Lectures on Least Squares Methods

Part I: Linear Least Squares

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Prerequisites

1. Differential calculus and integrals with multiple variables
2. Linear algebra, from fundamentals to eigenvalues, eigenvectors, and spectral theorem
3. All the previous notions extended to the complex field
4. Fundamentals of probability theory: distributions, expected value, variance, covariance and their properties, Bayes theorem

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Basic concepts and notation

1. The least squares problem arises whenever one has a physical system described by a model in the form $\mathbf{b} = H\boldsymbol{\theta}$
   - H is the response function describing the system, in this case a linear function, i.e. a matrix, with $\boldsymbol{\theta}$ as its argument
   - $\boldsymbol{\theta}$ are the parameters or inputs of the system (independent variables)
   - $\mathbf{b}$ are the observations or outputs of the system (dependent variables)

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   - $\boldsymbol{\theta}$ are the parameters or inputs of the system (independent variables)
   - $\mathbf{b}$ are the observations or outputs of the system (dependent variables)
2. Experimentally, observations are affected by uncertainty due to system and measurement noise, and finite measurement resolution: $\mathbf{b} \neq H\boldsymbol{\theta} \Rightarrow \mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$
   - $\mathbf{b}$ is a column vector with N components, representing observations
   - $\boldsymbol{\theta}$ is a column vector with p parameters that are characteristic of the system, and that must be estimated
   - H is a known $N \times p$ matrix; N: number of equations, p number of parameters.
   - $\boldsymbol{\varepsilon}$ is the noise and generally it is assumed: $\mathrm{E}[\boldsymbol{\varepsilon}] = 0$, and $\mathrm{cov}[\boldsymbol{\varepsilon}] = \sigma^2 I$ [a]

[a] Reminder: $\mathrm{cov}[\mathbf{X}] = \mathrm{E}\left[\mathbf{X}\mathbf{X}^T\right] - \mathrm{E}[\mathbf{X}]\,\mathrm{E}\left[\mathbf{X}^\dagger\right]$

Basic concepts and notation

3. Because of the noise, $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$ is in general an inconsistent system of N equations
   - One then seeks the optimal solution that minimizes the cost function

$$\phi(\boldsymbol{\theta}) = ||\mathbf{b} - H\boldsymbol{\theta}||^2 = (\mathbf{b} - H\boldsymbol{\theta})^T (\mathbf{b} - H\boldsymbol{\theta})$$

   - Thus, the least squares estimator is $\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} ||\mathbf{b} - H\boldsymbol{\theta}||^2$

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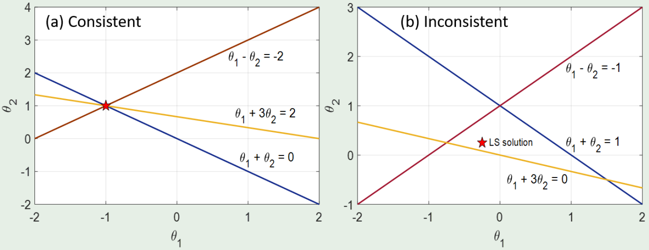
Example

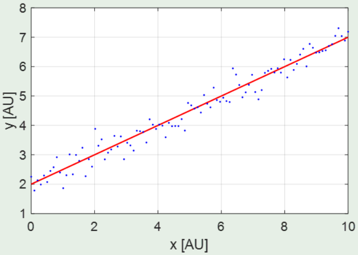
$$(a): \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \begin{pmatrix} 0 \\ -2 \\ 2 \end{pmatrix}$$

$$(b): \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$



At this level, only **b** is affected by the uncertainty. When **b** is changed, lines are just translated, slopes are not changed. When also H is affected by the uncertainty, slopes change: this is the Total Least Squares method, discussed later on.

LS regression examples



Linear regression, N observations, $p = 2$ parameters:

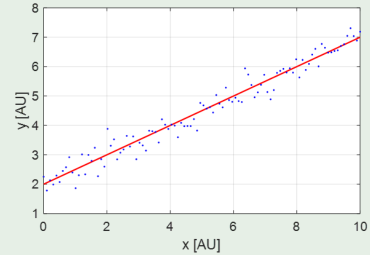
$$\mathbf{y} = m\mathbf{x} + q = \begin{pmatrix} \mathbf{x} & \mathbf{1} \end{pmatrix} \begin{pmatrix} m \\ q \end{pmatrix}$$

$$\mathbf{b} \equiv \mathbf{y}$$

$$H \equiv \begin{pmatrix} \mathbf{x} & \mathbf{1} \end{pmatrix}$$

$$\boldsymbol{\theta} \equiv \begin{pmatrix} m \\ q \end{pmatrix}$$

LS regression examples



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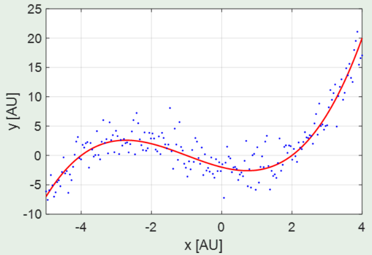


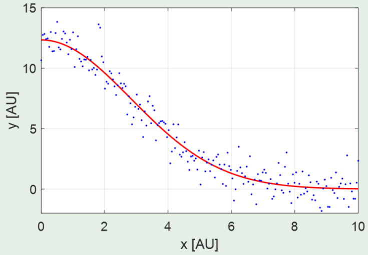
Polinomial regression, 3rd degree, N observations, $p = 4$ parameters:

$$\mathbf{y} = c_0 + c_1\mathbf{x} + c_2\mathbf{x}^2 + c_3\mathbf{x}^2 = \begin{pmatrix} \mathbf{x} & \mathbf{1} \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

$$\mathbf{b} \equiv \mathbf{y} \qquad H \equiv \begin{pmatrix} \mathbf{1} & \mathbf{x} & \mathbf{x}^2 & \mathbf{x}^3 \end{pmatrix}$$

$$\boldsymbol{\theta} \equiv \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

LS regression examples



Exponential regression, N observations, $p = 2$ parameters:

$$\mathbf{y} = A e^{b\mathbf{x}^2}$$

A non-linear problem. It can be linearized by using logarithms

$$\log \mathbf{y} = \log A + b\mathbf{x}^2 =$$
$$= C + b\mathbf{x}^2 = \begin{pmatrix} 1 & \mathbf{x}^2 \end{pmatrix} \begin{pmatrix} C \\ b \end{pmatrix}$$

Warning: the uncertainty estimated for C will propagate non-linearly on A

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General terminology for estimators

1. A sample is a series of N observations $\mathbf{z} = (z_1 \cdots z_N)$ of a random variable $\mathbf{Z}$

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2. A statistic is any function of the observations $g(\mathbf{z}) = g(z_1 \cdots z_N)$ not dependent on unknown parameters
3. Typically, formulating a hypothesis means assuming that observations are extracted from a probability density function p.d.f. $f(\mathbf{z} \,|\, \boldsymbol{\theta})$ dependent on some parameters $\boldsymbol{\theta} = (\theta_1 \cdots \theta_N)$ that must be determined

General terminology for estimators

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6. Tipically, observations are independent, hence the p.d.f. is $f_{sample} = f_1(z_1) f_2(z_2) \ldots f_N(z_N)$. If the sample consists of repeated observations of the same variable, then $f_1 = f_2 = \ldots = f_N = f$, and:

$$\mathrm{E}\left[\hat{\theta}(\mathbf{z})\right] = \int_D \hat{\theta}(\mathbf{z}) f_{sample}(\mathbf{z}|\theta)\, d\mathbf{z} = \int \ldots \int \hat{\theta}(\mathbf{z}) f_1(z_1) \ldots f_N(z_N)\, dz_1 \ldots dz_N$$

General terminology for estimators

Unbiased estimator example: the sample (or arithmetic) mean

The sample mean is an unbiased estimator of the expected value of a p.d.f. $f(z)$, given a sample of N observations z_i

$$\mu = \mathrm{E}[z] = \int z f(z)\, dz$$

$$\hat{\mu} = \bar{z} = \frac{1}{N} \sum_{i=1}^{N} z_i$$

$$\mathrm{E}[\hat{\mu}(\mathbf{z})] = \mathrm{E}\left[\frac{1}{N} \sum_{i=1}^{N} z_i\right] = \frac{1}{N} \sum_{i=1}^{N} \mathrm{E}[z_i] = \frac{1}{N} \sum_{i=1}^{N} \mu = \frac{1}{N} N\mu = \mu$$

$$b = \mathrm{E}[\hat{\mu}(\mathbf{z})] - \mu = \mu - \mu = 0$$

Biased estimator example: the sample variance

The sample variance

$$s^2 = \frac{1}{N} \sum_{i=1}^{N} (z_i - \bar{z})^2$$

is a biased estimator of the variance σ^2, indeed, without performing all calculations

$$\mathrm{E}\left[s^2\right] = \frac{N-1}{N}\sigma^2$$

An unbiased estimator can be easily obtained:

$$S^2 = \frac{1}{N-1} \sum_{i=1}^{N} (z_i - \bar{z})^2 = \frac{N}{N-1} s^2$$

$$\mathrm{E}\left[S^2\right] = \frac{N}{N-1}\mathrm{E}\left[s^2\right] = \sigma^2$$

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Review of linear algebra

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2. The rank of a matrix $A \in \mathbb{C}^{m\times n}$ is the maximum number of linearly independent columns or rows: $\mathrm{rank}\,(A) \leq \min\,(m, n)$; $\mathrm{rank}\,(A) = \mathrm{rank}\,\left(A^{\dagger}\right)$.

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3. The rank of a matrix is the dimension of the space generated by its columns: $\mathrm{rank}\,(A) = \dim\,[\mathrm{Span}\,(\mathbf{a}_1, \ldots, \mathbf{a}_n)]$, $\mathrm{Span}\,(\mathbf{a}_1, \ldots, \mathbf{a}_n) \equiv \left\{ \mathbf{v} : \mathbf{v} = \sum_i c_i \mathbf{a}_i \right\}$

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4. Kernel of A:
$\ker\,(A) \equiv \{\mathbf{v} : A\mathbf{v} = \mathbf{0}\}$, $\quad \forall A, (\mathbf{v} = \mathbf{0}) \in \ker\,(A)$, $\ \ker\,(A) \equiv \{\mathbf{0}\} \Rightarrow \dim\,[\ker\,(A)] = 0$
$\dim\,[\ker\,(A)]$ is called the nullity of A.

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Rank-nullity theorem

$$\forall A \in \mathbb{C}^{m\times n},\ \mathrm{rank}\,(A) + \dim\left[\ker\,(A)\right] = n$$

A useful lemma

$$\forall A \in \mathbb{C}^{m \times n},\ \mathrm{rank}\,(A) = \mathrm{rank}\left(A^\dagger A\right)$$

Review of linear algebra

A useful lemma

$$\forall A \in \mathbb{C}^{m\times n},\ \mathrm{rank}\left(A\right) = \mathrm{rank}\left(A^{\dagger}A\right)$$

Proof.

- From the rank-nullity theorem, it follows that:

$$\mathrm{rank}\left(A\right) + \dim\left[\ker\left(A\right)\right] = n = \mathrm{rank}\left(A^{\dagger}A\right) + \dim\left[\ker\left(A^{\dagger}A\right)\right]$$

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- Then, one can prove that ranks are equal by proving that kernels are the same, i.e. by showing that if $\mathbf{v} \in \ker(A)$, then $\mathbf{v} \in \ker\left(A^{\dagger}A\right)$, and *vice versa*:

$$\mathbf{v} \in \ker(A) \Rightarrow A\mathbf{v} = \mathbf{0} \Rightarrow A^{\dagger}A\mathbf{v} = \mathbf{0} \Rightarrow \mathbf{v} \in \ker\left(A^{\dagger}A\right)$$

$$\mathbf{v} \in \ker\left(A^{\dagger}A\right) \Rightarrow A^{\dagger}A\mathbf{v} = \mathbf{0} \Rightarrow \mathbf{v}^{\dagger}A^{\dagger}A\mathbf{v} = 0 \Rightarrow \|A\mathbf{v}\|^2 = 0 \Rightarrow A\mathbf{v} = \mathbf{0} \Rightarrow \mathbf{v} \in \ker(A)$$

□

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Ordinary Least Squares - OLS

OLS assumptions

- System $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$ has more equations the parameters $(N \geq p)$
- H is a full-rank matrix: $\mathrm{rank}\,(H) = p$.

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Consistent system

- When $\boldsymbol{\varepsilon} = 0$ the system is:

$$\mathbf{b} = H\boldsymbol{\theta} = \begin{pmatrix} \mathbf{h}_1 & \mathbf{h}_2 & \cdots & \mathbf{h}_p \end{pmatrix} \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_p \end{pmatrix} = \sum_{i=1}^{p} \theta_i \mathbf{h}_i$$

- The system has a solution when $\mathbf{b}$ is a linear combination of the columns of H:

$$\mathbf{b} \in \text{Span}\,(H) \Leftrightarrow rank\,(H) = \text{rank}\left[\begin{pmatrix} H & \mathbf{b} \end{pmatrix}\right]$$

When H is full-rank, the solution is unique.

Ordinary Least Squares - OLS

Inconsistent system

- In general $\boldsymbol{\varepsilon} \neq 0$ and the sistem is inconsistent: $rank\,(H) \neq \operatorname{rank}\left[\begin{pmatrix} H & \mathbf{b} \end{pmatrix}\right]$
- According to the lemma on the rank of $H^\dagger H$: $\operatorname{rank}(H) = p = \operatorname{rank}\left(H^\dagger H\right)$
- $H^\dagger H$ is a full-rank square $p \times p$ matrix, hence it is invertible

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Associated consistent system

- For the previous assumptions, the following system is consistent:

$$H^{\dagger}\mathbf{b} = H^{\dagger}H\boldsymbol{\theta} \Rightarrow \hat{\boldsymbol{\theta}} = \left(H^{\dagger}H\right)^{-1}H^{\dagger}\mathbf{b} = H^{+}\mathbf{b}$$

- The pseudo-inverse or Moore-Penrose matrix has been introduced:

$$H^{+} = \left(H^{\dagger}H\right)^{-1}H^{\dagger} \Rightarrow H^{+}H = I,\ HH^{+} \neq I$$

- H is a $N \times p$ matrix, and H^{+} is $p \times N$. When H is square ($N = p$), then $H^{+} = H^{-1}$

Ordinary Least Squares - OLS

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What does the solution $\hat{\boldsymbol{\theta}} = \left(H^\dagger H\right)^{-1} H^\dagger \mathbf{b} = H^+ \mathbf{b}$ mean?

Ordinary Least Squares - OLS

OLS problem

- Full-rank (p) inconsistent system: $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$, $\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} ||\mathbf{b} - H\boldsymbol{\theta}||^2$
- Associated consistent system: $H^\dagger \mathbf{b} = H^\dagger H\boldsymbol{\theta}$
- Cost function:

$$\phi(\boldsymbol{\theta}) = ||\mathbf{b} - H\boldsymbol{\theta}||^2 = (\mathbf{b} - H\boldsymbol{\theta})^\dagger (\mathbf{b} - H\boldsymbol{\theta}) =$$
$$= \boldsymbol{\theta}^\dagger H^\dagger H\boldsymbol{\theta} + \mathbf{b}^\dagger\mathbf{b} - \mathbf{b}^\dagger H\boldsymbol{\theta} - \boldsymbol{\theta}^\dagger H^\dagger \mathbf{b} = \boldsymbol{\theta}^\dagger H^\dagger H\boldsymbol{\theta} + \mathbf{b}^\dagger\mathbf{b} - 2\mathrm{Re}\left(\boldsymbol{\theta}^\dagger H^\dagger \mathbf{b}\right)$$

Ordinary Least Squares - OLS

OLS problem

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OLS solution of the full-rank inconsistent system

The solution of the associated consistent system:

$$\hat{\boldsymbol{\theta}} = \left(H^\dagger H\right)^{-1} H^\dagger\mathbf{b} = H^+\mathbf{b}$$

is also the solution that minimizes the cost function

Ordinary Least Squares - OLS

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Ordinary Least Squares - OLS

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Proof.

We give a simple proof for the real case. The complex case will be proved later in the more general context of singular value decomposition. When H is real:

$$\phi(\boldsymbol{\theta}) = \boldsymbol{\theta}^T H^T H \boldsymbol{\theta} + \mathbf{b}^T \mathbf{b} - 2\boldsymbol{\theta}^T H^T \mathbf{b} = \sum_{jkl} \theta_j H_{kj} H_{kl} \theta_l + \sum_j b_j^2 - 2 \sum_{jk} \theta_j H_{kj} b_k$$

The minimum is attained where the jacobian matrix (the gradient in this case) is zero:

$$\frac{\partial \phi}{\partial \theta_i} = \sum_{jkl} (\delta_{ij} H_{kj} H_{kl} \theta_l + \theta_j H_{kj} H_{kl} \delta_{il}) - 2 \sum_{jk} \delta_{ij} H_{kj} b_k = 2 \sum_{jk} H_{ji} H_{jk} \theta_k - 2 \sum_j H_{ji} b_j$$

OLS solution of the full-rank inconsistent system

The solution of the associated consistent system:

$$\hat{\boldsymbol{\theta}} = \left(H^{\dagger}H\right)^{-1} H^{\dagger}\mathbf{b} = H^{+}\mathbf{b}$$

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Proof.

The minimum is attained where the jacobian matrix (the gradient in this case) is zero:

$$\frac{\partial \phi}{\partial \theta_i} = 2\left(H^T H\boldsymbol{\theta}\right)_i - 2(H\mathbf{b})_i \Rightarrow \frac{\partial \phi}{\partial \boldsymbol{\theta}} = 2H^T H\boldsymbol{\theta} - 2H\mathbf{b} = 0 \Rightarrow H^T H\boldsymbol{\theta} = H\mathbf{b}$$

from which the solution follows. □

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We assumed: $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$, $\mathrm{E}[\boldsymbol{\varepsilon}] = 0$, and $\mathrm{cov}[\boldsymbol{\varepsilon}] = \sigma^2 I$, $N \geq p$
Observations $\mathbf{b}$ are homoscedastic (from the greek *homo* "same" *skedasis* "dispersion", i.e. they all have the same variance) and uncorrelated

Expected value of the OLS estimator

The OLS estimator $\boldsymbol{\theta} = H^{+}\mathbf{b}$ is unbiased: $\mathrm{E}\left[\hat{\boldsymbol{\theta}}\right] = \boldsymbol{\theta}$

Properties of the OLS estimator

We assumed: $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$, $\mathrm{E}[\boldsymbol{\varepsilon}] = 0$, and $\mathrm{cov}[\boldsymbol{\varepsilon}] = \sigma^2 I$, $N \geq p$
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Proof.

By a straightforward calculation:

$$\mathrm{E}\left[\hat{\boldsymbol{\theta}}\right] = \mathrm{E}\left[\left(H^{\dagger}H\right)^{-1}H^{\dagger}\mathbf{b}\right] = \mathrm{E}\left[\left(H^{\dagger}H\right)^{-1}H^{\dagger}(H\boldsymbol{\theta} + \boldsymbol{\varepsilon})\right] =$$

$$= \left(H^{\dagger}H\right)^{-1}H^{\dagger}H\mathrm{E}[\boldsymbol{\theta}] + \left(H^{\dagger}H\right)^{-1}H^{\dagger}\mathrm{E}[\boldsymbol{\varepsilon}] = \boldsymbol{\theta}$$

□

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By a straightforward calculation[a]:

$$\mathrm{cov}\left[\hat{\boldsymbol{\theta}}\right] = \mathrm{cov}\left[\left(H^\dagger H\right)^{-1} H^\dagger \mathbf{b}\right] = \mathrm{cov}\left[\boldsymbol{\theta} + \left(H^\dagger H\right)^{-1} H^\dagger \boldsymbol{\varepsilon}\right] =$$

$$= \left(H^\dagger H\right)^{-1} H^\dagger \mathrm{cov}\left[\boldsymbol{\varepsilon}\right] H \left(H^\dagger H\right)^{-1} = \left(H^\dagger H\right)^{-1} H^\dagger \sigma^2 I H \left(H^\dagger H\right)^{-1} = \sigma^2 \left(H^\dagger H\right)^{-1}$$

□

[a] Reminder: $\mathrm{cov}\left[A\mathbf{X}\right] = A\,\mathrm{cov}\left[\mathbf{X}\right] A^\dagger$

Properties of the OLS estimator

A reminder on positive semi-definite and definite matrices

- A Hermitian matrix $A = A^\dagger$ is positive semi-definite (respectively definite) iff $\mathbf{z}^\dagger A\mathbf{z} \geq 0$ (respectively $\mathbf{z}^\dagger A\mathbf{z} > 0$), $\forall \mathbf{z} \in \mathbb{C}^n$

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- The diagonal elements of a positive semi-definite (respectively definite) matrix A are always real positive semi-definite (respectively definite) values, indeed, by using the standard basis on $\mathbb{C}^n$, $\mathbf{z} \equiv \mathbf{e}_i$: $A_{ii} = \mathbf{e}_i^T A\mathbf{e}_i \geq 0$ (respectively $A_{ii} > 0$).

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- A matrix of the form $A^\dagger A$ is always positive semi-definite, indeed $\mathbf{z}^\dagger A^\dagger A\mathbf{z} = \|A\mathbf{z}\|^2 \geq 0$ by definition of norm.

Properties of the OLS estimator

Assumptions: $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$, $\mathrm{E}\left[\boldsymbol{\varepsilon}\right] = 0$, and $\mathrm{cov}\left[\boldsymbol{\varepsilon}\right] = \sigma^2 I$, $N \geq p$

Gauss-Markov theorem

- The OLS estimator $\hat{\boldsymbol{\theta}}$ is the unbiased linear estimator with minimum variance, i.e., given any other unbiased linear estimator $\hat{\boldsymbol{\theta}}_L = C\mathbf{b}$, then

$$\mathrm{var}\left[\hat{\boldsymbol{\theta}}_L\right] \geq \mathrm{var}\left[\hat{\boldsymbol{\theta}}\right]$$

- The OLS estimator $\hat{\boldsymbol{\theta}}$ is the best linear unbiased estimator (BLUE), i.e., it has minimum squared error:

$$\mathrm{E}\left[\left\|\hat{\boldsymbol{\theta}}_L - \boldsymbol{\theta}\right\|^2\right] \geq \mathrm{E}\left[\left\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\right\|^2\right]$$

Properties of the OLS estimator

Proof.

- For the first point: first we need an unbiased $\hat{\boldsymbol{\theta}}_L$. C can always be written as $C = H^{+} + D$, for a suitable D:

$$\mathrm{E}\left[\hat{\boldsymbol{\theta}}_L\right] = \mathrm{E}\left[C\mathbf{b}\right] = \mathrm{E}\left[\left(\left(H^{\dagger}H\right)^{-1}H^{\dagger} + D\right)(H\boldsymbol{\theta} + \boldsymbol{\varepsilon})\right]$$

$$= \left(\left(H^{\dagger}H\right)^{-1}H^{\dagger} + D\right)H\boldsymbol{\theta} = (I + DH)\,\boldsymbol{\theta}$$

Hence $\hat{\boldsymbol{\theta}}_L$ is unbiased iff $DH = 0$. Then:

$$\mathrm{var}\left[\hat{\boldsymbol{\theta}}_L\right] = \mathrm{diag}\left(\mathrm{cov}\left[C\mathbf{b}\right]\right) = \mathrm{diag}\left(C\,\mathrm{cov}\left[\mathbf{b}\right]C^{\dagger}\right) = \mathrm{diag}\left(\sigma^2 CC^{\dagger}\right)$$

$$\sigma^2 CC^{\dagger} = \sigma^2\left(\left(H^{\dagger}H\right)^{-1}H^{\dagger} + D\right)\left(H\left(H^{\dagger}H\right)^{-1} + D^{\dagger}\right)$$

$$= \sigma^2\left(H^{\dagger}H\right)^{-1} + \sigma^2\left(H^{\dagger}H\right)^{-1}(DH)^{\dagger} + \sigma^2 DH\left(H^{\dagger}H\right)^{-1} + \sigma^2 DD^{\dagger}$$

$$= \mathrm{cov}\left[\hat{\boldsymbol{\theta}}\right] + \sigma^2 DD^{\dagger}$$

Since $DD^{\dagger}$ is positive semi-definite, then $\mathrm{var}\left[\hat{\boldsymbol{\theta}}_L\right] \geq \mathrm{var}\left[\hat{\boldsymbol{\theta}}\right]$

Properties of the OLS estimator

Proof.

- The second point follows from the first, and from the fact that $\hat{\boldsymbol{\theta}}_L$ and $\hat{\boldsymbol{\theta}}$ are unbiased.

$$\mathrm{var}\left[\hat{\boldsymbol{\theta}}_L\right] \geq \mathrm{var}\left[\hat{\boldsymbol{\theta}}\right]$$

$$\sum_i \mathrm{var}\left[\hat{\theta}_{L,i}\right] = \mathrm{E}\left[\left\|\hat{\boldsymbol{\theta}}_L - \mathrm{E}\left[\hat{\boldsymbol{\theta}}_L\right]\right\|^2\right] \geq \mathrm{E}\left[\left\|\hat{\boldsymbol{\theta}} - \mathrm{E}\left[\hat{\boldsymbol{\theta}}\right]\right\|^2\right] = \sum_i \mathrm{var}\left[\hat{\theta}_i\right]$$

$$\mathrm{E}\left[\left\|\hat{\boldsymbol{\theta}}_L - \boldsymbol{\theta}\right\|^2\right] \geq \mathrm{E}\left[\left\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\right\|^2\right] \qquad \square$$

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Weighted least squares

- Let us now consider the case: $\operatorname{cov}[\mathbf{b}] = \operatorname{cov}[\boldsymbol{\varepsilon}] = \boldsymbol{\Sigma} = \sigma_i^2\delta_{ij}$ (i.e. $\boldsymbol{\Sigma}$ is a diagonal matrix). When the variances σ_i^2 have different values, the random variable is called heteroscedastic.

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- Accordingly: $H_w = W^{\frac{1}{2}}H$, $\boldsymbol{\varepsilon}_w = W^{\frac{1}{2}}\boldsymbol{\varepsilon}$, and

$$\text{cov}\,[\mathbf{b}_w] = \text{cov}\,[\boldsymbol{\varepsilon}_w] = \text{cov}\left[W^{\frac{1}{2}}\boldsymbol{\varepsilon}\right] = W^{\frac{1}{2}}\boldsymbol{\Sigma}W^{\frac{1}{2}} = I,$$

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- Thus, the weighted LS estimator for the system $\mathbf{b}_w = H_w\boldsymbol{\theta} + \boldsymbol{\varepsilon}_w$ is BLUE:

$$\hat{\boldsymbol{\theta}} = \left(H_w^\dagger H_w\right)^{-1} H_w^\dagger \mathbf{b_w} = \left(H^\dagger W H\right)^{-1} H^\dagger W \mathbf{b} = H_w^+ \mathbf{b}$$

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Lemma 1

A positive definite complex square matrix A is invertible. If A is positive semi-definite, but not positive definite, it is not invertible.

Proof.

If A is positive definite, it has only non-zero eigenvalues: $\forall \mathbf{z} \neq 0$, $A\mathbf{z} \neq 0$. Hence $\dim(\ker A) = 0$, and A is full-rank. Therefore, A is invertible. Otherwise, if A is positive semi-definite but not definite, it has a 0 eigenvalue and $\dim(\ker A) \neq 0 \Rightarrow A$ not invertible. □

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Lemma 2

The covariance matrix $\operatorname{cov}[\mathbf{b}]$ of a sample **b** is positive definite and invertible iff for any non-zero **z**, $\operatorname{var}\left[\mathbf{z}^\dagger \mathbf{b}\right] \neq 0$.

Proof.

Since the covariance is positive semi-definite by definition, it is invertible only if it is also positive definite. If $\operatorname{cov}[\mathbf{b}]$ is positive definite, then $\operatorname{var}\left[\mathbf{z}^\dagger \mathbf{b}\right] \neq 0$, indeed $0 \neq \mathbf{z}^\dagger \operatorname{cov}[\mathbf{b}]\, \mathbf{z}$ $= \operatorname{cov}\left[\mathbf{z}^\dagger \mathbf{b}\right] = \operatorname{var}\left[\mathbf{z}^\dagger \mathbf{b}\right]$, since $\mathbf{z}^\dagger \mathbf{b}$ is a scalar. Conversely, if for any non-zero **z**, $\operatorname{var}\left[\mathbf{z}^\dagger \mathbf{b}\right] \neq 0$, then $\operatorname{cov}[\mathbf{b}]$ is positive definite, hence invertible. □

Weighted least squares

- If $\Sigma = \mathrm{cov}\left[\mathbf{b}\right]$ is positive definite, its inverse can be factorized by Cholensky decomposition as $\Sigma^{-1} = \Omega\Omega^{\dagger}$, where Ω is an invertible lower-triangular matrix.

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Generalized Weighted Least Squares

The weighted observations $\mathbf{b}_\Omega$ are homoscedastic and non-autocorrelated, therefore, the weighted LS estimator for the system $\mathbf{b}_\Omega = H_\Omega \boldsymbol{\theta} + \boldsymbol{\varepsilon}_\Omega$ is BLUE by Gauss-Markov theorem:

$$\hat{\boldsymbol{\theta}} = \left(H_\Omega^\dagger H_\Omega\right)^{-1} H_\Omega^\dagger \mathbf{b}_\Omega = \left(H^\dagger \Omega\Omega^\dagger H\right)^{-1} H^\dagger \Omega\Omega^\dagger \mathbf{b} = \left(H^\dagger \Sigma^{-1} H\right)^{-1} H^\dagger \Sigma^{-1} \mathbf{b} = H_\Omega^{+} \mathbf{b}$$

$$\mathrm{cov}\left[\hat{\boldsymbol{\theta}}\right] = \left(H_\Omega^\dagger H_\Omega\right)^{-1} = \left(H^\dagger \Omega\Omega^\dagger H\right)^{-1} = \left(H^\dagger \Sigma^{-1} H\right)^{-1}$$

Proof.

- $\mathrm{E}\left[\boldsymbol{\varepsilon}_\Omega\right] = \mathrm{E}\left[\Omega^\dagger \boldsymbol{\varepsilon}\right] = \Omega^\dagger \mathrm{E}\left[\boldsymbol{\varepsilon}\right] = 0$
- $\mathrm{cov}\left[\boldsymbol{\varepsilon}_\Omega\right] = \mathrm{cov}\left[\Omega^\dagger \boldsymbol{\varepsilon}\right] = \Omega^\dagger \mathrm{cov}\left[\boldsymbol{\varepsilon}\right] \Omega = \Omega^\dagger \Sigma \Omega = \Omega^\dagger \left(\Omega\Omega^\dagger\right)^{-1} \Omega = \Omega^\dagger \left(\Omega^\dagger\right)^{-1} \Omega^{-1}\Omega = I.$
- The assumptions of the Gauss-Markov theorem are therefore satisfied.

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Summary on the OLS estimator

- Given a system $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$, with N observations, p parameters, $\mathrm{rank} H = p$, $\mathrm{E}[\boldsymbol{\varepsilon}] = 0$, $\mathrm{cov}[\boldsymbol{\varepsilon}] = \Sigma$ positive definite, the OLS estimator is:

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So far, so good! BUT when $\mathrm{rank} H < p$, $H^\dagger H$ is not invertible and $\hat{\boldsymbol{\theta}}$ is not defined.

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How to proceed then when $\mathrm{rank}(H) < p$?

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Under-determined linear system

- In this section we consider the case $N < p$ and $\mathrm{rank}\,(H) = N$, i.e. a system with less equations than parameters.
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- The most general case $(\mathrm{rank}\,(H) \leq \min\,(N, p)$, $\forall N$ and $\forall p)$ will be treated later on.
- Since $\mathbf{b} \in \mathbb{C}^N$ and $\mathrm{rank}\,(H) = N$, then $\mathrm{rank}\,(H) = \mathrm{rank}\left[\begin{pmatrix} H & \mathbf{b} \end{pmatrix}\right]$, and the undetermined system $H\boldsymbol{\theta} = \mathbf{b}$ is consistent.
- For the rank-nullity theorem $\dim\,(\ker H) = p - N$, therefore, there exist nonzero vectors $\mathbf{v} \in \ker H$, s.t. $H\mathbf{v} = 0 \Rightarrow H\,(\boldsymbol{\theta} + \mathbf{v}) = H\boldsymbol{\theta} = \mathbf{b}$, i.e., the system has infinite solutions.
- The solution can be made unique by requiring that $\|\boldsymbol{\theta}\|^2 = \boldsymbol{\theta}^\dagger\boldsymbol{\theta}$ is minimum.
- Hence we have the following constrained optimization problem:

$$\begin{cases} \hat{\boldsymbol{\theta}} = \arg\min\limits_{\boldsymbol{\theta}} \|\boldsymbol{\theta}\|^2 \\ \mathbf{g}\,(\boldsymbol{\theta}) = H\boldsymbol{\theta} - \mathbf{b} = 0 \end{cases}$$

Under-determined linear system

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- The problem can be solved by using Lagrange multipliers. As for the the full-rank system, we now treat only the system in the real field. The complex case will be treated later on. Let us define the Lagrangian function with the Lagrange multiplier $\boldsymbol{\lambda} \in \mathbb{R}^N$:

$$L(\boldsymbol{\theta}, \lambda) = \boldsymbol{\theta}^T\boldsymbol{\theta} + \boldsymbol{\lambda}^T\mathbf{g}(\boldsymbol{\theta}) = \boldsymbol{\theta}^T\boldsymbol{\theta} + \boldsymbol{\lambda}^T(H\boldsymbol{\theta} - \mathbf{b})$$

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- The constrained problem becomes an unconstrained problem. Imposing the gradient is zero, the constraint is directly included in the second equation:

$$\begin{cases} \frac{\partial L}{\partial \boldsymbol{\theta}} = 2\boldsymbol{\theta} + H^T\boldsymbol{\lambda} = 0 \\ \frac{\partial L}{\partial \boldsymbol{\lambda}} = H\boldsymbol{\theta} - \mathbf{b} = \mathbf{g}(\boldsymbol{\theta}) = 0 \end{cases}$$

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- Therefore: $\boldsymbol{\theta} = -\frac{1}{2}H^T\boldsymbol{\lambda} \Rightarrow -\frac{1}{2}HH^T\boldsymbol{\lambda} = \mathbf{b} \Rightarrow \boldsymbol{\lambda} = -2\left(HH^T\right)^{-1}\mathbf{b}$, and finally:

$$\hat{\boldsymbol{\theta}} = H^\dagger \left(HH^\dagger\right)^{-1} \mathbf{b}$$

Transpose ^{T} has been substituted with conjugate transpose †, since the solution is correct also in the complex field, as will be proved later on. $HH^\dagger$ is invertible because it is an $N \times N$ matrix and $\mathrm{rank}(H) = N$.

Under-determined linear system

LS solution of the underdetermined linear system

The system $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$, with $N < p$, $\operatorname{rank} H = N$, $\mathrm{E}[\boldsymbol{\varepsilon}] = 0$, $\operatorname{cov}[\boldsymbol{\varepsilon}] = \sigma^2 I$, has the following LS solution:

$$\hat{\boldsymbol{\theta}} = H^\dagger \left(HH^\dagger\right)^{-1} \mathbf{b} \Rightarrow \operatorname{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2 H^\dagger \left(HH^\dagger\right)^{-2} H$$

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Proof.

Theorem already proved, except for the covariance:

$$\mathrm{cov}\left[\hat{\boldsymbol{\theta}}\right] = \mathrm{cov}\left[H^{+}\mathbf{b}\right] = \mathrm{cov}\left[H^{\dagger}\left(HH^{\dagger}\right)^{-1}\mathbf{b}\right] = H^{\dagger}\left(HH^{\dagger}\right)^{-1}\mathrm{cov}\left[\boldsymbol{\varepsilon}\right]\left(HH^{\dagger}\right)^{-1} H =$$

$$= \sigma^2 H^{\dagger}\left(HH^{\dagger}\right)^{-1}\left(HH^{\dagger}\right)^{-1} H = \sigma^2 H^{\dagger}\left(HH^{\dagger}\right)^{-2} H$$

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- In the next section, Singular Value Decomposition will be introduced and demonstrated.

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- Since $A^\dagger A$ and $AA^\dagger$ are Hermitian, they have an orthonormal basis of eigenvectors. E.g.:

$$A^\dagger AV = A^\dagger A\begin{bmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_p \end{bmatrix} = \\ = V\begin{bmatrix} \sigma_1^2 & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \sigma_r^2 & \vdots \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} \end{bmatrix}_{p\times p} = V\Sigma_p^2 \quad ; \qquad AA^\dagger U = AA^\dagger\begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_N \end{bmatrix} = \\ = U\begin{bmatrix} \sigma_1^2 & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \sigma_r^2 & \vdots \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} \end{bmatrix}_{N\times N} = U\Sigma_N^2$$

- Same symbols σ_i^2 have been used for both Σ_N^2 and Σ_p^2, indeed, as it will be proved in the following, the eigenvalues of $A^\dagger A$ and $AA^\dagger$ are the same.

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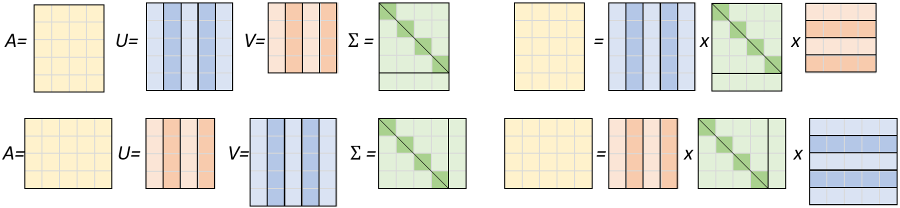
Singular Value Decomposition

Singular Value Decomposition

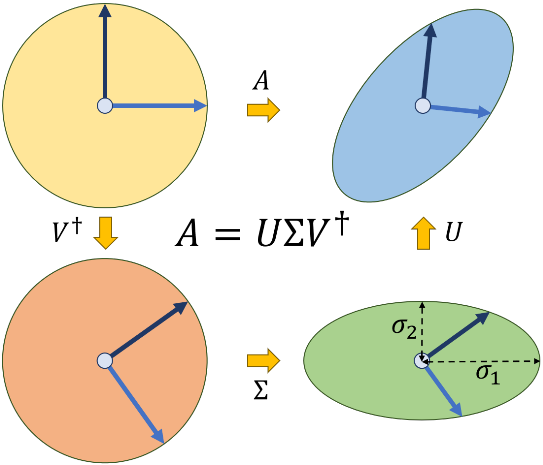
Any matrix $A \in \mathbb{C}^{N \times p}$, of any rank $r \leq \min(N, p)$, can be factorized in the form $A = U \Sigma V^{\dagger}$,

- $\Sigma \in \mathbb{R}^{N \times p}$ is a diagonal matrix with r positive elements that can always be ordered as $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r$; σ_i are the so called singular values
- $U \in \mathbb{C}^{N \times N}$ and $V \in \mathbb{C}^{p \times p}$ are unitary matrices
- U, V and Σ can be found by solving the eigenvalue problems $A^{\dagger} A V = V \Sigma_p^2$ and $A A^{\dagger} U = U \Sigma_N^2$, where $\Sigma_p^2 = \Sigma^{\dagger} \Sigma$ and $\Sigma_N^2 = \Sigma \Sigma^{\dagger}$.



Singular Value Decomposition

- Geometrical interpretation: rotation, scaling and rotation



Singular Value Decomposition

Proof.

- Let us first consider the case $N \geq p$. Any matrix $A \in \mathbb{C}^{N \times p}$ is a linear application that is completely defined by the values it takes on a given basis $\mathbf{v}_{1\ldots p}$ of the domain $\mathbb{C}^p$:

$$\begin{cases} A\mathbf{v}_1 = \sigma_1 \mathbf{u}_1 \\ \vdots \\ A\mathbf{v}_p = \sigma_p \mathbf{u}_p \end{cases}$$

- $\mathbf{u}_i \in \mathbb{C}^N$ are unit vectors, $\sigma_i \geq 0$, and it is always possible to reorder the basis so that the σ_i are in descending order.

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- This choice implies that also $\tilde{U} = [\mathbf{u}_1 \ \cdots \ \mathbf{u}_p]$ are orthonormal. Indeed, if $\sigma_{i,j} \neq 0$:

$$\mathbf{u}_i^\dagger \mathbf{u}_j = \frac{1}{\sigma_i \sigma_j} \mathbf{v}_i^\dagger A^\dagger A \mathbf{v}_j = \frac{\lambda_j}{\sigma_i \sigma_j} \mathbf{v}_i^\dagger \mathbf{v}_j = \frac{\lambda_j}{\sigma_i \sigma_j} \delta_{ij} \Rightarrow \begin{cases} i \neq j \Rightarrow \mathbf{u}_i^\dagger \mathbf{u}_j = 0 \\ i = j \Rightarrow \mathbf{u}_i^\dagger \mathbf{u}_j = \|\mathbf{u_i}\|^2 = 1 \end{cases}$$

$\lambda_i = \sigma_i^2$ because each $\mathbf{u}_i$ is a unit vector by construction.

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- When $i > r$, $\sigma_i = 0$, and it is always possible to complete $[\mathbf{u}_1 \ \cdots \ \mathbf{u}_r]$ to $[\mathbf{u}_1 \ \cdots \ \mathbf{u}_p]$ by adding $p - r$ orthonormal vectors however chosen (e.g., Gram-Schmidt).

Singular Value Decomposition

Proof.

- We came up to: $AV = A\left[\mathbf{v}_1 \;\; \cdots \;\; \mathbf{v}_p\right] = \left[\mathbf{u}_1 \;\; \cdots \;\; \mathbf{u}_p\right] \operatorname{diag}\left(\sigma_1 \;\; \cdots \;\; \sigma_r \;\; 0_{r+1} \;\; \cdots \;\; 0_p\right) = \tilde{U}\tilde{\Sigma}$.

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- $\tilde{U}$ can be completed to a basis of $\mathbb{C}^N$:

$$AV = \begin{bmatrix} \tilde{U} & \mathbf{u}_{p+1} \cdots \mathbf{u}_N \end{bmatrix} \begin{bmatrix} \tilde{\Sigma} \\ \mathbf{0}_{(N-p)\times p} \end{bmatrix} = U\Sigma$$

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- The eigenvalue problems for U, V and Σ can be derived as follows:

$$V^\dagger A^\dagger AV = \Sigma^\dagger U^\dagger U\Sigma = \Sigma^\dagger\Sigma = \Sigma_p^2 \Rightarrow A^\dagger AV = V\Sigma_p^2$$

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- For the case $N < p$, let us define $\bar{N} = p$ and $\bar{p} = N$, and $\bar{A} = A^\dagger \in \mathbb{C}^{\bar{N}\times\bar{p}}$, $\bar{N} > \bar{p}$:

$$\begin{array}{ccc} \bar{A} = \bar{U}\bar{\Sigma}\bar{V}^\dagger & \bar{A}^\dagger\bar{A}\bar{V} = \bar{V}\bar{\Sigma}_{\bar{p}}^2 & \bar{A}\bar{A}^\dagger\bar{U}\bar{\Sigma}_{\bar{N}}^2 \\ & AA^\dagger\bar{V} = \bar{V}\bar{\Sigma}_{\bar{p}}^2 & A^\dagger A\bar{U}\bar{\Sigma}_{\bar{N}}^2 \\ \bar{V} = U & \bar{U} = V & \bar{\Sigma} = \Sigma^\dagger \end{array}$$

$$\bar{A} = A^\dagger = V\Sigma^\dagger U^\dagger \Rightarrow A = U\Sigma V^\dagger \quad \square$$

Singular Value Decomposition

$N \geq p \Rightarrow A = U\Sigma V^\dagger =$

- $$\begin{pmatrix} \mathbf{u}_1 & \cdots & \mathbf{u}_N \end{pmatrix} \begin{pmatrix} \sigma_1 & \cdots & \cdots & \cdots \\ \vdots & \ddots & & \vdots \\ \vdots & & \sigma_r & \vdots \\ \cdots & \cdots & \cdots & 0_{(p-r)\times(p-r)} \\ & & 0_{(N-p)\times p} & \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^\dagger \\ \vdots \\ \mathbf{v}_p^\dagger \end{pmatrix}$$

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Alternative expression of the SVD

$$A = U\Sigma V^\dagger = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\dagger \quad \forall A \in \mathbb{C}^{N\times p}, \forall N, \forall p$$

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Introduction to the general LS solution

- For $N \geq p$ and $\mathrm{rank}\,(H) = r = p$, the OLS solution of the inconsistent system $\mathbf{b} = H\boldsymbol{\theta}$ is $\hat{\boldsymbol{\theta}} = \left(H^{\dagger}H\right)^{-1}H^{\dagger}\mathbf{b} = H^{+}\mathbf{b}$. A corrected observation vector $\hat{\mathbf{b}} = H\hat{\boldsymbol{\theta}}$ is defined, s.t. the cost function $\phi = \left\|\mathbf{b} - \hat{\mathbf{b}}\right\|^2 = \left\|\mathbf{b} - H\hat{\boldsymbol{\theta}}\right\|^2$ is minimum.

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- The solution can be made unique and it will be shown that:

General SVD pseudo-inverse

- The general form of the pseudo-inverse of $H = U\Sigma V^\dagger$ is $H^+ = V\Sigma^+ U^\dagger$.
- The unique LS solution $\hat{\boldsymbol{\theta}} = H^+\mathbf{b}$ is s.t. both $\left\|\mathbf{b} - H\hat{\boldsymbol{\theta}}\right\|^2$ and $\left\|\hat{\boldsymbol{\theta}}\right\|^2$ are minimum.
- $HH^+H = H$ is always true, but $H^+H = I$ or $HH^+ = I$ do not hold in general.
- $OLS : r = p \leq N \Rightarrow H^+ = \left(H^\dagger H\right)^{-1} H^\dagger$, $r = N < p \Rightarrow H^+ = H^\dagger \left(HH^\dagger\right)^{-1}$.
- $HH^+ = (HH^+)^\dagger$, $H^+H = (H^+H)^\dagger$

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- Remark: as it will be shown, the pseudo-inverse of Σ, Σ^+ is obtained by transposing Σ and by replacing the elements of the diagonal with the reciprocals of their respective nonzero elements of Σ. E.g.:

$$\Sigma = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \Rightarrow \Sigma^+ = \begin{pmatrix} 1/3 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

- $N \geq p,\ \ r = p \Rightarrow \Sigma^+\Sigma = I$;
- $N \leq p,\ \ r = N \Rightarrow \Sigma\Sigma^+ = I$;
- $r < \min(N, p) \Rightarrow \Sigma^+\Sigma \neq I$, and $\Sigma\Sigma^+ \neq I$, but $\Sigma\Sigma^+\Sigma = \Sigma$ is always true.
- $\Sigma\Sigma^+ = (\Sigma\Sigma^+)^T = {\Sigma^+}^T\Sigma^T$; $\Sigma^+\Sigma = (\Sigma^+\Sigma)^T = \Sigma^T{\Sigma^+}^T$

General LS solution

An explanatory example on Σ and Σ^+

- If Σ is $N \times p$, then Σ^+ is $p \times N$, $\Sigma^+\Sigma$ is $p \times p$ and $\Sigma\Sigma^+$ is $N \times N$. E.g.:

$$\Sigma = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \Sigma^+ = \begin{pmatrix} 1/3 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \quad \Sigma\Sigma^+ = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

- Matrices in the same form as $\Sigma\Sigma^+$, with only 0 and 1, can be called selection matrices of rank r, and denoted by the symbol I_n^r, where the superscript denotes rank, while the subscript denotes dimensions. Hence, $\Sigma\Sigma^+ = I_N^r$ and $\Sigma^+\Sigma = I_p^r$; obviously, $\mathrm{tr}\,(\Sigma\Sigma^+) = \mathrm{tr}\,(\Sigma^+\Sigma) = r$. In this example $\Sigma\Sigma^+ = I_4^2$.

General LS solution

Proof.

- $H = U\Sigma V^\dagger = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\dagger$
- Unitarity: $\mathbf{v}_i^\dagger \mathbf{v}_j = \mathbf{u}_i^\dagger \mathbf{u}_j = \delta_{ij}$

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- Cost function with SVD: $\|\mathbf{b} - H\boldsymbol{\theta}\|^2 = \left\|\mathbf{b} - U\Sigma V^\dagger \boldsymbol{\theta}\right\|^2 = \left\|U^\dagger \mathbf{b} - \Sigma V^\dagger \boldsymbol{\theta}\right\|^2$

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- By defining $\mathbf{y} \equiv V^\dagger\boldsymbol{\theta}$ and $\mathbf{c} \equiv U^\dagger\mathbf{b}$:
  $\|\mathbf{b} - H\boldsymbol{\theta}\|^2 = \|\mathbf{c} - \Sigma\mathbf{y}\|^2 = \sum_{i=1}^{r} |c_i - \sigma_i y_i|^2 + \sum_{i=r+1}^{p} |c_i|^2.$

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- The cost function is minimum for $y_i = c_i/\sigma_i$, $i = 1, \ldots, r$:

$$\mathbf{y} = \begin{pmatrix} c_1/\sigma_1 \\ \vdots \\ c_r/\sigma_r \\ \mathbf{0} \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} = U^\dagger \mathbf{b} = \begin{pmatrix} \mathbf{u}_1^\dagger \\ \vdots \\ \mathbf{u}_N^\dagger \end{pmatrix} \mathbf{b}$$

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- Since $i \le r, j > r \Rightarrow \mathbf{v}_i^\dagger \mathbf{v}_j = 0$, then $\hat{\boldsymbol{\theta}} \perp \mathbf{v}_{\text{ker}} \Rightarrow \left\| \hat{\boldsymbol{\theta}} + \mathbf{v}_{\text{ker}} \right\|^2 = \left\| \hat{\boldsymbol{\theta}} \right\|^2 + \left\| \mathbf{v}_{\text{ker}} \right\|^2 \ge \left\| \hat{\boldsymbol{\theta}} \right\|^2$

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- In general the pseudoinverse A^+ of a matrix A is exactly the inverse A^{-1} when A is invertible, i.e. when A is a full-rank square matrix.

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- Indeed, be $A = U\Sigma V^\dagger$ and $A^+ = V\Sigma^+ U^\dagger$; since A is square, both Σ and Σ^+ are square; since A is full-rank, all the diagonal elements of both Σ and Σ^+ are non-zero, hence $\Sigma\Sigma^+ = \Sigma^+\Sigma = I$.

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- Thus:

$$AA^+ = U\Sigma V^\dagger V\Sigma^+ U^\dagger = U\Sigma\Sigma^+ U^\dagger = UIU^\dagger = I$$
$$A^+A = V\Sigma^+ U^\dagger U\Sigma V^\dagger = V\Sigma^+\Sigma V^\dagger = VIV^\dagger = I$$

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- With these expressions it is easy to verify that

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$$H^{+}H^{+\dagger} = V\Sigma^{+}\Sigma^{+T}V^{\dagger} = \left(H^{\dagger}H\right)^{-1} = \left(H^{\dagger}H\right)^{+}$$

- Similarly, it can be proved that:

$$H^{+\dagger}H^{+} = U\Sigma^{+T}\Sigma^{+}U^{\dagger} = \left(HH^{\dagger}\right)^{-1} = \left(HH^{\dagger}\right)^{+}$$

General LS solution

Proof.

- $HH^+H = U\Sigma V^\dagger V\Sigma^+ U^\dagger U\Sigma V^\dagger = U\Sigma\Sigma^+\Sigma V^\dagger = U\Sigma V^\dagger = H$

General LS solution

Proof.

- $HH^{+}H = U\Sigma V^{\dagger} V \Sigma^{+} U^{\dagger} U \Sigma V^{\dagger} = U\Sigma\Sigma^{+}\Sigma V^{\dagger} = U\Sigma V^{\dagger} = H$
- $N \geq p,\ \ r = p \Rightarrow \Sigma^{+}\Sigma = I \Rightarrow H^{+}H = V\Sigma^{+}U^{\dagger}U\Sigma V^{\dagger} = V\Sigma^{+}\Sigma V^{\dagger} = VV^{\dagger} = I;$
- $N \geq p,\ \ r = p \Rightarrow \left(H^{\dagger}H\right)^{-1}H^{\dagger} = \left(H^{\dagger}H\right)^{+}H^{\dagger} = V\Sigma^{+}\Sigma^{+T}V^{\dagger}V\Sigma^{T}U^{\dagger} = V\Sigma^{+}U^{\dagger}$

General LS solution

Proof.

- $HH^+H = U\Sigma V^\dagger V\Sigma^+ U^\dagger U\Sigma V^\dagger = U\Sigma\Sigma^+\Sigma V^\dagger = U\Sigma V^\dagger = H$
- $N \geq p,\ \ r = p \Rightarrow \Sigma^+\Sigma = I \Rightarrow H^+H = V\Sigma^+ U^\dagger U\Sigma V^\dagger = V\Sigma^+\Sigma V^\dagger = VV^\dagger = I;$
- $N \geq p,\ \ r = p \Rightarrow \left(H^\dagger H\right)^{-1} H^\dagger = \left(H^\dagger H\right)^+ H^\dagger = V\Sigma^+\Sigma^{+T} V^\dagger V\Sigma^T U^\dagger = V\Sigma^+ U^\dagger$
- $N \leq p,\ \ r = N \Rightarrow \Sigma\Sigma^+ = I \Rightarrow HH^+ = U\Sigma V^\dagger V\Sigma^+ U^\dagger = U\Sigma\Sigma^+ U^\dagger = UU^\dagger = I;$
- $N \leq p,\ \ r = N \Rightarrow H^\dagger\left(HH^\dagger\right)^{-1} = H^\dagger\left(HH^\dagger\right)^+ = V\Sigma^T U^\dagger U\Sigma^{+T}\Sigma^+ U^\dagger = V\Sigma^+ U^\dagger$

General LS solution

Proof.

- $HH^+H = U\Sigma V^\dagger V\Sigma^+ U^\dagger U\Sigma V^\dagger = U\Sigma\Sigma^+\Sigma V^\dagger = U\Sigma V^\dagger = H$
- $N \geq p,\ r = p \Rightarrow \Sigma^+\Sigma = I \Rightarrow H^+H = V\Sigma^+ U^\dagger U\Sigma V^\dagger = V\Sigma^+\Sigma V^\dagger = VV^\dagger = I;$
- $N \geq p,\ r = p \Rightarrow \left(H^\dagger H\right)^{-1} H^\dagger = \left(H^\dagger H\right)^{+} H^\dagger = V\Sigma^+\Sigma^{+T} V^\dagger V\Sigma^T U^\dagger = V\Sigma^+ U^\dagger$
- $N \leq p,\ r = N \Rightarrow \Sigma\Sigma^+ = I \Rightarrow HH^+ = U\Sigma V^\dagger V\Sigma^+ U^\dagger = U\Sigma\Sigma^+ U^\dagger = UU^\dagger = I;$
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- Proof that $HH^+ = (HH^+)^\dagger$, $H^+H = (H^+H)^\dagger$ is now obvious □

General SVD pseudo-inverse

- The general form of the pseudo-inverse of $H = U\Sigma V^\dagger$ is $H^+ = V\Sigma^+ U^\dagger$.
- The unique LS solution $\hat{\boldsymbol{\theta}} = H^+\mathbf{b}$ is s.t. both $\left\|\mathbf{b} - H\hat{\boldsymbol{\theta}}\right\|^2$ and $\left\|\hat{\boldsymbol{\theta}}\right\|^2$ are minimum.
- $HH^+H = H$ is always true, but $H^+H = I$ or $HH^+ = I$ do not hold in general.
- $OLS : r = p \leq N \Rightarrow H^+ = \left(H^\dagger H\right)^{-1} H^\dagger,\ r = N < p \Rightarrow H^+ = H^\dagger\left(HH^\dagger\right)^{-1}.$
- $HH^+ = (HH^+)^\dagger,\ H^+H = (H^+H)^\dagger$

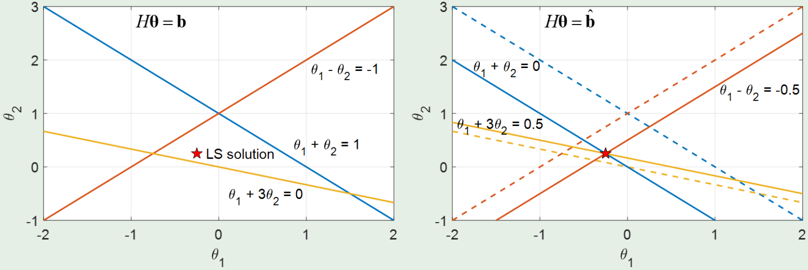
General LS solution

Example

- With Matlab, the SVD can be obtained by using the command `[U, S, V] = svd(H)`

$$H\boldsymbol{\theta} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 3 \end{pmatrix}\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = \mathbf{b} \qquad \hat{\boldsymbol{\theta}} = \begin{pmatrix} -0.25 \\ 0.25 \end{pmatrix} \qquad \hat{\mathbf{b}} = H\hat{\boldsymbol{\theta}} = \begin{pmatrix} 0 \\ -0.5 \\ 0.5 \end{pmatrix} \qquad H\boldsymbol{\theta} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 3 \end{pmatrix}\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \begin{pmatrix} 0 \\ -0.5 \\ 0.5 \end{pmatrix} = \hat{\mathbf{b}}$$

$$U = \begin{pmatrix} 0.3651 & 0.4472 & -0.8165 \\ -0.1826 & 0.8944 & 0.4082 \\ 0.9129 & 0 & 0.4082 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 3.4641 & 0 \\ 0 & 1.4142 \\ 0 & 0 \end{pmatrix} \qquad V = \begin{pmatrix} 0.3162 & 0.9487 \\ 0.9487 & -0.3162 \end{pmatrix}$$



General LS solution

An explanatory example on V

- In the following we will have to deal with product of the form $V^\dagger V_r$ or $V_r^\dagger V$, where V_r is the matrix formed by taking the first r columns of V, hence it is useful to visualize these products. If V is $p \times p$:

$$V^\dagger V_r = \begin{bmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 1 \end{pmatrix}_{r\times r} \\ \begin{pmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{pmatrix}_{(p-r)\times r} \end{bmatrix} = \begin{bmatrix} I_r \\ 0_{(p-r)\times r} \end{bmatrix}$$

$$V_r^\dagger V = \begin{bmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 1 \end{pmatrix}_{r\times r} & \begin{pmatrix} 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \end{pmatrix}_{r\times(p-r)} \end{bmatrix} = \begin{bmatrix} I_r & 0_{r\times(p-r)} \end{bmatrix}$$

- They can be called expansion or selection matrices and denoted by the symbol $I_{p\times r}$ or $I_{r\times p}$. Obviously, entirely similar results apply to U.

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Geometrical interpretation of LS

- Let us define the residual: $\mathbf{r} = \mathbf{b} - H\hat{\boldsymbol{\theta}} = \mathbf{b} - HH^{+}\mathbf{b} = \left(I - HH^{+}\right)\mathbf{b} = P_{H\perp}\mathbf{b}$

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- Let us also define $P_{H\|} = (I - P_{H\perp}) = HH^{+}$

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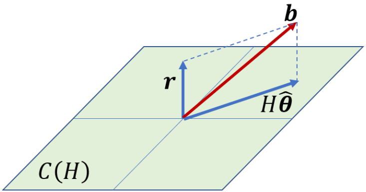
- $P_{H\perp}$ and $P_{H\|}$ are orthogonal projections



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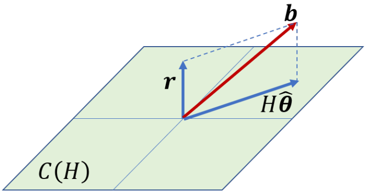
- $P_{H\perp}$ and $P_{H\|}$ are orthogonal projections
- It is straightforward to prove they are idempotent and symmetric
- $P_{H\perp}P_{H\perp} = P_{H\perp}$, $P_{H\|}P_{H\|} = P_{H\|}$ idempotency
- $P_{H\perp}{}^{\dagger} = P_{H\perp}$, $P_{H\|}{}^{\dagger} = P_{H\|}$ symmetry



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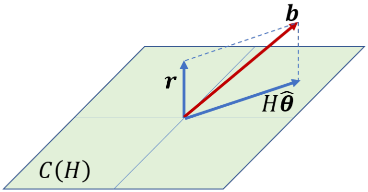
- Also $P_{H\perp}P_{H\|} = 0$



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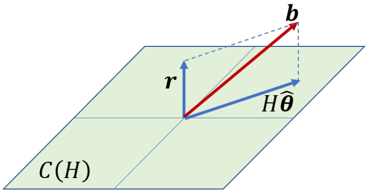

- Since $P_{H\|}\mathbf{b} = H\hat{\boldsymbol{\theta}}$, $P_{H\|}$ projects $\mathbf{b}$ onto column space $C(H)$ of H

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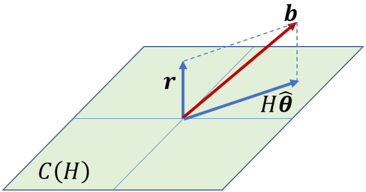

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- $P_{H\perp}$ projects $\mathbf{b}$ onto space $C_{\perp}(H)$ orthogonal to $C(H)$

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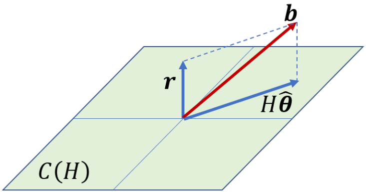
- Let us also define $P_{H\parallel} = (I - P_{H\perp}) = HH^{+}$

- $P_{H\perp}$ and $P_{H\parallel}$ are orthogonal projections
- It is straightforward to prove they are idempotent and symmetric
- $P_{H\perp}P_{H\perp} = P_{H\perp}$, $P_{H\parallel}P_{H\parallel} = P_{H\parallel}$ idempotency
- ${P_{H\perp}}^{\dagger} = P_{H\perp}$, ${P_{H\parallel}}^{\dagger} = P_{H\parallel}$ symmetry
- Also $P_{H\perp}P_{H\parallel} = 0$



- Since $P_{H\parallel}\mathbf{b} = H\hat{\boldsymbol{\theta}}$, $P_{H\parallel}$ projects $\mathbf{b}$ onto column space $C(H)$ of H
- $P_{H\perp}$ projects $\mathbf{b}$ onto space $C_{\perp}(H)$ orthogonal to $C(H)$
- The residual $\mathbf{r}$ accounts for the observed component of $\mathbf{b}$ that are not accounted for by the model $H\hat{\boldsymbol{\theta}}$

Geometrical interpretation of LS

- Since $\mathbf{r} = P_{H\perp}\mathbf{b}$, $P_{H\perp}$ is also called residual maker matrix.

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Geometrical interpretation of LS

- Since $\mathbf{r} = P_{H\perp}\mathbf{b}$, $P_{H\perp}$ is also called residual maker matrix.
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- Hence, $\mathbf{r} = P_{H\perp}\mathbf{b} = P_{H\perp}\left(H\boldsymbol{\theta} + \boldsymbol{\varepsilon}\right) = P_{H\perp}\boldsymbol{\varepsilon}$

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- Thus, the cost function is $\phi = \|\mathbf{r}\|^2 = \mathbf{r}^{\dagger}\mathbf{r} = \boldsymbol{\varepsilon}^{\dagger}P_{H\perp}^{\dagger}P_{H\perp}\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\dagger}P_{H\perp}\boldsymbol{\varepsilon}$

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- Hence, $\mathbf{r} = P_{H\perp}\mathbf{b} = P_{H\perp}\left(H\boldsymbol{\theta} + \boldsymbol{\varepsilon}\right) = P_{H\perp}\boldsymbol{\varepsilon}$
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- The expected value can be computed easily:

$$
\begin{aligned}
\mathrm{E}\left[\phi\left(\hat{\boldsymbol{\theta}}\right)\right] &= \mathrm{E}\left[\boldsymbol{\varepsilon}^\dagger P_{H\perp}\boldsymbol{\varepsilon}\right] = \mathrm{E}\left[\mathrm{tr}\left(\boldsymbol{\varepsilon}^\dagger P_{H\perp}\boldsymbol{\varepsilon}\right)\right] = \mathrm{E}\left[\mathrm{tr}\left(P_{H\perp}\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\dagger\right)\right] = \\
&= \mathrm{tr}\left(P_{H\perp}\mathrm{E}\left[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\dagger\right]\right) = \mathrm{tr}\left(P_{H\perp}\mathrm{cov}\left[\boldsymbol{\varepsilon}\right]\right) = \mathrm{tr}\left(P_{H\perp}\sigma^2 I\right) = \sigma^2\mathrm{tr}P_{H\perp} \\
\mathrm{tr}P_{H\perp} &= \mathrm{tr}\left(I_N - HH^{+}\right) = \mathrm{tr}\left(I_N - U\Sigma\Sigma^{+}U^\dagger\right) = N - \mathrm{tr}\left(\Sigma^{+}U^\dagger U\Sigma\right) = \\
&= N - \mathrm{tr}\left(\Sigma^{+}\Sigma\right) = N - \mathrm{tr}I_p^r = N - r
\end{aligned}
$$

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- Since $\mathbf{r} = P_{H\perp}\mathbf{b}$, $P_{H\perp}$ is also called residual maker matrix.
- Also $P_{H\perp}H = \left(I - HH^{+}\right)H = H - HH^{+}H = H - H = 0$.
- Hence, $\mathbf{r} = P_{H\perp}\mathbf{b} = P_{H\perp}\left(H\boldsymbol{\theta} + \boldsymbol{\varepsilon}\right) = P_{H\perp}\boldsymbol{\varepsilon}$
- Thus, the cost function is $\phi = \|\mathbf{r}\|^2 = \mathbf{r}^\dagger\mathbf{r} = \boldsymbol{\varepsilon}^\dagger P_{H\perp}^\dagger P_{H\perp}\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^\dagger P_{H\perp}\boldsymbol{\varepsilon}$
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$$= \mathrm{tr}\left(P_{H\perp}\mathrm{E}\left[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^\dagger\right]\right) = \mathrm{tr}\left(P_{H\perp}\mathrm{cov}\left[\boldsymbol{\varepsilon}\right]\right) = \mathrm{tr}\left(P_{H\perp}\sigma^2 I\right) = \sigma^2\mathrm{tr}P_{H\perp}$$

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$$= N - \mathrm{tr}\left(\Sigma^{+}\Sigma\right) = N - \mathrm{tr}I_p^r = N - r$$

Estimator of σ^2

If σ^2 is not known a priori, an unbiased estimator can be obtained from the residual:

$$\hat{\sigma}^2 = \frac{\phi\left(\hat{\boldsymbol{\theta}}\right)}{N-r} = \frac{\left\|\mathbf{r}\left(\hat{\boldsymbol{\theta}}\right)\right\|^2}{N-r} \Rightarrow \mathrm{E}\left[\hat{\sigma}^2\right] = \frac{\mathrm{E}\left[\phi\left(\hat{\boldsymbol{\theta}}\right)\right]}{N-r} = \frac{\sigma^2\left(N-r\right)}{N-r} = \sigma^2$$

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Properties of the general LS estimator

Covariance of the general LS estimator

1. For the general LS estimator, when $\mathrm{cov}\left[\boldsymbol{\varepsilon}\right] = \sigma^2 I$:

$$\hat{\boldsymbol{\theta}} = V\boldsymbol{\Sigma}^{+}U^{\dagger}\mathbf{b} \Rightarrow \mathrm{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2 V\boldsymbol{\Sigma}^{+}\boldsymbol{\Sigma}^{+T}V^{\dagger}$$

2. When $N \geq p$, and $\mathrm{rank}H = p$ (OLS):

$$\hat{\boldsymbol{\theta}} = \left(H^{\dagger}H\right)^{-1}H^{\dagger}\mathbf{b} \Rightarrow \mathrm{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2\left(H^{\dagger}H\right)^{-1}$$

3. When $N < p$, and $\mathrm{rank}H = N$:

$$\hat{\boldsymbol{\theta}} = H^{\dagger}\left(HH^{\dagger}\right)^{-1}\mathbf{b} \Rightarrow \mathrm{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2 H^{\dagger}\left(HH^{\dagger}\right)^{-2}H$$

The general covariance expression 1 yields the same values as the particular expressions 2 and 3, valid under the specified assumptions.

Properties of the general LS estimator

Proof.

1. $\text{cov}\,[\mathbf{b}] = \text{cov}\,[\varepsilon] = \sigma^2 I \Rightarrow$

$$\text{cov}\left[\hat{\boldsymbol{\theta}}\right] = \text{cov}\left[H^{+}\mathbf{b}\right] = \text{cov}\left[V\Sigma^{+}U^{\dagger}\mathbf{b}\right] = V\Sigma^{+}U^{\dagger}\text{cov}\,[\varepsilon]\,U\Sigma^{+T}V^{\dagger} = \sigma^2 V\Sigma^{+}\Sigma^{+T}V^{\dagger}$$

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$$\text{cov}\left[\hat{\boldsymbol{\theta}}\right] = \text{cov}\left[H^+\mathbf{b}\right] = \text{cov}\left[V\Sigma^+ U^\dagger \mathbf{b}\right] = V\Sigma^+ U^\dagger \text{cov}\left[\boldsymbol{\varepsilon}\right] U\Sigma^{+T} V^\dagger = \sigma^2 V\Sigma^+\Sigma^{+T} V^\dagger$$

2. $\text{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2 \left(H^\dagger H\right)^{-1} = \sigma^2 \left(H^\dagger H\right)^{+} = \sigma^2 V\Sigma^+ U^\dagger U\Sigma^{+T} V^\dagger = \sigma^2 V\Sigma^+\Sigma^{+T} V^\dagger$

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2. $\text{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2\left(H^\dagger H\right)^{-1} = \sigma^2\left(H^\dagger H\right)^{+} = \sigma^2 V\Sigma^+U^\dagger U\Sigma^{+T}V^\dagger = \sigma^2 V\Sigma^+\Sigma^{+T}V^\dagger$

3. $\text{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2 H^\dagger\left(HH^\dagger\right)^{-1}\left(HH^\dagger\right)^{-1}H =$

$$\sigma^2 V\Sigma^T\Sigma^{+T}\Sigma^+\Sigma^{+T}\Sigma^+\Sigma V^\dagger = \sigma^2 V\Sigma^+\Sigma\Sigma^+\Sigma^{+T}\Sigma^+\Sigma V^\dagger$$

Since $\Sigma\Sigma^+ = I$ when $\text{rank}H = N$, we get

$$\sigma^2 V\Sigma^+\Sigma^{+T}\Sigma^+\Sigma V^\dagger = \sigma^2 V\Sigma^+\Sigma^{+T}\Sigma^T\Sigma^{+T}V^\dagger = \sigma^2 V\Sigma^+\Sigma^{+T}\Sigma^T\Sigma^{+T}V^\dagger =$$

$$= \sigma^2 V\Sigma^+\left(\Sigma\Sigma^+\right)^T\Sigma^{+T}V^\dagger = \sigma^2 V\Sigma^+\Sigma^{+T}V^\dagger$$

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$$= V\Sigma^{+}\Sigma V^{\dagger}\boldsymbol{\theta} + V\Sigma^{+}U^{\dagger}\mathrm{E}\left[\boldsymbol{\varepsilon}\right] = V\Sigma^{+}\Sigma V^{\dagger}\boldsymbol{\theta}$$

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$$= V\Sigma^{+}\Sigma V^{\dagger}\boldsymbol{\theta} + V\Sigma^{+}U^{\dagger}\mathrm{E}\left[\boldsymbol{\varepsilon}\right] = V\Sigma^{+}\Sigma V^{\dagger}\boldsymbol{\theta}$$

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Properties of the general LS estimator

- Is the Gauss-Markov theorem valid for the general LS estimator $\hat{\boldsymbol{\theta}} = V\Sigma^{+}U^{\dagger}\mathbf{b}$?

- Gauss-Markov theorem assumptions:
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  - LS estimator is unbiased: let's check...

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- Gauss-Markov is not valid for the general LS estimator, hence in general $\hat{\boldsymbol{\theta}}$ is not BLUE.
- We will see how, for any rank r, it is always possible to extract r independent BLUE estimators from $\hat{\boldsymbol{\theta}}$.

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- Be $r = \text{rank} H \leq \min(N, p)$ and $\hat{\boldsymbol{\theta}} = H^+ \mathbf{b} = V\boldsymbol{\Sigma}^+ U^\dagger \mathbf{b}$ the generalized LS estimator.
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- There are infinite possible choices of $\boldsymbol{\lambda}_i^\dagger$.

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Estimable linear functions

Definition of estimable linear function

A linear function $\lambda(\boldsymbol{\theta}) \equiv \boldsymbol{\lambda}^\dagger \boldsymbol{\theta}$ of the unknown parameter $\boldsymbol{\theta}$ is estimable if, given observations $\mathbf{b}$ s.t. $\mathrm{E}[\mathbf{b}] = \mathrm{E}[H\boldsymbol{\theta} + \boldsymbol{\varepsilon}] = H\boldsymbol{\theta}$, there exists an unbiased linear estimator $\mathbf{a}^\dagger \mathbf{b}$ for some $\mathbf{a}$, s.t. $\mathrm{E}\left[\mathbf{a}^\dagger \mathbf{b}\right] = \boldsymbol{\lambda}^\dagger \boldsymbol{\theta}$.

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Lemma: estimator of minimum variance

- The unique unbiased estimator $\mathbf{a}_{\|}^{\dagger}\mathbf{b}$ has minimum variance, i.e., for any other unbiased estimator $\mathbf{a}^{\dagger}\mathbf{b}$ s.t. $\mathrm{E}\left[\mathbf{a}^{\dagger}\mathbf{b}\right] = \boldsymbol{\lambda}^{\dagger}\boldsymbol{\theta}$, then $\mathrm{var}\left[\mathbf{a}^{\dagger}\mathbf{b}\right] \geq \mathrm{var}\left[\mathbf{a}_{\|}^{\dagger}\mathbf{b}\right]$.
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- $$\mathrm{var}\left[\mathbf{a}^{\dagger}\mathbf{b}\right] = \mathbf{a}^{\dagger}\mathrm{cov}\,[\mathbf{b}]\,\mathbf{a} = \sigma^{2}\left\|\mathbf{a}\right\|^{2} = \sigma^{2}\left(\left\|\mathbf{a}_{||}\right\|^{2} + \left\|\mathbf{a}_{\perp}\right\|^{2}\right) =$$
$$= \mathrm{var}\left[\mathbf{a}_{||}^{\dagger}\mathbf{b}\right] + \sigma^{2}\left\|\mathbf{a}_{\perp}\right\|^{2} \geq \mathrm{var}\left[\mathbf{a}_{||}^{\dagger}\mathbf{b}\right].$$

Estimable linear functions

Lemma: estimator of minimum variance

- The unique unbiased estimator $\mathbf{a}_{\|}^{\dagger}\mathbf{b}$ has minimum variance, i.e., for any other unbiased estimator $\mathbf{a}^{\dagger}\mathbf{b}$ s.t. $\mathrm{E}\left[\mathbf{a}^{\dagger}\mathbf{b}\right] = \boldsymbol{\lambda}^{\dagger}\boldsymbol{\theta}$, then $\mathrm{var}\left[\mathbf{a}^{\dagger}\mathbf{b}\right] \geq \mathrm{var}\left[\mathbf{a}_{\|}^{\dagger}\mathbf{b}\right]$.
- The unique unbiased estimator $\mathbf{a}_{\|}^{\dagger}\mathbf{b}$ is BLUE, i.e. $\mathrm{E}\left[\left|\mathbf{a}^{\dagger}\mathbf{b} - \boldsymbol{\lambda}^{\dagger}\boldsymbol{\theta}\right|^2\right] \geq \mathrm{E}\left[\left|\mathbf{a}_{\|}^{\dagger}\mathbf{b} - \boldsymbol{\lambda}^{\dagger}\boldsymbol{\theta}\right|^2\right]$.

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- $\mathrm{var}\left[\mathbf{a}^{\dagger}\mathbf{b}\right] = \mathrm{E}\left[\left|\mathbf{a}^{\dagger}\mathbf{b} - \mathrm{E}\left[\mathbf{a}^{\dagger}\mathbf{b}\right]\right|^2\right] = \mathrm{E}\left[\left|\mathbf{a}^{\dagger}\mathbf{b} - \boldsymbol{\lambda}^{\dagger}\boldsymbol{\theta}\right|^2\right]$, and BLUEness follows from the first part of the lemma. □

Estimable linear functions

Lemma: definition of the unbiased estimator

- The unique unbiased estimator $\mathbf{a}_{||}^{\dagger}\mathbf{b}$ for $\boldsymbol{\lambda}^{\dagger}\boldsymbol{\theta}$, where $\boldsymbol{\lambda}^{\dagger} = \mathbf{a}_{||}^{\dagger}H \in R(H)$ is defined as $\mathbf{a}_{||}^{\dagger}\mathbf{b} = \boldsymbol{\lambda}^{\dagger}\hat{\boldsymbol{\theta}}$, where $\hat{\boldsymbol{\theta}}$ is the general LS estimator $\hat{\boldsymbol{\theta}} = H^{+}\mathbf{b} = V\boldsymbol{\Sigma}^{+}U^{\dagger}\mathbf{b}$.

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Proof.

- Since $\mathbf{a}_{||} \in C(H)$ and $\mathbf{a}_{||} = P_{H||}\mathbf{a}_{||}$:

$$\mathbf{a}_{||}^{\dagger}\mathbf{b} = \mathbf{a}_{||}^{\dagger}P_{H||}^{\dagger}\mathbf{b} = \mathbf{a}_{||}^{\dagger}P_{H||}\mathbf{b} = \mathbf{a}_{||}^{\dagger}H\hat{\boldsymbol{\theta}} = \boldsymbol{\lambda}^{\dagger}\hat{\boldsymbol{\theta}}. \square$$

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Generalized Gauss-Markov theorem

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Generalized Gauss-Markov theorem

- Given any system $\mathbf{b} = H\boldsymbol{\theta} + \boldsymbol{\varepsilon}$ with N equations and p unknown parameters, s.t. $\mathrm{E}\left[\boldsymbol{\varepsilon}\right] = 0$ and $\mathrm{cov}\left[\boldsymbol{\varepsilon}\right] = \sigma^2 I_N$.
- Be $r = \mathrm{rank} H \leq \min\left(N, p\right)$ and $\hat{\boldsymbol{\theta}} = H^+\mathbf{b} = V\boldsymbol{\Sigma}^+U^\dagger\mathbf{b}$ the generalized LS estimator.
- Be $\boldsymbol{\lambda}_i^\dagger, \;\; i = 1\cdots r$, any set of linearly independent vectors $\in R\left(H\right)$.
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- By all the previous lemmas, $\boldsymbol{\lambda}_i^\dagger\hat{\boldsymbol{\theta}}$ is the unbiased, minimum variance, and BLUE estimator of $\boldsymbol{\lambda}_i^\dagger\boldsymbol{\theta}$. $\square$

Covariance of the generalized Gauss-Markov estimator

- Let us define $\Lambda = [\boldsymbol{\lambda}_1 \ \cdots \ \boldsymbol{\lambda}_r]$. Hence, the generalized Gauss-Markov estimators can be collected in the single expression $\Lambda^\dagger \hat{\boldsymbol{\theta}}$.

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- By noticing that $R(H) = R\left(H^\dagger H\right)$, it is possible to choose $\boldsymbol{\lambda}_i^\dagger = \mathbf{a}_i^\dagger H^\dagger H$, $\mathbf{a}_i \in C(H)$. Let us define $A = [\mathbf{a}_1 \ \cdots \ \mathbf{a}_r] \Rightarrow \Lambda^\dagger = A^\dagger H^\dagger H$. The covariance is then

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- If $\Lambda = V_r$, where V_r are the first r columns of V, the covariance is diagonal, and $V_r^\dagger \hat{\boldsymbol{\theta}}$ are the principal components of $\hat{\boldsymbol{\theta}}$:

$$\mathrm{cov}\left[\Lambda^\dagger \hat{\boldsymbol{\theta}}\right] = \sigma^2 V_r^\dagger V \Sigma^+ \Sigma^{+T} V^\dagger V_r = \sigma^2 I_{r\times p} \Sigma^+ \Sigma^{+T} I_{p\times r} = \sigma^2 \mathrm{diag}\left(1/\sigma_1^2 \ \cdots \ 1/\sigma_r^2\right)$$

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Remark on V_r

- $\boldsymbol{\lambda} \in R(H)$. Are we confident that the columns $\mathbf{v}$ of $\Lambda = V_r$ are in $R(H)$?

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- Since $C\left(H^{\dagger}\right) \equiv R(H)$, it is proved that $\mathbf{v} \in R(H)$.

Generalized Gauss-Markov theorem

Example

- Let us consider the following system:

$$H\boldsymbol{\theta} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

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- Clearly, it is $r = \mathrm{rank} H = 2$. SVD yields the following matrices:

$$U = \begin{bmatrix} -0.5 & -0.5 & -0.5 & -0.5 \\ -0.5 & -0.5 & 0.5 & 0.5 \\ -0.5 & 0.5 & 0.5 & -0.5 \\ -0.5 & 0.5 & -0.5 & 0.5 \end{bmatrix} \quad V = \begin{bmatrix} -8.165 & 0 & -0.5774 \\ -0.4082 & -0.7071 & 0.5774 \\ -0.4082 & 0.7071 & 0.5774 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} 2.4495 & 0 & 0 \\ 0 & 1.4142 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \Sigma^+ = \begin{bmatrix} 0.4082 & 0 & 0 & 0 \\ 0 & 0.7071 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

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- Thus, $\left\|\mathbf{b}_0 - \hat{\mathbf{b}}_0\right\|^2 = 0$ is effectively minimized, but even without noise, it is not possible to estimate parameters correctly, since the system is under-determined.

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- Thus, $\left\|\mathbf{b}_0 - \hat{\mathbf{b}}_0\right\|^2 = 0$ is effectively minimized, but even without noise, it is not possible to estimate parameters correctly, since the system is under-determined.
- But if check principal components: $V_r^\dagger \boldsymbol{\theta} = [-1.633\ 0]^\dagger$ and $V_r^\dagger \hat{\boldsymbol{\theta}} = [-1.633\ 0]^\dagger$, perfectly matching.

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- We add Gaussian noise with $\sigma = 0.1$: $\mathbf{b} = \mathbf{b}_0 + \boldsymbol{\varepsilon} = [1.9196\ 2.0697\ 2.0835\ 1.9756]^\dagger$.

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- The LS estimator yields $\hat{\boldsymbol{\theta}} = V\Sigma^+U^\dagger = [1.3414\ 0.6532\ 0.6882]^\dagger$, with covariance:

$$\operatorname{cov}\left[\hat{\boldsymbol{\theta}}\right] = \sigma^2 V \boldsymbol{\Sigma}^+ \boldsymbol{\Sigma}^{+T} V^\dagger = \begin{bmatrix} 0.0011 & 0.0006 & 0.0006 \\ 0.0006 & 0.0028 & -0.0022 \\ 0.0006 & -0.0022 & 0.0028 \end{bmatrix}$$

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- Principal components: $V_r^\dagger\boldsymbol{\theta} = [-1.633\ 0]^\dagger$ and $V_r^\dagger\hat{\boldsymbol{\theta}} = [-1.6429\ 0.0247]^\dagger$, with:

$$\mathrm{cov}\left[V_r^\dagger\hat{\boldsymbol{\theta}}\right] = \sigma^2 V_r^\dagger V\boldsymbol{\Sigma}^+\boldsymbol{\Sigma}^{+T}V^\dagger V_r = \sigma^2 \mathrm{diag}\left(1/\sigma_1^2\ \cdots\ 1/\sigma_r^2\right) = \begin{bmatrix} 0.0017 & 0 \\ 0 & 0.0050 \end{bmatrix}$$