Chapter 3

Applications

- Least-squares
- Least-norm
- Total least-squares
- Low-rank approximation

The first three sections are discuss the linear system of equations $Ax = y$. The matrix $A \in \mathbb{R}^{m\times n}$ and the vector $y \in \mathbb{R}^m$ are given data. The vector $x \in \mathbb{R}^n$ is an unknown. Assuming that A is full rank, the system $Ax = y$ is called

- *overdetermined* if $m > n$ (in this case it has more equations than unknowns) and
- *underdetermined* if $m < n$ (in this case it has more unknowns than equations).

For most vectors $y \in \mathbb{R}^m$, an overdetermined system has no solution x, and for any $y \in \mathbb{R}^m$ an underdetermined system has infinitely many solutions x. In the case of an overdetermined system, it is of interested to find an approximate solution. An important example is the least squares approximate solution, which minimizes the 2-norm of the equation error.

In the case of an underdetermined system, it is of interested to find a particular solution. The least-norm solution is an example of a particular solution, It minimizes the 2-norm of the solution. Note that the least-squares approximate solution is (most of the time) not a solution, while the least-norm solution is (aways) one of infinitely many solutions.

3.1 Least-squares

The least-squares method for solving approximately an overdetermined system $Ax = y$ of equations is defined as follows. Choose x such that the 2-norm of the residual (equation error)

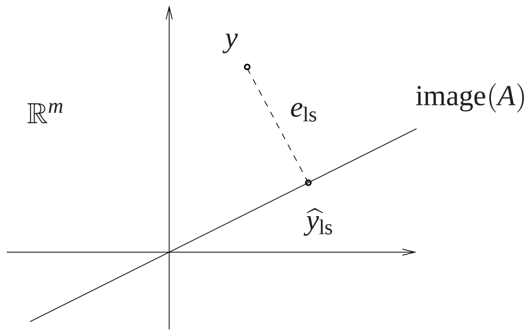
$$e(x) := y - Ax$$

is minimized. A minimizer

$$\widehat{x}_{\text{ls}} := \arg\min_{x} \|\underbrace{y - Ax}_{e(x)}\|_2 \tag{3.1}$$

is called a *least-squares approximate solution* of the system $Ax = y$.

A geometric interpretation of the least-squares approximation problem (3.1) projection of y onto the image of A.



Here $\widehat{y}_{\text{ls}} := A\widehat{x}_{\text{ls}}$ is the projection, which is the least-squares approximation of y and $e_{\text{ls}} := \widehat{y}_{\text{ls}} - A\widehat{x}_{\text{ls}}$ is the approximation error.

Let a_i be the ith row of A. We refer to the vector $\text{col}(a_i, y_i)$ as a "data point". We have,

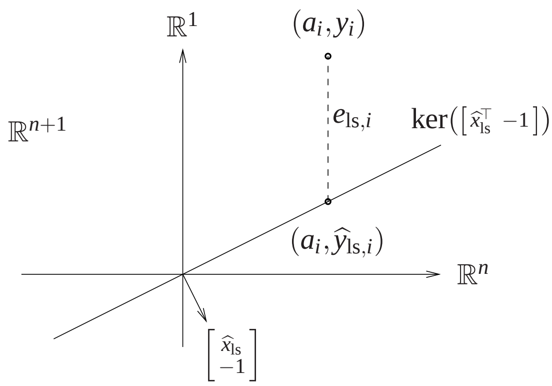
$$\begin{aligned} A\widehat{x}_{\text{ls}} = \widehat{y}_{\text{ls}} \quad &\iff \quad \begin{bmatrix} A & \widehat{y}_{\text{ls}} \end{bmatrix} \begin{bmatrix} \widehat{x}_{\text{ls}} \\ -1 \end{bmatrix} = 0 \\ &\iff \quad \begin{bmatrix} a_i & \widehat{y}_{\text{ls},i} \end{bmatrix} \begin{bmatrix}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

so that for all i, $(a_i, \widehat{y}_{\text{ls},i})$ lies on the subspace perpendicular to $(\widehat{x}_{\text{ls}}, -1)$. $(a_i, \widehat{y}_{\text{ls},i})$ is an the least-squares approximation of the i data point $\text{col}(a_i, y_i)$.

$$(a_i, \widehat{y}_{\text{ls},i}) = (a_i, \widehat{y}_{\text{ls},i}) + (0, e_{\text{ls},i}),$$

and $(0, e_{\text{ls},i})$ is the least-squares approximation error. Note that $e_{\text{ls},i}$ is the vertical distance from (a_i, y_i) to the subspace.

The above derivation suggestions another geometric interpretation of the least-squares approximation.



Note that the former geometric interpretation is in the space $\mathbb{R}^m$, while the latter is in the (data space) $\mathbb{R}^{n+1}$.

Exercise problem 49. [Derivation of solution x_{ln} via Lagrange multipliers] Assuming that $m \geq n = \text{rank}(A)$, i.e., A is full column rank, show that

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

□

Notes:

- $A_{\text{ls}} := (A^\top A)^{-1} A^\top$ is a left-inverse of A
- $\widehat{x}_{\text{ls}}$ is a linear function of y (given by the matrix A_{ls})
- If A is square, $\widehat{x}_{\text{ls}} = A^{-1} y$ (i.e., $A_{\text{ls}} = A^{-1}$)
- $\widehat{x}_{\text{ls}}$ 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 image of A and orthogonality principle

The $m \times m$ matrix

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

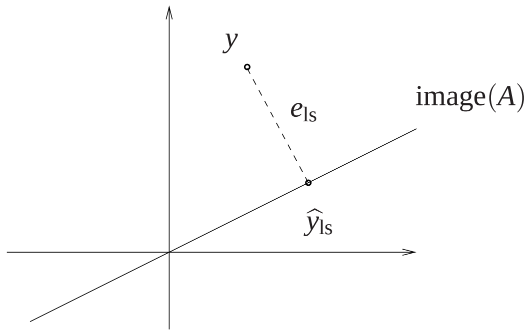
is the orthogonal projector onto the subspace $\mathscr{L} := \text{image}(A)$. Suppose that the columns of A form an orthonormal basis for $\mathscr{L}$. Then, recall that $\Pi_{\text{image}(Q)} := AA^\top$.

The least-squares residual vector

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

is orthogonal to image(A)

$$\langle e_{\text{ls}}, A\widehat{x}_{\text{ls}}\rangle = y^\top \left(I_m - A(A^\top A)^{-1}A^\top\right)A\widehat{x}_{\text{ls}} = 0. \tag{3.2}$$



Exercise problem 50. Show that the orthogonality condition (3.2) is a necessary and sufficient condition for $\widehat{x}_{\text{ls}}$ being a least squares approximate solution to $Ax = b$.

□

Least-squares via QR factorization

Let $A = QR$ be the QR factorization of A. We have,

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

so that

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

Exercise problem 51 (Least-squares with an increasing number of columns in A). Let $A =: \begin{bmatrix} a_1 & \cdots & a_n \end{bmatrix}$ and consider the sequence of least squares problems

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

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

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

□

Weighted least-squares

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

$$\|e\|_W^2 := e^\top We.$$

and the weighted least-squares approximate solution

$$\widehat{x}_{W,\text{ls}} := \arg\min_x \|y - Ax\|_W^2.$$

Exercise problem 52. Show that

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

and that the least-squares orthogonality principle holds for the weighted least-squares problem as well by replacing the inner product $\langle e, y\rangle$ by the weighted inner product

$$\langle e, y\rangle_W := e^\top Wy.$$

$\square$

Recursive least-squares

The least-squares criterion is

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

where $a_i^\top$ is the ith row of A. We consider the sequence of least-squares problems

$$\text{minimize} \quad \sum_{i=1}^k (y_i - a_i^\top x)^2$$

the solutions of which are

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

The meaning is that the measurements (a_i, y_i) come sequentially (in time) and we aim to compute a solution each time a new data point arrives. Instead of recomputing the solution from scratch, we can recursively update $\widehat{x}_{\text{ls}}(k-1)$ in order to obtain $\widehat{x}_{\text{ls}}(k)$.

Recursive algorithm

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

On each step, the algorithm requires inversion of an $n \times n$ matrix, which requires $O(n^3)$ operations. At certain k, $P(k)$ being invertible implies that $P(k')$ is invertible, for all $k' > k$.

The computational complexity of the algorithm can be decreased to $O(n^2)$ operations per step by using the following result about the inverse of matrix with rank-1 update

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

Multiobjective least-squares

Least-squares minimizes the cost function

$$J_1(x) := \|Ax - y\|_2^2.$$

Consider a second cost function

$$J_2(x) := \|Bx - z\|_2^2,$$

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. A common example is $J_2(x) := \|x\|_2^2$ — minimize J_1 with small x.

The set of achievable objectives is

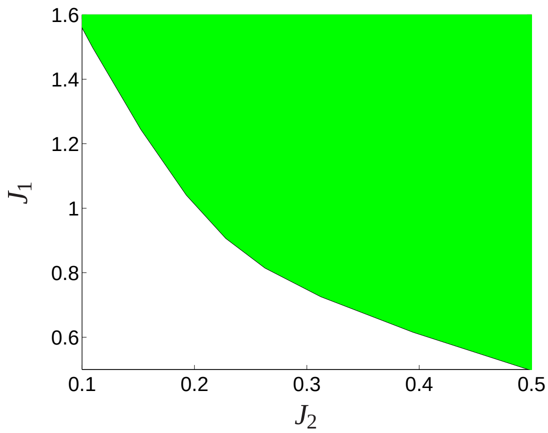
$$\{\,(\alpha,\beta) \in \mathbb{R}^2 \mid \exists\, x \in \mathbb{R}^n \text{ subject to } J_1(x) = \alpha,\ J_2(x) = \beta\,\}$$

Its boundary is the optimal trade-off curve and the corresponding x's are called *Pareto optimal*.

A common method for "solving" multiobjective optimization problems is secularization. For any $\mu \geq 0$, the problem

$$\widehat{x}(\mu) = \arg\min_x J_1(x) + \mu J_2(x)$$

produces a Pareto optimal point. For a convex problem (such as the the multiobjective least-squares), by varying $\mu \in [0,\infty)$, $\widehat{x}(\mu)$ sweeps all Pareto optimal solutions.



Regularized least-squares

Exercise problem 53. Show that the solution of the *Tychonov regularization* problem

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

is

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

□

Note that $\widehat{x}_{\text{reg}}$ exists for any $\mu > 0$, independent on size and rank of A. The parameter μ controls the trade-off between

- fitting accuracy $\|Ax - b\|_2$, and
- solution size $\|x\|_2$.

For small μ, the solution is larger but gives better fit. For large μ, the solution is smaller but the fit is worse. In the extreme case $\mu = 0$, assuming that the system $Ax = b$ is overdetermined, the regularized least-squares problem is equivalent to the standard least-squares problem, which does not constrain the size of x. In the other extreme $\mu \to 0$, assuming that $Ax = b$ is underdetermined, the regularized least-squares problem tends to the least-norm problem.

3.2 Least-norm

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

$$\mathscr{A} := \{\, x \in \mathbb{R}^n \mid Ax = y \,\} = \{\, x_{\mathrm{p}} + z \mid z \in \ker(A) \,\} = x_{\mathrm{p}} + \ker(A).$$

where x_{p} is a particular solution, i.e., $Ax_{\mathrm{p}} = y$. The least-norm solution is defined by the optimization problem

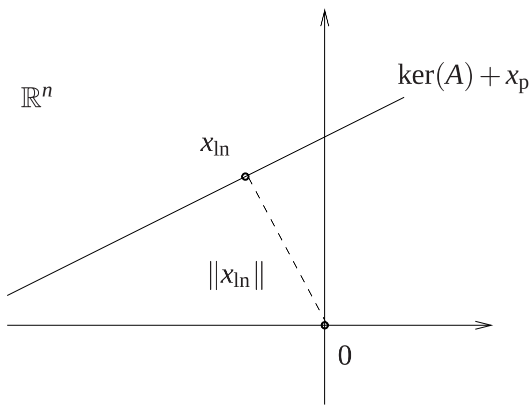
$$x_{\mathrm{ln}}^2 := \arg\min_x \|x\|_2 \quad \text{subject to} \quad Ax = y. \tag{3.3}$$

Exercise problem 54 (Derivation of solution x_{ln} via Lagrange multipliers). Assuming that $n \geq m = \operatorname{rank}(A)$, i.e., A is full row rank, show that

$$x_{\mathrm{ln}} = A^\top (AA^\top)^{-1} y.$$

□

A geometric interpretation of (1.3) is the projection of 0 onto the solution set $\mathscr{A}$.



Exercise problem 55. The orthogonality principle for least-norm is $x_{\mathrm{ln}} \perp \ker(A)$. Show that it is a necessary and sufficient condition for optimality of x_{ln}

□

Let $A^\top = QR$ be the QR factorization of $A^\top$. The right inverse of A is

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

so that

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

3.3 Total least-squares

The least-squares method minimizes the 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 total least-squares method is motivated by the asymmetry of the least-squares method: both A and b are given data, but only b is corrected. The total least squares problem is defined by the optimization problem

$$\text{minimize}_{x,\widetilde{A},\widetilde{y}} \quad \left\| \begin{bmatrix} \widetilde{A} & \widetilde{y} \end{bmatrix} \right\|_{\mathrm{F}} \quad \text{subject to} \quad (A + \widetilde{A})x = y + \widetilde{y}$$

Here $\widetilde{A}$ is the correction on A and $\widetilde{y}$ is the correction on y. The Frobenius norm $\|C\|_{\mathrm{F}}$ of $C \in \mathbb{R}^{m\times n}$ is defined as

$$\|C\|_{\mathrm{F}} := \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} c_{ij}^2}.$$

Geometric interpretation of the total least squares criterion

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

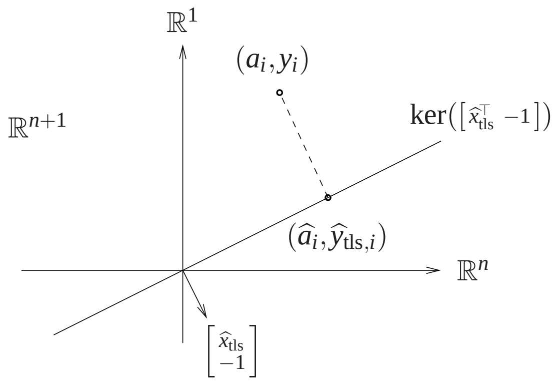
$$\begin{bmatrix} a_1 \\ \vdots \\ a_m \end{bmatrix} x = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}, \qquad \text{where} \quad x \in \mathbb{R}. \tag{3.4}$$

A geometric interpretation of the total least squares problem (3.4) is: fit a line

$$\mathscr{L}(x) := \{\, (a,b) \mid ax = b \,\}$$

passing through the origin to the points $(a_1, y_1), \ldots, (a_m, y_m)$.

- least squares minimizes sum of squared *vertical* distances from (a_i, y_i) to $\mathscr{L}(x)$,
- total least squares minimizes sum of squared *orthogonal* distances from (a_i, y_i) to $\mathscr{L}(x)$.



Solution of the total least squares problem

Theorem 56. *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 total least squares solution exists if and only if $v_{n+1,n+1} \neq 0$ (last element of v_{n+1}) and is unique if and only if $\sigma_n \neq \sigma_{n+1}$.

In the case when a total least squares solution exists and is unique, it is given by

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

and the corresponding total least squares corrections are

$$\begin{bmatrix} \widetilde{A}_{\text{tls}} & \widetilde{y}_{\text{tls}} \end{bmatrix} = -\sigma_{n+1} u_{n+1} v_{n+1}^\top.$$

3.4 Low-rank approximation

The low-rank approximation problem is defined as: Given a matrix $A \in \mathbb{R}^{m\times n}$, $m \geq n$, and an integer r, $0 < r < n$, find

$$\widehat{A}^* := \arg\min_{\widehat{A}} \|A - \widehat{A}\| \quad \text{subject to} \quad \operatorname{rank}(\widehat{A}) \leq r. \tag{3.5}$$

$\widehat{A}^*$ is an optimal rank-r approximation of A with respect to the norm $\|\cdot\|$, e.g.,

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

Theorem 57 (Solution via SVD). *Let $A = U\Sigma V^\top$ be the SVD of A and define*

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

An solution to (3.5) is

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

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

3.5 Notes and references

Least-squares and least-norm are standard topics in both numerical linear algebra and engineering. Numerical aspects of the problem are considered in [Bjö96]. For an overview of total least squares problem, see [MV07]

Bibliography

[Bjö96] Å. Björck. *Numerical Methods for Least Squares Problems*. SIAM, 1996.

[MV07] I. Markovsky and S. Van Huffel. Overview of total least squares methods. *Signal Processing*, 87:2283–2302, 2007.