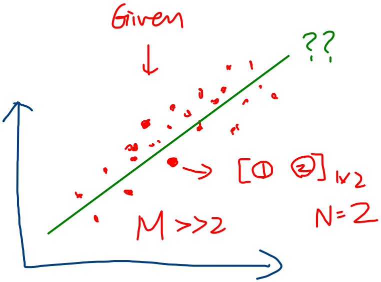
Outline

1. Motivations
2. Jordan Canonical Form
   - Definition and Examples
   - The Integer Power of a Matrix
3. Singular Value Decomposition (SVD)
   - Definition and Properties
   - Matrix Norms and SVD
4. Principal Component Analysis (PCA)



$y = ax + b$

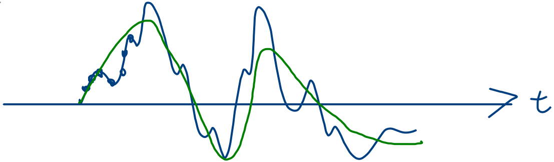
The Data Vectors

- Consider a set of data vectors (row vectors)

$$\mathbf{x}_m = \begin{bmatrix} x_{m,1} & x_{m,2} & x_{m,3} & \dots & x_{m,N} \end{bmatrix}_{1 \times N}, \tag{87}$$

for $m = 1, 2, \dots \boxed{M}$.

- The number of data vectors: M
- The length of a data vector: N
- Usually $M \gg N$.
- Applications
  - Audio signals
  - Images
  - Communication signals
  - Array signal processing (linear arrays or planar arrays)



Mean Subtraction

- The mean vector $\overline{\mathbf{x}}$ (as a row vector) is

$$\overline{\mathbf{x}} = \frac{1}{M}\sum_{m=1}^{M}\mathbf{x}_m. \tag{88}$$

$\underline{x}_1 =$

$\underline{x}_2 =$

$\vdots$

$\underline{x}_M =$

average

$\overline{\underline{x}} =$ $1 \times N$

- The new data vector $\mathbf{a}_m$ after subtracting the mean vector from $\mathbf{x}_m$

$$\mathbf{a}_m \triangleq \mathbf{x}_m - \overline{\mathbf{x}}. \tag{89}$$

$m = 1 \sim M$

↳ row vectors

$1 \times N$

The Data Matrix

$a_m = \boxed{}$ $1 \times N$

$m = 1 \sim M$

$A = \boxed{\; \cdot \quad \cdot \; \cdots \;}$

- The data matrix $\mathbf{A} \in \mathbb{C}^{M \times N}$

(89)

$$\mathbf{A} \triangleq \begin{bmatrix} \boxed{\phantom{\mathbf{a}_1}} \\ \mathbf{a}_1 \\ \mathbf{a}_2 \boxed{} \\ \vdots \\ \mathbf{a}_M \boxed{} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 - \overline{\mathbf{x}} \\ \mathbf{x}_2 - \overline{\mathbf{x}} \\ \vdots \\ \mathbf{x}_M - \overline{\mathbf{x}} \end{bmatrix}. \tag{90}$$

$M \times N$

- The data vector $\mathbf{x}_m$ can be expressed as

to be compressed

$$\mathbf{x}_m = \mathbf{e}_m^{\mathsf{T}} \mathbf{A} + \overline{\mathbf{x}}, \tag{91}$$

where $\mathbf{e}_m \in \mathbb{C}^M$ satisfies

$$[\mathbf{e}_m]_i = \begin{cases} 1 & \text{if } i = m, \\ 0 & \text{if } i \neq m. \end{cases} \tag{92}$$

$$e_m = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow m^{th}$$

$$\underline{\underline{A}} = \begin{bmatrix} \underline{a}_1 \\ \vdots \\ \underline{a}_M \end{bmatrix}$$

$$(*) \quad \boxed{\underline{a}_1}_{\,1\times N} = \boxed{\begin{matrix} 1 & 0 & 0 & \cdots & 0 \end{matrix}}_{\,1\times M} \boxed{\underline{\underline{A}}}_{\,M\times N}$$

The m^{th}

$$\underbrace{\underline{x}_m - \underline{\bar{x}}} = \underline{a}_m = \boxed{\begin{matrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{matrix}} \underline{\underline{A}} = \underbrace{\underline{e}_m^T \underline{\underline{A}}}$$

SVD of $\mathbf{A}$

$A = \begin{bmatrix} - & - & - \\ - & \times & \zeta \\ & \times & \times \end{bmatrix}$

- According to Page 37, the SVD of $\mathbf{A}$ is

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\mathsf{H}} \quad (93)$$

components

$$= \sum_{i=1}^{N} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{H}} \quad (94)$$

"N terms"

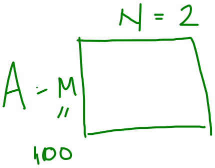
$$= \sigma_1 \mathbf{u}_1 \mathbf{v}_1^{\mathsf{H}} + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^{\mathsf{H}} + \sigma_3 \mathbf{u}_3 \mathbf{v}_3^{\mathsf{H}} + \cdots + \sigma_N \mathbf{u}_N \mathbf{v}_N^{\mathsf{H}}. \quad (95)$$

- The singular values satisfy

$$\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \cdots \geq \sigma_N \geq 0. \quad (96)$$

- The ith component of $\mathbf{A}$ is $\sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{H}}$.

Dimensionality Reduction (1/2)



- We approximate the matrix $\mathbf{A}$ by L components:

$$\widehat{\mathbf{A}} \triangleq \sum_{i=1}^{L} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{H}} \tag{97}$$

$$= \sigma_1 \mathbf{u}_1 \mathbf{v}_1^{\mathsf{H}} + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^{\mathsf{H}} + \sigma_3 \mathbf{u}_3 \mathbf{v}_3^{\mathsf{H}} + \cdots + \sigma_L \mathbf{u}_L \mathbf{v}_L^{\mathsf{H}}. \tag{98}$$

- Dimensional reduction: $L \leq N$.

$L = 1$: $\hat{A} = \sigma_1 \, u_1 \, \boxed{v_1^H}$

1x1 100x1 1x2

σ_1 : 1 number

u_1 : 100 numbers

v_1 : 2 numbers

Dimensionality Reduction (2/2)

- According to (91) and (97), we define the approximated data vectors

$$\widehat{\mathbf{x}}_m \triangleq \mathbf{e}_m^{\mathsf{T}}\widehat{\mathbf{A}} + \overline{\mathbf{x}} = \left(\sum_{i=1}^{L} \overset{\text{scalar}}{\boxed{\sigma_i\left(\mathbf{e}_m^{\mathsf{T}}\mathbf{u}_i\right)}}\overset{\text{row vector.}}{\boxed{\mathbf{v}_i^{\mathsf{H}}}}\right) + \overline{\mathbf{x}}. \quad (99)$$

M×1

  - $\boxed{\mathbf{e}_m^{\mathsf{T}}\mathbf{u}_i}$ is the mth entry of $\mathbf{u}_i$.
  - $\sigma_i\left(\mathbf{e}_m^{\mathsf{T}}\mathbf{u}_i\right)$ is the combination coefficient.
  - The set $\{\mathbf{v}_1^{\mathsf{H}}, \mathbf{v}_2^{\mathsf{H}}, \ldots, \mathbf{v}_L^{\mathsf{H}}\}$ contains the axes.
- A general form of the approximated data vectors is

$$\left(\sum_{i=1}^{L} c_i\mathbf{v}_i^{\mathsf{H}}\right) + \overline{\mathbf{x}}, \quad (100)$$

where $c_i \in \mathbb{C}$ for $i = 1, 2, \ldots L$.

An Example of the PCA (1/4)

Problem

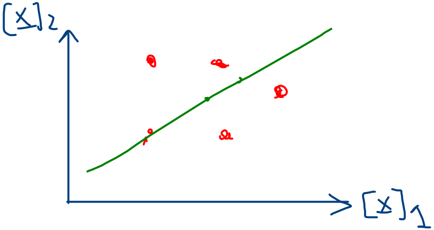
Use the PCA with $L = 1$ to find a regression line that approximates the points in $\mathbb{R}^2$

$$\mathbf{x}_1 = \begin{bmatrix} 7 & 8 \end{bmatrix}_{1\times 2}, \quad \mathbf{x}_2 = \begin{bmatrix} 9 & 8 \end{bmatrix}, \quad \mathbf{x}_3 = \begin{bmatrix} 10 & 10 \end{bmatrix}, \quad \mathbf{x}_4 = \begin{bmatrix} 11 & 12 \end{bmatrix}, \quad \mathbf{x}_5 = \begin{bmatrix} 13 & 12 \end{bmatrix}.$$

We assume that the combination coefficients are real numbers.

- (Solution) The number of data $M = 5$.
- The length of the data vector $N = 2$.
- The mean vector

$c = 0$
$c = 1$
$c =$



$$\overline{\mathbf{x}} = \begin{bmatrix} 10 & 10 \end{bmatrix}.$$

An Example of the PCA (2/4)

- The new data vectors

$$\underline{\mathbf{a}_1} = \begin{bmatrix} -3 & -2 \end{bmatrix}, \quad \mathbf{a}_2 = \begin{bmatrix} -1 & -2 \end{bmatrix}, \quad \mathbf{a}_3 = \begin{bmatrix} 0 & 0 \end{bmatrix}, \quad \mathbf{a}_4 = \begin{bmatrix} 1 & 2 \end{bmatrix}, \quad \underline{\mathbf{a}_5} = \begin{bmatrix} 3 & 2 \end{bmatrix}.$$

- The data matrix $\mathbf{A}$ and its SVD

$$\mathbf{A} = \begin{array}{cl} \begin{bmatrix} -3 & -2 \\ -1 & -2 \\ 0 & 0 \\ 1 & 2 \\ 3 & 2 \end{bmatrix}. & \begin{array}{l} \underline{a_1} \\ \underline{a_2} \\ \\ \\ \underline{a_5} \end{array} \end{array} \tag{101}$$

5×2

An Example of the PCA (3/4)

- The SVD of $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\mathsf{H}}$, where

$$
\mathbf{U} = \begin{array}{c} \begin{bmatrix} -0.6116 & 0.3549 & 0 & 0.0393 & 0.7060 \\ -0.3549 & -0.6116 & 0 & 0.7060 & -0.0393 \\ 0 & 0 & 1.0000 & 0 & 0 \\ 0.3549 & 0.6116 & 0 & 0.7060 & -0.0393 \\ 0.6116 & -0.3549 & 0 & 0.0393 & 0.7060 \end{bmatrix} \\ \begin{array}{ccccc} \underline{u}_1 & \quad\underline{u}_2 & \quad\underline{u}_3 & \quad\underline{u}_4 & \quad\underline{u}_5 \end{array} \end{array}, \quad \mathbf{\Sigma} = \begin{bmatrix} \boxed{5.8416} & 0 \\ 0 & \boxed{1.3695} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix},
$$

$\sigma_1 = 5.8416$, $\sigma_2 = 1.3695$

$$
\mathbf{V} = \begin{array}{c} \begin{bmatrix} 0.7497 & -0.6618 \\ 0.6618 & 0.7497 \end{bmatrix} \\ \begin{array}{cc} \underline{v}_1 & \quad\underline{v}_2 \end{array} \end{array}.
$$

An Example of the PCA (4/4)

- For $L = 1$ in (97), we obtain

$$\widehat{\mathbf{A}} = \underbrace{(5.8416)}_{\sigma_1} \underbrace{\begin{bmatrix} -0.6116 \\ -0.3549 \\ 0 \\ 0.3549 \\ 0.6116 \end{bmatrix}}_{\mathbf{u}_1} \underbrace{\begin{bmatrix} 0.7497 & -0.6618 \end{bmatrix}}_{\mathbf{v}_1^{\mathsf{H}}}.$$

- According to (100) and page 61, an approximation of the data points is

$$\underbrace{\begin{bmatrix} 10 & 10 \end{bmatrix}}_{\bar{x}} + c \underbrace{\begin{bmatrix} 0.7497 & -0.6618 \end{bmatrix}}_{v_1^H}, \rightarrow$$

$[\underline{x}]_1 = 10 + 0.7497c$

$[\underline{x}]_2 = 10 - 0.6618c$

where $\boxed{c \in \mathbb{R}}$.

Selected Topics in Engineering Mathematics: Least Squares Problems

LS

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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

Motivation

$N \times 1$

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

$$\mathbf{A}\mathbf{x} = \mathbf{b}. \tag{1}$$

  - The data matrix $\mathbf{A} \in \mathbb{C}^{M\times N}$ is given.
  - The observation vector $\mathbf{b} \in \mathbb{C}^{M}$ is given. $M \times 1$
- The number of equations is $\boxed{M}$.
- The number of unknowns is N.
- Underdetermined systems: $M < N$
- Overdetermined systems: $M > N$

$M<N$

$M=N$

$M>N$

Questions

- How many solutions to (1)?

Examples of (1)

rank($\underline{\underline{A}}$)

$$\begin{bmatrix} 1 \\ 3 \end{bmatrix} \begin{bmatrix} \overset{1}{x_1} \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

Underdetermined Systems

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

The solutions to (2) are

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

→ infinitely many solution

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

Overdetermined Systems

$$\underbrace{\begin{bmatrix} 1 \\ 3 \end{bmatrix}}_{\substack{\mathbf{A} \\ 2\times 1}} \underbrace{\begin{bmatrix} x_1 \end{bmatrix}}_{\mathbf{x}\ 1\times 1} = \underbrace{\begin{bmatrix} 3 \\ 2 \end{bmatrix}}_{\mathbf{b}\ 2\times 1}. \tag{3}$$

↗ $\frac{1}{3}$

There are no solutions to (3).

Usually, an overdetermine system has no exact solution.

The Least Squares Problem (1/2)

$A\underline{x} = \underline{b}$

- We aim to find a solution such that

$x = ?$

$$\mathbf{A}\mathbf{x} \approx \mathbf{b}. \qquad (4)$$

$A\underline{x}$ $\approx$ $\underline{b}$

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

$\| \cdot \|_p \in \mathbb{R}$

$3 \geq 2$

$$\|\boxed{\mathbf{A}\mathbf{x} - \mathbf{b}}\|_p, \quad \in \mathbb{R} \qquad (5)$$

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

$p = ?$ $\begin{cases} 1 \\ 2 \\ \infty \end{cases}$

The Least Squares Problem (2/2)

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

minimize

$$\min_{\mathbf{x}\in\mathbb{C}^N} \overbrace{\|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2}^{\text{objective function}} \rightarrow \ell_2 \text{ norm} \qquad (6)$$

- The LS problem (6) is tractable for two reasons

convex function ($\|\cdot\|_p \quad p \in [1, \infty)$

  1. The solutions to (6) can be found readily.
     - Completion of squares
     - The (complex) derivatives of the objective function $\frac{\partial}{\partial x^*}$

SVD

$U \Sigma V^H$

  2. The ℓ_2 norm is invariant under unitary transformations. Namely,

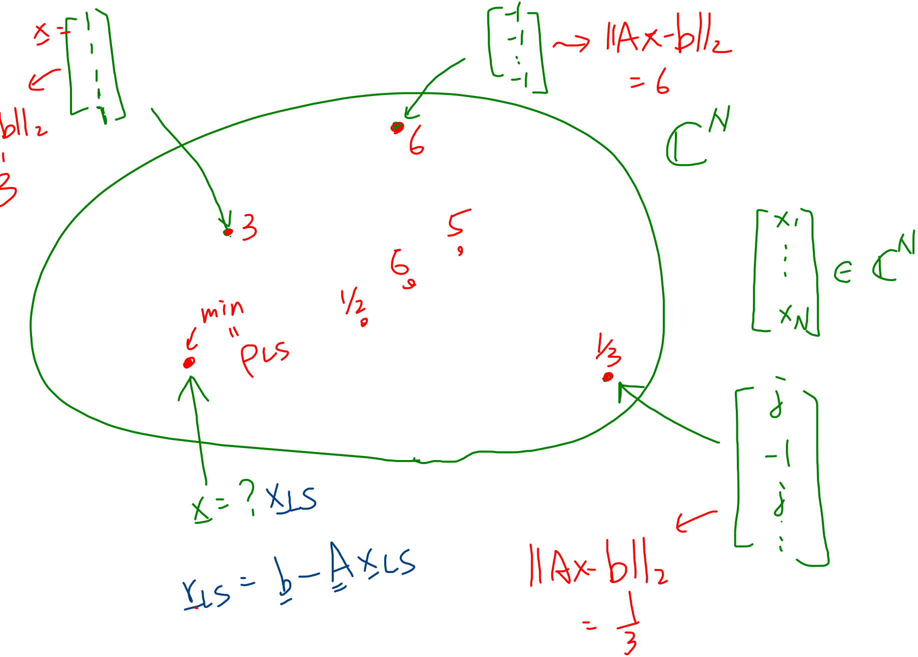
$$\underline{\|\mathbf{U}\mathbf{v}\|_2 = \|\mathbf{v}\|_2}\,, \qquad (7)$$

v $\quad$ Uv

for a unitary matrix $\mathbf{U}$.

LS:

$$\min_{\underline{x} \in \mathbb{C}^N} \|\underline{\underline{A}}\underline{x} - \underline{b}\|_2$$



$$\underline{r}_{LS} = \underline{b} - \underline{\underline{A}}\,\underline{x}_{LS}$$

Outline

$$\| \underline{\underline{A}} \underline{x} - \underline{b} \|_2$$

rank.

The LS Solution(s)

$A = \begin{pmatrix} \vdots \end{pmatrix}$

$$\min_{\mathbf{x}\in\mathbb{C}^N} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2 \tag{8}$$

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

Questions

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

The Normal Equation

x_{LS}

$A = M \times N$

$\text{rank}(A) = N$

Normal Equation

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

A

$$\boxed{\mathbf{A}^{\mathsf{H}}\mathbf{A}\mathbf{x}_{\mathrm{LS}}} = \boxed{\mathbf{A}^{\mathsf{H}}\mathbf{b}}. \tag{9}$$

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

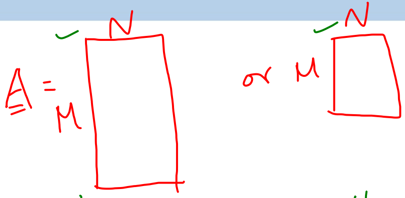
$$\underline{\underline{A}}\,\underline{x} \underset{=}{\approx} \underline{b}$$

$$\mathbf{r}_{\mathrm{LS}} \triangleq \mathbf{b} - \mathbf{A}\mathbf{x}_{\mathrm{LS}}. \tag{10}$$

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

$$\rho_{\mathrm{LS}} \triangleq \left\|\mathbf{A}\mathbf{x}_{\mathrm{LS}} - \mathbf{b}\right\|_2 . \tag{11}$$

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
  - $\operatorname{rank}(\mathbf{A}) = N$.
  - $\operatorname{rank}(\boxed{\mathbf{A}^{\mathsf{H}}\mathbf{A}}) = N$. (full rank)
  - $\mathbf{A}^{\mathsf{H}}\mathbf{A}$ is invertible.

- If $\mathbf{A}$ has full column rank, then the LS solution can be uniquely found by

$$\mathbf{x}_{\mathrm{LS}} \triangleq \boxed{\left(\mathbf{A}^{\mathsf{H}}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathsf{H}}}\mathbf{b}. \tag{12}$$

A^+

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

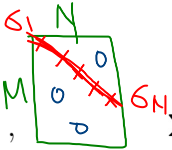
σ_i SVD u_i v_i

The LS Solution and the SVD (1/4)

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

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathsf{H}} = \sum_{i=1}^{N} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{H}}. \tag{13}$$

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



$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_N \\ \mathbf{0}_{(M-N)\times N} \end{bmatrix}, \qquad \boldsymbol{\Sigma}_N = \text{diag}\left(\sigma_1, \sigma_2, \ldots, \sigma_N\right). \tag{14}$$

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

$$\mathbf{U} = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \ldots & \mathbf{u}_M \end{bmatrix}, \qquad \mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \ldots & \mathbf{v}_N \end{bmatrix}. \tag{15}$$

The LS Solution and the SVD (2/4)

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

$$\mathbf{U}^{\mathsf{H}}\mathbf{U} = \mathbf{I}_M, \qquad \mathbf{V}^{\mathsf{H}}\mathbf{V} = \mathbf{I}_N. \tag{16}$$

- Substituting (13) into (12) leads to

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

$$= \left(\mathbf{V}\boldsymbol{\Sigma}^{\mathsf{H}}\overbrace{\mathbf{U}^{\mathsf{H}}\mathbf{U}}^{I}\boldsymbol{\Sigma}\mathbf{V}^{\mathsf{H}}\right)^{-1} \mathbf{V}\boldsymbol{\Sigma}^{\mathsf{H}}\mathbf{U}^{\mathsf{H}}\mathbf{b} \tag{18}$$

$$= \mathbf{V}\left(\boldsymbol{\Sigma}^{\mathsf{H}}\boldsymbol{\Sigma}\right)^{-1} \overbrace{\mathbf{V}^{\mathsf{H}}\mathbf{V}}^{I}\boldsymbol{\Sigma}^{\mathsf{H}}\mathbf{U}^{\mathsf{H}}\mathbf{b} \tag{19}$$

$$= \mathbf{V}\left(\boldsymbol{\Sigma}^{\mathsf{H}}\boldsymbol{\Sigma}\right)^{-1}\boldsymbol{\Sigma}^{\mathsf{H}}\boxed{\mathbf{U}^{\mathsf{H}}\mathbf{b}.} \tag{20}$$

The LS Solution and the SVD (3/4)

- From (14), the matrix associated with $\mathbf{\Sigma}$ can be expressed as

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

$$= \left(\mathbf{\Sigma}_N^{\mathsf{H}}\mathbf{\Sigma}_N\right)^{-1}\begin{bmatrix}\mathbf{\Sigma}_N^{\mathsf{H}} & \mathbf{0}_{N\times(M-N)}\end{bmatrix} \tag{22}$$

$$= \begin{bmatrix}\mathbf{\Sigma}_N^{-1} & \mathbf{0}_{N\times(M-N)}\end{bmatrix} \tag{23}$$

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

The LS Solution and the SVD (4/4)

Gram-Schmidt process

$\underline{w} = \alpha_1 \underline{v}_1 + \alpha_2 \underline{v}_2$

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

$$\mathbf{x}_{\mathrm{LS}} = \sum_{i=1}^{N} \frac{\mathbf{u}_i^{\mathsf{H}}\mathbf{b}}{\sigma_i}\mathbf{v}_i, \tag{25}$$

singular values

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

If $\underline{v}_1 \perp \underline{v}_2$

$\langle \underline{w}, \underline{v}_1 \rangle$

$\underline{w} \approx \frac{\langle \underline{w}, \underline{v}_1 \rangle}{\langle \underline{v}_1, \underline{v}_1 \rangle} \underline{v}_1 +$

$\alpha_1 = \frac{\langle \underline{w}, \underline{v}_1 \rangle}{\langle \underline{v}_1, \underline{v}_1 \rangle}$

$= \alpha_1 \langle v_1, v_1 \rangle + \alpha_2 \cancel{\langle v_2, v_1 \rangle} = 0$

The Size of the Minimum Residual

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

$\rho_{LS} = \| \underline{\underline{A}} x_{LS} - b \|_2$

$$\rho_{\mathrm{LS}}^2 = \sum_{i=N+1}^{M} \left| \mathbf{u}_i^{\mathsf{H}} \mathbf{b} \right|^2. \tag{26}$$

error

Outline

A full column rank

Motivation

- (The normal equation of LS problems) If $\overset{p}{\boxed{\mathbf{A} \text{ has full column rank}}}$, then there is an unique LS solution $\mathbf{x}_{\mathrm{LS}}$ and

$$\mathbf{A}^{\mathsf{H}}\mathbf{A}\mathbf{x}_{\mathrm{LS}} = \mathbf{A}^{\mathsf{H}}\mathbf{b}. \tag{27}$$

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

$\sim p \to \ldots$

$$\mathrm{rank}(\mathbf{A}) = r < N. \tag{28}$$

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

- Logical reasoning:

$$p \to q \qquad \equiv \qquad \sim q \to \sim p \tag{29}$$

Example 1

- We consider the following equations

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

- The associated LS problem is cast as

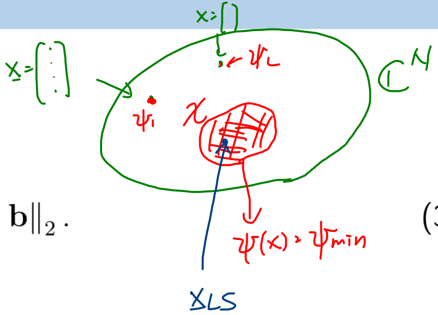
$$\min_{\mathbf{x}\in\mathbb{C}^N} \overbrace{\|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2}^{=0} \tag{31}$$

$\psi_{min} = 0$

Observations

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

The Minimum 2-Norm Solution



- We define the objective function

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

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

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

- 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:

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

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* $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathsf{H}} \in \mathbb{C}^{M\times N}$ *with* $\operatorname{rank}(\mathbf{A}) = r$. *The singular vectors satisfy*

$\sigma_1 \sim \sigma_r > 0$

$$\mathbf{U} \triangleq \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_M \end{bmatrix}, \qquad \mathbf{V} \triangleq \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_N \end{bmatrix}. \tag{35}$$

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

$$\mathbf{x}_{\mathrm{LS}} = \sum_{i=1}^{r} \frac{\mathbf{u}_i^{\mathsf{H}}\mathbf{b}}{\sigma_i}\mathbf{v}_i \tag{36}$$

$= A^+ b$

$= (V\Sigma^+ \boxed{U^H) b}$

(25)

minimizes $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2$ *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 $\mathbf{A}$

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

- The set of minimizers

real /imag

$Ax = b$

$$\mathcal{X} = \left\{ \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbb{C}^2 \;\middle|\; x_1 + 2x_2 = 1 \right\}. \tag{38}$$

$1 + j0$

The LS Solution in Example 1

$x_1, x_2 \in \mathbb{C}$

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

$$\mathbf{x}_{\mathrm{LS}} \triangleq \arg\min_{\boxed{\mathbf{x}\in\mathcal{X}}} \|\mathbf{x}\|_2 = \arg\min_{\mathbf{x}\in\mathcal{X}} \sqrt{|x_1|^2 + |x_2|^2} \tag{39}$$

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

$$x_1 = \mathrm{Re}\{x_1\} + \jmath \overset{0}{\mathrm{Im}\{x_1\}}, \tag{40}$$

$$x_2 = \mathrm{Re}\{x_2\} + \jmath \underset{0}{\mathrm{Im}\{x_2\}}. \tag{41}$$

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

$$\mathbf{x}_{\mathrm{LS}} \triangleq \arg\min_{\mathbf{x}\in\mathcal{X}} \sqrt{(\mathrm{Re}\{x_1\})^2 + (\underset{0}{\cancel{\mathrm{Im}\{x_1\}}})^2 + (\mathrm{Re}\{x_2\})^2 + (\underset{0}{\cancel{\mathrm{Im}\{x_2\}}})^2} \tag{42a}$$

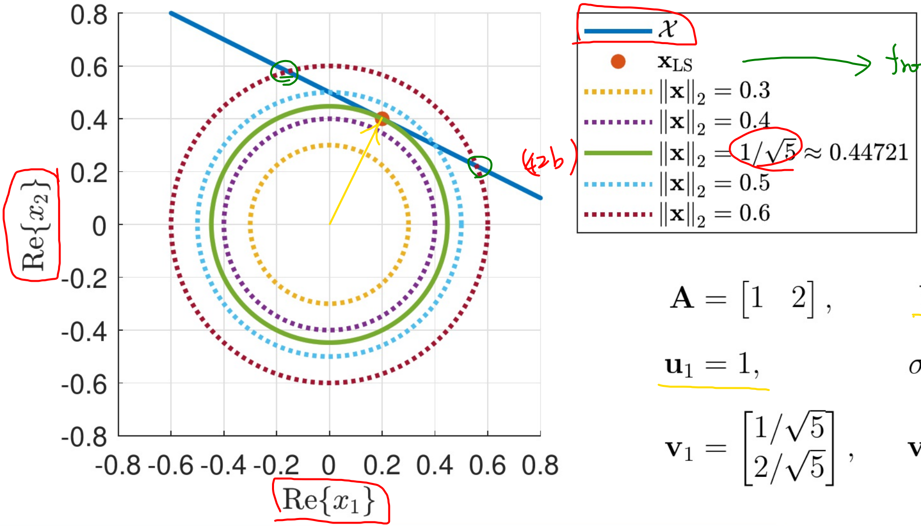
subject to

$$\mathrm{Re}\{x_1\} + 2\mathrm{Re}\{x_2\} = 1, \tag{42b}$$

$$\underset{0}{\cancel{\mathrm{Im}\{x_1\}}} + 2\underset{0}{\cancel{\mathrm{Im}\{x_2\}}} = 0. \tag{42c}$$

Illustration of the LS Solution

(42b) : $\mathrm{Re}\{x_1\} + 2\,\mathrm{Re}\{x_2\} = 1$



from (36)

$$\sum_{i=1}^{r} \frac{u_i^H b}{\sigma_i} v_i$$

$(r = 1)$

$$= \frac{u_1^H b}{\sigma_1} v_1$$

coef 1, $\sqrt{5}$ vec

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

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

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

Outline

Normal eq. $\rightarrow$ $x_{LS} = (A^H A)^{-1} A^H b$

$$A^H A x = A^H b$$

$$x_{LS} = \sum_{i=1}^{\square} \frac{u_i^H b}{\sigma_i} v_i$$

LS $\quad Ax \approx b$

$$x_{LS} = A^{\dagger} b$$

$Ax = b$

If A^{-1} exists, then $x = A^{-1} b$

Pseudo-inverse Using the SVD

$\sigma_1 \sim \sigma_r > 0$

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

$$\Sigma = \begin{array}{cc} & N \\ M & \begin{bmatrix} \sigma_1 & & & & & \\ & \sigma_2 & & & & \\ & & \ddots & & & \\ & & & \sigma_r & & \\ & & & & 0 & \\ & & & & & \ddots \; 0 \end{bmatrix} \end{array}$$

$$\boldsymbol{\Sigma}^{\dagger} \triangleq \begin{array}{cc} & M \\ N & \begin{bmatrix} \sigma_1^{-1} & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & \sigma_2^{-1} & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_r^{-1} & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \end{bmatrix} \end{array} \in \mathbb{C}^{N\times M}. \tag{43}$$

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

$$\mathbf{A}^{\dagger} \triangleq \mathbf{V}\boldsymbol{\Sigma}^{\dagger}\mathbf{U}^{\mathsf{H}} \in \mathbb{C}^{N\times M}. \tag{44}$$

$$\underline{\underline{A}} = \underline{\underline{U}}\,\underline{\underline{\Sigma}}\,\underline{\underline{V}}^H = \square_{M \times N}$$

$$\underline{\underline{A}}^{\dagger} = \underline{\underline{V}}\,\underline{\underline{\Sigma}}^{\dagger}\,\underline{\underline{U}}^H = \square_{N \times M}$$

Example of the Pseudo-Inverse

$\underline{\underline{A}}\,\underline{\underline{A}}^{+} = \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 1/5 \\ 2/5 \end{bmatrix}$

$= 1$

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

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

- The pseudo-inverse of $\mathbf{A}$

$\underline{\underline{V}} \quad \underline{\underline{\Sigma}}^{+} \quad \underline{\underline{U}}^{H}$

$$\mathbf{A}^\dagger = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 \end{bmatrix} \begin{bmatrix} \sigma_1^{-1} \\ 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \end{bmatrix}^{\mathsf{H}} = \begin{bmatrix} 1/5 \\ 2/5 \end{bmatrix}. \tag{46}$$

$\underline{\underline{A}}^{+}\underline{\underline{A}} = \begin{bmatrix} 1/5 \\ 2/5 \end{bmatrix} \begin{bmatrix} 1 & 2 \end{bmatrix} = \begin{bmatrix} x & x \\ x & x \end{bmatrix}$

$x_{LS} \overset{?}{=} \underline{\underline{A}}^{+} b$

Properties of the Pseudo-Inverse (1/5)

$[\underline{A}\underline{x} \approx \underline{b}]$

LS: $\min \|\underline{A}\underline{x} - \underline{b}\|_2$

- 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 $\mathbf{x}_{\mathrm{LS}}$ satisfies

$$\mathbf{x}_{\mathrm{LS}} = \mathbf{A}^\dagger \mathbf{b}. \tag{47}$$

- Remarks
  - Comparison: (25) and (36).
  - Initially, we aim to solve $\mathbf{Ax} = \mathbf{b}$. $\rightsquigarrow$ $x = \underline{A}^{-1} \underline{b}$

Properties of the Pseudo-Inverse (2/5)

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

full column rank

(12)

$$\mathbf{A}^{\dagger} = \left(\mathbf{A}^{\mathsf{H}}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathsf{H}}. \tag{48}$$

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

full rank

N

A = M

$$\begin{aligned}
\mathbf{A}^{\dagger} &= \left(\mathbf{A}^{\mathsf{H}}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathsf{H}} && (49)\\
&= \mathbf{A}^{-1}\left(\cancel{\mathbf{A}^{\mathsf{H}}}\right)^{-1}\cancel{\mathbf{A}^{\mathsf{H}}} && (50)\\
&= \mathbf{A}^{-1}. && (51)
\end{aligned}$$

Properties of the Pseudo-Inverse (3/5)

$A^\dagger = V \Sigma^\dagger U^H$

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

Inverse A^{-1} (exists)

$A A^{-1} = I \Rightarrow A A^{-1} A = A$

$A^{-1} A = I$

$A A^\dagger \overset{?}{\neq} I$

$$\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}, \tag{52}$$

$$\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger, \tag{53}$$

$$\left(\mathbf{A}\mathbf{A}^\dagger\right)^{\mathsf{H}} = \mathbf{A}\mathbf{A}^\dagger, \tag{54}$$

$$\left(\mathbf{A}^\dagger\mathbf{A}\right)^{\mathsf{H}} = \mathbf{A}^\dagger\mathbf{A}. \tag{55}$$

- (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

$$\mathbf{A}\mathbf{A}^\dagger = \sum_{i=1}^{r} \mathbf{u}_i \mathbf{u}_i^{\mathsf{H}}, \tag{56}$$

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

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

$$\mathbf{A}^\dagger\mathbf{A} = \sum_{i=1}^{r} \mathbf{v}_i \mathbf{v}_i^{\mathsf{H}}, \tag{57}$$

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

Properties of the Pseudo-Inverse (5/5)

- The size of the minimum residual satisfies

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

Outline

Concluding Remarks

- The LS problem

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

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

$Ax \approx b$