls}} \end{bmatrix} = -\sigma_{n+1} u_{n+1} v_{n+1}^\top$

(Corollary of the low-rank approximation theorem, see page 17.)

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