

Selected Topics in Engineering Mathematics: Least Squares Problems

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Reference

- ① R. A. Horn and C. R. Johnson, Matrix Analysis, 2nd ed., New York: Cambridge University Press, 2013.
[HJ2013]
- ② G. H. Golub and C. F. Van Loan, Matrix Computations, 4th ed., Baltimore: The Johns Hopkins University Press, 2013.
[GVL2013]
- ③ J.-J. Ding. (2023). Selected Topics in Engineering Mathematics [PowerPoint slides].

Outline

- 1 Problem Formulation
- 2 The Full-Rank LS Problem
- 3 The Rank-Deficient LS Problem
- 4 The Pseudo-Inverse of a Matrix
- 5 Concluding Remarks

Motivation

- Find a vector $\mathbf{x} \in \mathbb{C}^N$ such that

$$\mathbf{Ax} = \mathbf{b}. \quad (1)$$

- The **data matrix** $\mathbf{A} \in \mathbb{C}^{M \times N}$ is given.
- The **observation vector** $\mathbf{b} \in \mathbb{C}^M$ is given.
- The number of equations is M .
- The number of unknowns is N .
- Underdetermined systems: $M < N$
- Overdetermined systems: $M > N$

Questions

- How many solutions to (1)?

Examples of (1)

Underdetermined Systems

$$\underbrace{\begin{bmatrix} 1 & 2 \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} 0 \end{bmatrix}}_{\mathbf{b}}. \quad (2)$$

The solutions to (2) are

$$\mathbf{x} = \begin{bmatrix} -2c \\ c \end{bmatrix},$$

where $c \in \mathbb{C}$.

Overdetermined Systems

$$\underbrace{\begin{bmatrix} 1 \\ 3 \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} x_1 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} 3 \\ 2 \end{bmatrix}}_{\mathbf{b}}. \quad (3)$$

There are **no solutions** to (3).

Usually, an overdetermine system has no exact solution.

The Least Squares Problem (1/2)

- We aim to find a solution such that

$$\mathbf{Ax} \approx \mathbf{b}. \quad (4)$$

- The vector p -norm measures the proximity of \mathbf{Ax} to \mathbf{b} .

$$\|\mathbf{Ax} - \mathbf{b}\|_p, \quad (5)$$

where $p \in [1, \infty)$.

The Least Squares Problem (2/2)

The Least Squares (LS) Problem ($p = 2$)

$$\min_{\mathbf{x} \in \mathbb{C}^N} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2 \quad (6)$$

- The LS problem (6) is tractable for two reasons
 - ① The solutions to (6) can be found readily.
 - Completion of squares
 - The (complex) derivatives of the objective function
 - ② The ℓ_2 norm is invariant under unitary transformations. Namely,

$$\|\mathbf{U}\mathbf{v}\|_2 = \|\mathbf{v}\|_2, \quad (7)$$

for a unitary matrix \mathbf{U} .

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The LS Solution(s)

$$\min_{\mathbf{x} \in \mathbb{C}^N} \|\mathbf{Ax} - \mathbf{b}\|_2 \quad (8)$$

- Let \mathbf{x}_{LS} be a solution to the LS problem (6).

Questions

- Does \mathbf{x}_{LS} exist?
- How do we find \mathbf{x}_{LS} ?
- Is the LS solution \mathbf{x}_{LS} unique?

The Normal Equation

Normal Equation

If \mathbf{A} has full column rank, then there is a unique LS solution \mathbf{x}_{LS} , and it satisfies

$$\mathbf{A}^H \mathbf{A} \mathbf{x}_{LS} = \mathbf{A}^H \mathbf{b}. \quad (9)$$

- See Section 5.3.1 in [GVL2013] for the complete arguments
- The **minimum residual** \mathbf{r}_{LS}

$$\mathbf{r}_{LS} \triangleq \mathbf{b} - \mathbf{A} \mathbf{x}_{LS}. \quad (10)$$

- The size of \mathbf{r}_{LS}

$$\rho_{LS} \triangleq \|\mathbf{A} \mathbf{x}_{LS} - \mathbf{b}\|_2. \quad (11)$$

Remarks on the Normal Equation

- Assume that $\mathbf{A} \in \mathbb{C}^{M \times N}$ and $M \geq N$.
- If \mathbf{A} has full column rank, then
 - $\text{rank}(\mathbf{A}) = N$.
 - $\text{rank}(\mathbf{A}^H \mathbf{A}) = N$.
 - $\mathbf{A}^H \mathbf{A}$ is invertible.
- If \mathbf{A} has full column rank, then the LS solution can be uniquely found by

$$\mathbf{x}_{\text{LS}} \triangleq (\mathbf{A}^H \mathbf{A})^{-1} \mathbf{A}^H \mathbf{b}. \quad (12)$$

- Interpretations of \mathbf{x}_{LS}
 - Wiener-Hopf equation in Adaptive Signal Processing
 - Singular values and singular vectors of \mathbf{A}

The LS Solution and the SVD (1/4)

- We assume that $\text{rank}(\mathbf{A}) = N$.
- The SVD of \mathbf{A} is denoted by

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H = \sum_{i=1}^N \sigma_i \mathbf{u}_i \mathbf{v}_i^H. \quad (13)$$

- The matrix $\mathbf{\Sigma}$ is

$$\mathbf{\Sigma} = \begin{bmatrix} \mathbf{\Sigma}_N \\ \mathbf{0}_{(M-N) \times N} \end{bmatrix}, \quad \mathbf{\Sigma}_N = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_N). \quad (14)$$

- The singular values satisfy $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_N > 0$.
- The **unitary matrices \mathbf{U} and \mathbf{V}** comprise left and right singular vectors.

$$\mathbf{U} = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \dots \quad \mathbf{u}_M], \quad \mathbf{V} = [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \dots \quad \mathbf{v}_N]. \quad (15)$$

The LS Solution and the SVD (2/4)

- The unitary matrices \mathbf{U} and \mathbf{V} satisfy

$$\mathbf{U}^H \mathbf{U} = \mathbf{I}_M, \quad \mathbf{V}^H \mathbf{V} = \mathbf{I}_N, \quad (16)$$

- Substituting (13) into (12) leads to

$$\mathbf{x}_{LS} = \left((\mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^H)^H (\mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^H) \right)^{-1} (\mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^H)^H \mathbf{b} \quad (17)$$

$$= (\mathbf{V} \boldsymbol{\Sigma}^H \mathbf{U}^H \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^H)^{-1} \mathbf{V} \boldsymbol{\Sigma}^H \mathbf{U}^H \mathbf{b} \quad (18)$$

$$= \mathbf{V} (\boldsymbol{\Sigma}^H \boldsymbol{\Sigma})^{-1} \mathbf{V}^H \mathbf{V} \boldsymbol{\Sigma}^H \mathbf{U}^H \mathbf{b} \quad (19)$$

$$= \mathbf{V} (\boldsymbol{\Sigma}^H \boldsymbol{\Sigma})^{-1} \boldsymbol{\Sigma}^H \mathbf{U}^H \mathbf{b}. \quad (20)$$

The LS Solution and the SVD (3/4)

- From (14), the matrix associated with Σ can be expressed as

$$(\Sigma^H \Sigma)^{-1} \Sigma^H = \left(\begin{bmatrix} \Sigma_N \\ \mathbf{0}_{(M-N) \times N} \end{bmatrix}^H \begin{bmatrix} \Sigma_N \\ \mathbf{0}_{(M-N) \times N} \end{bmatrix} \right)^{-1} \begin{bmatrix} \Sigma_N \\ \mathbf{0}_{(M-N) \times N} \end{bmatrix}^H \quad (21)$$

$$= (\Sigma_N^H \Sigma_N)^{-1} [\Sigma_N^H \quad \mathbf{0}_{N \times (M-N)}] \quad (22)$$

$$= [\Sigma_N^{-1} \quad \mathbf{0}_{N \times (M-N)}] \quad (23)$$

$$= \begin{bmatrix} \sigma_1^{-1} & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \sigma_2^{-1} & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_N^{-1} & 0 & \dots & 0 \end{bmatrix}. \quad (24)$$

The LS Solution and the SVD (4/4)

- Substituting (24) and (15) into (20) gives

$$\mathbf{x}_{LS} = \sum_{i=1}^N \frac{\mathbf{u}_i^H \mathbf{b}}{\sigma_i} \mathbf{v}_i. \quad (25)$$

- \mathbf{x}_{LS} is a **linear combination** of $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N\}$.
- Two factors influence the combination coefficients
 - 1 The inner product $\langle \mathbf{b}, \mathbf{u}_i \rangle \triangleq \mathbf{u}_i^H \mathbf{b}$
 - 2 The singular value σ_i

The Size of the Minimum Residual

- (Exercise) It can be shown that the size of the minimum residual (denoted by ρ_{LS}) satisfies

$$\rho_{\text{LS}}^2 = \sum_{i=N+1}^M |\mathbf{u}_i^H \mathbf{b}|^2. \quad (26)$$

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Motivation

- (The normal equation of LS problems) If \mathbf{A} has full column rank, then there is a unique LS solution \mathbf{x}_{LS} and

$$\mathbf{A}^H \mathbf{A} \mathbf{x}_{LS} = \mathbf{A}^H \mathbf{b}. \quad (27)$$

- What if \mathbf{A} is rank-deficient? Namely, $\mathbf{A} \in \mathbb{C}^{M \times N}$, and

$$\text{rank}(\mathbf{A}) = r < N. \quad (28)$$

- Logical reasoning:

$$p \rightarrow q \quad \equiv \quad \sim q \rightarrow \sim p \quad (29)$$

Example 1

- We consider the following equations

$$\underbrace{\begin{bmatrix} 1 & 2 \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} 1 \end{bmatrix}}_{\mathbf{b}}. \quad (30)$$

- The associated LS problem is cast as

$$\min_{\mathbf{x} \in \mathbb{C}^N} \|\mathbf{Ax} - \mathbf{b}\|_2 \quad (31)$$

Observations

- There are infinitely many solutions to (30).
- If \mathbf{x}^* is a solution to (30), then $\|\mathbf{Ax}^* - \mathbf{b}\|_2 = 0$.
- The LS problem (31) has **an infinite number of solutions**.

The Minimum 2-Norm Solution

- We define the objective function

$$\psi(\mathbf{x}) \triangleq \|\mathbf{Ax} - \mathbf{b}\|_2. \quad (32)$$

- The minimum of $\psi(\mathbf{x})$ is denoted by ψ_{\min} .
- The set of all minimizers

$$\mathcal{X} \triangleq \{\mathbf{x} \in \mathbb{C}^N \mid \psi(\mathbf{x}) = \psi_{\min}\}. \quad (33)$$

- The set \mathcal{X} is convex [GVL2013, Section 5.5.1].
- Among the vectors in \mathcal{X} , we select the unique element with **the minimum 2-norm**:

$$\mathbf{x}_{\text{LS}} \triangleq \arg \min_{\mathbf{x} \in \mathcal{X}} \|\mathbf{x}\|_2 \quad (34)$$

The Rank-Deficient LS Solution with the Minimum 2-Norm

Theorem (Revised from Theorem 5.5.1 in [GVL2013])

Let the SVD of \mathbf{A} be $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H \in \mathbb{C}^{M \times N}$ with $\text{rank}(\mathbf{A}) = r$. The singular vectors satisfy

$$\mathbf{U} \triangleq [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \dots \quad \mathbf{u}_M], \quad \mathbf{V} \triangleq [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \dots \quad \mathbf{v}_N]. \quad (35)$$

Assume that $\mathbf{b} \in \mathbb{C}^M$. Then

$$\mathbf{x}_{\text{LS}} = \sum_{i=1}^r \frac{\mathbf{u}_i^H \mathbf{b}}{\sigma_i} \mathbf{v}_i \quad (36)$$

minimizes $\|\mathbf{Ax} - \mathbf{b}\|_2$ and has the smallest 2-norm of all minimizers.

The LS Solution in Example 1

- We consider the matrix $\mathbf{A} = \begin{bmatrix} 1 & 2 \end{bmatrix}$ in (30).
- The rank of \mathbf{A} is 1.
- The SVD of \mathbf{A}

$$\mathbf{u}_1 = 1, \quad \sigma_1 = \sqrt{5}, \quad \mathbf{v}_1 = \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} -2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix}. \quad (37)$$

- The set of minimizers

$$\mathcal{X} = \left\{ \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbb{C}^2 \mid x_1 + 2x_2 = 1 \right\}. \quad (38)$$

The LS Solution in Example 1

- The rank-deficient LS solution with the minimum 2-norm

$$\mathbf{x}_{\text{LS}} \triangleq \arg \min_{\mathbf{x} \in \mathcal{X}} \|\mathbf{x}\|_2 = \arg \min_{\mathbf{x} \in \mathcal{X}} \sqrt{|x_1|^2 + |x_2|^2} \quad (39)$$

- We decompose the elements x_1 and x_2 into the real and imaginary parts:

$$x_1 = \text{Re}\{x_1\} + j\text{Im}\{x_1\}, \quad (40)$$

$$x_2 = \text{Re}\{x_2\} + j\text{Im}\{x_2\}. \quad (41)$$

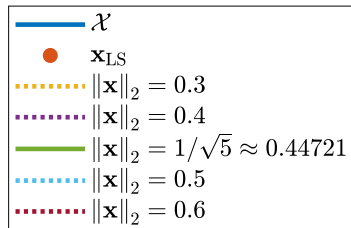
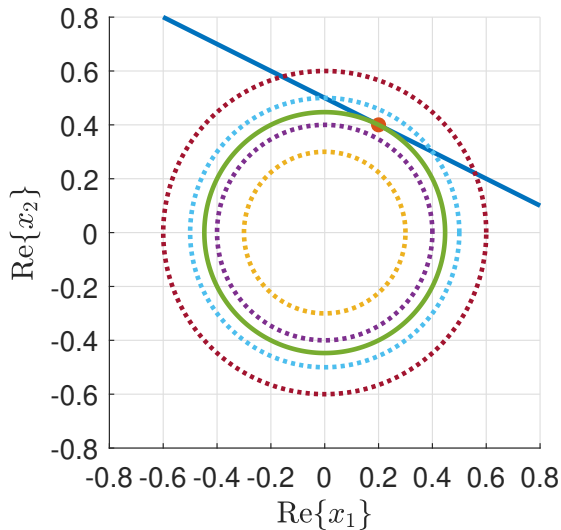
- The LS solution \mathbf{x}_{LS}

$$\mathbf{x}_{\text{LS}} \triangleq \arg \min_{\mathbf{x} \in \mathcal{X}} \sqrt{(\text{Re}\{x_1\})^2 + (\text{Im}\{x_1\})^2 + (\text{Re}\{x_2\})^2 + (\text{Im}\{x_2\})^2} \quad (42a)$$

$$\text{subject to} \quad \text{Re}\{x_1\} + 2\text{Re}\{x_2\} = 1, \quad (42b)$$

$$\text{Im}\{x_1\} + 2\text{Im}\{x_2\} = 0. \quad (42c)$$

Illustration of the LS Solution



$$\mathbf{A} = \begin{bmatrix} 1 & 2 \end{bmatrix}, \quad \mathbf{b} = 1,$$

$$\mathbf{u}_1 = 1, \quad \sigma_1 = \sqrt{5},$$

$$\mathbf{v}_1 = \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} -2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix}.$$

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Pseudo-inverse Using the SVD

- Let $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H \in \mathbb{C}^{M \times N}$ where $\text{rank}(\mathbf{A}) = r \leq \min\{M, N\}$ (c.f. page 21).
- We define a matrix $\mathbf{\Sigma}^\dagger$ (c.f. page 14)

$$\mathbf{\Sigma}^\dagger \triangleq \begin{bmatrix} \sigma_1^{-1} & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \sigma_2^{-1} & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_r^{-1} & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \end{bmatrix} \in \mathbb{C}^{N \times M}. \quad (43)$$

- The pseudo-inverse of \mathbf{A} is defined as

$$\mathbf{A}^\dagger \triangleq \mathbf{V}\mathbf{\Sigma}^\dagger\mathbf{U}^H \in \mathbb{C}^{N \times M}. \quad (44)$$

Example of the Pseudo-Inverse

- We consider the matrix $\mathbf{A} = \begin{bmatrix} 1 & 2 \end{bmatrix}$ in (30).
- The rank of \mathbf{A} is 1.
- The SVD of \mathbf{A}

$$\mathbf{u}_1 = 1, \quad \sigma_1 = \sqrt{5}, \quad \mathbf{v}_1 = \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} -2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix}. \quad (45)$$

- The pseudo-inverse of \mathbf{A}

$$\mathbf{A}^\dagger = [\mathbf{v}_1 \quad \mathbf{v}_2] \begin{bmatrix} \sigma_1^{-1} \\ 0 \end{bmatrix} [\mathbf{u}_1]^\mathbf{H} = \begin{bmatrix} 1/5 \\ 2/5 \end{bmatrix}. \quad (46)$$

Properties of the Pseudo-Inverse (1/5)

- Let $\mathbf{A} \in \mathbb{C}^{M \times N}$
- Let \mathbf{A}^\dagger be the pseudo-inverse of \mathbf{A}
- Let $\mathbf{b} \in \mathbb{C}^M$.
- The LS solution \mathbf{x}_{LS} satisfies

$$\mathbf{x}_{\text{LS}} = \mathbf{A}^\dagger \mathbf{b}. \quad (47)$$

- Remarks
 - Comparison: (25) and (36).
 - Initially, we aim to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$.

Properties of the Pseudo-Inverse (2/5)

- If $\text{rank}(\mathbf{A}) = N$, then

$$\mathbf{A}^\dagger = (\mathbf{A}^H \mathbf{A})^{-1} \mathbf{A}^H. \quad (48)$$

- If $M = N = \text{rank}(\mathbf{A})$, then

$$\mathbf{A}^\dagger = (\mathbf{A}^H \mathbf{A})^{-1} \mathbf{A}^H \quad (49)$$

$$= \mathbf{A}^{-1} (\mathbf{A}^H)^{-1} \mathbf{A}^H \quad (50)$$

$$= \mathbf{A}^{-1}. \quad (51)$$

Properties of the Pseudo-Inverse (3/5)

- The pseudo-inverse \mathbf{A}^\dagger satisfies **the four Moore-Penrose conditions**:

$$\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}, \quad (52)$$

$$\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger, \quad (53)$$

$$(\mathbf{A}\mathbf{A}^\dagger)^H = \mathbf{A}\mathbf{A}^\dagger, \quad (54)$$

$$(\mathbf{A}^\dagger\mathbf{A})^H = \mathbf{A}^\dagger\mathbf{A}. \quad (55)$$

- (Exercise) Prove the four Moore-Penrose conditions.

Properties of the Pseudo-Inverse (4/5)

- The matrix $\mathbf{A}\mathbf{A}^\dagger$ can be expressed as

$$\mathbf{A}\mathbf{A}^\dagger = \sum_{i=1}^r \mathbf{u}_i \mathbf{u}_i^H, \quad (56)$$

where $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_r$ are the left singular vectors of \mathbf{A} .

- The matrix $\mathbf{A}^\dagger \mathbf{A}$ can be expressed as

$$\mathbf{A}^\dagger \mathbf{A} = \sum_{i=1}^r \mathbf{v}_i \mathbf{v}_i^H, \quad (57)$$

where $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r$ are the right singular vectors of \mathbf{A} .

Properties of the Pseudo-Inverse (5/5)

- The size of the minimum residual satisfies

$$\rho_{LS} = \left\| (\mathbf{I} - \mathbf{A}\mathbf{A}^\dagger) \mathbf{b} \right\|_2. \quad (58)$$

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Concluding Remarks

- The LS problem

$$\min_{\mathbf{x} \in \mathbb{C}^N} \|\mathbf{Ax} - \mathbf{b}\|_2$$

- Normal equations
- Full-rank LS
- Rank-deficient LS
- Pseudo inverse
- Extensions
 - Weighted least squares (WLS)
 - Total least squares (TLS)
 - Constrained least squares (CLS)
 - Recursive least squares (RLS)