

Numerical Linear Algebra Homework Project 2: Least Squares, Orthogonalization, and the SVD

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Problem 1

(1) Suppose we are given m pairs of data points, $(x_1, y_1), \dots, (x_m, y_m)$. We want to find a linear combination of prescribed functions ϕ_1, \dots, ϕ_n whose values at the points $x_i \in [a, b]$, $1 \leq i \leq m$, approximate the values y_1, \dots, y_m as well as possible. More precisely, the problem is to find a function of the form $f(x) = \alpha_1 \phi_1(x) + \dots + \alpha_n \phi_n(x)$ such that

$$\sum_{i=1}^m [y_i - f(x_i)]^2 \leq \sum_{i=1}^m [y_i - g(x_i)]^2 \quad \forall g \in \text{Span}(\phi_1, \dots, \phi_n), \quad (1)$$

where, usually, $m > n$. It is possible to rephrase the problem as:

$$f = \arg \min_{f \in \text{Span}(\phi_1, \dots, \phi_n)} \sum_{i=1}^m [y_i - f(x_i)]^2. \quad (2)$$

Now we can define a column vector $\mathbf{z} \in \mathbb{R}^n$ such that:

$$[\mathbf{z}]_i = \alpha_i \quad (3)$$

and a matrix A such that:

$$[A\mathbf{z}]_i = f(x_i) = \alpha_1 \phi_1(x_i) + \dots + \alpha_n \phi_n(x_i). \quad (4)$$

In this way, the element of the i -th row and j -th column of the matrix A is:

$$[A]_{ij} = a_{ij} = \phi_j(x_i). \quad (5)$$

Finally, defining a column vector $\mathbf{b} \in \mathbb{R}^n$ such that:

$$[\mathbf{b}]_i = y_i \quad (6)$$

we can rewrite the (2) as follows:

$$\tilde{\mathbf{z}} = \arg \min_{\mathbf{z} \in \mathbb{R}^n} \|\mathbf{b} - A\mathbf{z}\|_2^2 = \arg \min_{\mathbf{z} \in \mathbb{R}^n} \|\mathbf{b} - A\mathbf{z}\|_2, \quad (7)$$

where the function f can be built from $\tilde{\mathbf{z}}$.

(2) Now we suppose to take $\phi_k = x^{k-1}$, $1 \leq k \leq n$. Under this assumption, the matrix A takes the form:

$$A = \begin{bmatrix} x_1^0 & \dots & x_1^{n-1} \\ \vdots & \ddots & \vdots \\ x_m^0 & \dots & x_m^{n-1} \end{bmatrix}. \quad (8)$$

We want to prove that, assuming that $x_i \neq x_j$ for $i \neq j$, A has full rank: $\text{rank}(A) = n$.

Proof: Proving that $\text{rank}(A) = n$ is equivalent to prove that $\dim(\ker(A)) = 0$, that means

that $\nexists \mathbf{v} \in \mathbb{R}^n$ s.t. $\mathbf{v} \in \ker(A)$. We want to prove this statement by contraddiction, therefore, we look for a vector $\mathbf{v} \in \mathbb{R}^n$, with $\mathbf{v} \neq \underline{0}$, such that $A\mathbf{v} = \underline{0}$, that means:

$$\begin{cases} v_1x_1^0 + \dots + v_nx_1^{n-1} = 0 \\ \vdots \\ v_1x_m^0 + \dots + v_nx_m^{n-1} = 0 \end{cases} \quad (9)$$

Defining the polynomial

$$p_{\mathbf{v}}^{(n-1)}(x) = \sum_{i=1}^n v_i x^{i-1} \quad (10)$$

we can observe that, for any choice of $\mathbf{v} \neq \underline{0}$, $p_{\mathbf{v}}^{(n-1)}(x)$ admits at most $n - 1$ different roots, therefore $\nexists \mathbf{v} \neq \underline{0}$ such that $A\mathbf{v} = \underline{0}$. This concludes the proof. \square

(3) Consider the problem of finding the best fit with a quadratic function $f(x) = \alpha_1 + \alpha_2x + \alpha_3x^2$ for the following data:

x_i	8	10	12	16	20	30	40	60	100
y_i	0.88	1.22	1.64	2.72	3.96	7.66	11.96	21.56	43.16

In the following we report the code that solves the normal equations:

$$A^T A \mathbf{v} = A^T \mathbf{b} \quad (11)$$

using the Cholesky factorization algorithm and then compares the result with the one found using the QR factorization of the matrix A .

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Using the previous functions we have computed the solution to the minimization problem, obtaining the following results:

Cholesky: $x = [-1.91914925269909, 0.278213536291725, 0.001739400875055]$

QR factorization: $x = [-1.91914925269904, 0.278213536291722, 0.001739400875055]$

From these results we can observe that, for this problem, both the algorithms perform in a similar way. In fact, the results differ at most in the 15th digit. In figure 1 we show the input data and the solutions to the least square problem.

(4) The following code computes the residual $\mathbf{r} = \mathbf{d} - C\hat{\mathbf{x}}$ where $\hat{\mathbf{x}} = [-1.919, 0.2782, 0.001739]$ is the approximate solution of the least squares problem.

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The results that we obtain are:

Residual: $\mathbf{r} = [0.009503999999993, 0.716895999999906, 62.090847999905236]$

Norm 2 of the residual: $\|\mathbf{r}\|_2 = 62.09498720144942$

The value of the residual may seem strange, in fact, if we compute the relative error we find:

$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2} = 7.728184292875672\text{e-}05. \quad (12)$$

However, we can observe that, from the relation

$$\frac{1}{k_2(C)} \frac{\|\mathbf{r}\|_2}{\|\mathbf{d}\|_2} \leq \frac{\|\mathbf{x} - \hat{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2} \leq k_2(C) \frac{\|\mathbf{r}\|_2}{\|\mathbf{d}\|_2} \quad (13)$$

we can obtain the following relation for \mathbf{r} :

$$\frac{\|\mathbf{d}\|_2}{k_2(C)} \frac{\|\mathbf{x} - \hat{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2} \leq \|\mathbf{r}\|_2 \leq k_2(C) \|\mathbf{d}\|_2 \frac{\|\mathbf{x} - \hat{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2}. \quad (14)$$

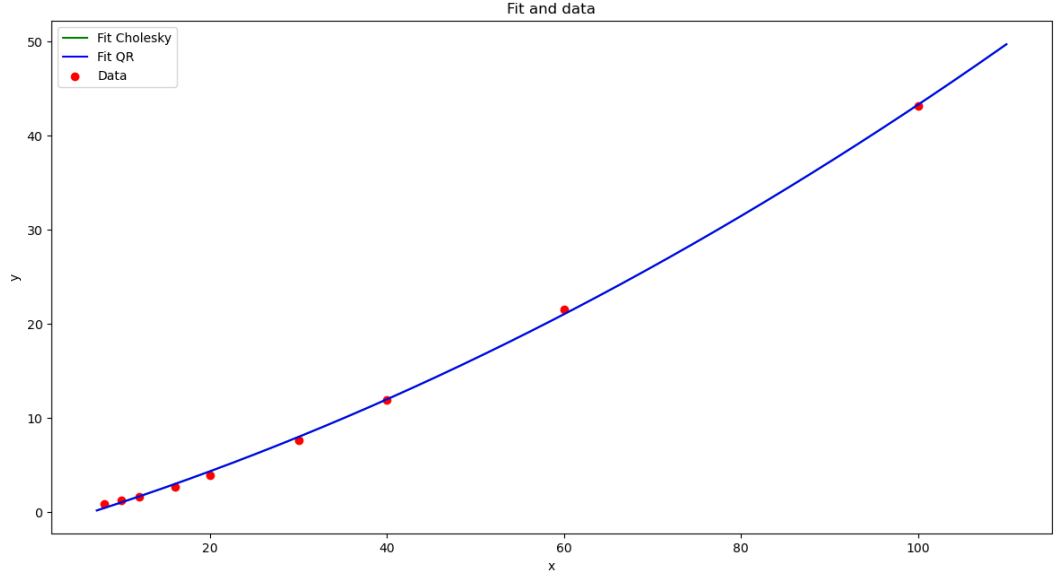


Figure 1

With the following python code we have computed the bounds to the residual. *** INSERIRE CODICE***

From the output of the previous code we know that:

$$5 \times 10^{-7} \lesssim \|\mathbf{r}\|_2 \lesssim 3 \times 10^9 \quad (15)$$

this big range is due to the value of $k_2(C) \simeq 8 \times 10^7$ that suggests us that we should not use the residual to measure the accuracy of the solution when the problem is ill-conditioned as in this case.

Problem 2

(1) Let $A \in \mathbb{R}^{m \times n}$, with $\text{rank}(A) = n$, let $A = QR$ be the (full) QR factorization of A , with $Q \in \mathbb{R}^{m \times m}$ orthogonal and $R \in \mathbb{R}^{m \times n}$ upper trapezoidal. Also, let $A = Q_1 R_1$ be the reduced QR factorization of A with $Q_1 \in \mathbb{R}^{m \times n}$ having orthonormal columns and $R_1 \in \mathbb{R}^{m \times m}$ upper triangular. Show that R_1 is nonsingular, and that the columns $\mathbf{q}_1, \dots, \mathbf{q}_n$ of Q_1 form an orthonormal basis for $\text{Ran}(A)$, the column space of A . Also, find an orthonormal basis for $\text{Null}(A^T)$, the null space of A^T .

We start showing that R_1 is nonsingular. Since A has full rank, we know that:

$$A\mathbf{x} = \mathbf{0} \Leftrightarrow \mathbf{x} = \mathbf{0} \quad (16)$$

and multiplying both sides for Q_1^T knowing that $Q_1^T Q_1 = I_n$ we obtain

$$R_1 \mathbf{x} = \mathbf{0} \Leftrightarrow \mathbf{x} = \mathbf{0}, \quad (17)$$

that concludes the proof.

Now we want to show that the columns $\mathbf{q}_1, \dots, \mathbf{q}_n$ of Q_1 form an orthonormal basis for $\text{Ran}(A)$. We start observing that

$$\forall \mathbf{y} \in \text{Ran}(A) \exists \mathbf{x} \in \mathbb{R}^n : \mathbf{y} = A\mathbf{x} = Q_1 R_1 \mathbf{x} \quad (18)$$

and we know this from the definition of range of a matrix. In a similar way, knowing that R_1 is nonsingular and therefore is a bijective map from \mathbb{R}^n to \mathbb{R}^n , we can put $\mathbf{x}' = R_1\mathbf{x}$ and say that:

$$\forall \mathbf{y} \in \text{Ran}(A) \exists \mathbf{x} \in \mathbb{R}^n : \mathbf{y} = A\mathbf{x} = Q_1\mathbf{x}', \quad (19)$$

that means that $\text{Ran}(A) = \text{Ran}(Q_1) = \text{Span}\{\mathbf{q}_1, \dots, \mathbf{q}_n\}$.

Now we want to find an orthonormal basis for $\text{Null}(A^T)$. Knowing that $\text{Null}(A^T) = (\text{Ran}(A))^\perp$ we can, immediately, find the solution. In fact:

$$(\text{Ran}(A))^\perp = \text{Span}\{\mathbf{q}_1, \dots, \mathbf{q}_n\}^\perp = \text{Span}\{\mathbf{q}_{n+1}, \dots, \mathbf{q}_m\}. \quad (20)$$

This concludes the proof. \square

(2) Given the full rank matrix

$$A = \begin{bmatrix} 1.07 & 1.10 \\ 1.07 & 1.11 \\ 1.07 & 1.15 \end{bmatrix}, \quad (21)$$

compute $A^T A$ in $\beta = 10$, $t = 3$ digit arithmetic and verify if $A^T A$ is positive definite. We performed the prescribed calculation using the rounding function

$$\text{fl}(x) = \arg \min_{y \in \mathbb{F}} |y - x| \quad (22)$$

where $\mathbb{F} = \{\pm(0.d_1 d_2 d_3) \times 10^p : d_i \in 0, \dots, 9, -2046 \leq p \leq 2046\}$ and, when there is ambiguity, we approximate always away from 0. Moreover, the rounding function has been applied at each step of the calculation, meaning that, if we consider $\mathbf{v}, \mathbf{u} \in \mathbb{R}^n$

$$\mathbf{v}^T \mathbf{u} = \text{fl} \left(\sum_{i=1}^n \text{fl}(v_i u_i) \right). \quad (23)$$

The result of the calculation is the following:

$$A^T A = \begin{bmatrix} 3.42 & 3.6 \\ 3.6 & 3.76 \end{bmatrix}. \quad (24)$$

The last matrix is indefinite, in fact $\text{Det}(A^T A) = 3.42 \times 3.76 - 3.6^2 = 12.8592 - 12.96 < 0$.

(3) Compute the QR factorization of the matrix

$$A = \begin{bmatrix} 1.07 & 1.10 \\ 1.07 & 1.11 \\ 1.07 & 1.15 \end{bmatrix} = [\mathbf{a}_1 \ \mathbf{a}_2] \quad (25)$$

in 3 digit arithmetic, i.e. with $\beta = 10$, $t = 3$. The $\text{fl}(x)$ function has been applied at each step, as in the previous exercise.

We want to compute $H_1 A$:

$$H_1 A = \begin{bmatrix} r_{11} & \mathbf{r}_1^T \\ \mathbf{0} & A_1 \end{bmatrix}. \quad (26)$$

$$r_{11} = -\text{sgn}(a_{11}) \|\mathbf{a}_1\|_2 = \|\mathbf{a}_1\|_2 = \sqrt{1.14 \times 3} = \sqrt{3.42} = -1.85 \quad (27)$$

$$\hat{\mathbf{u}}_1 = \mathbf{a}_1 + r_{11} \mathbf{e}_1 = \begin{pmatrix} 1.07 \\ 1.07 \\ 1.07 \end{pmatrix} + 1.85 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 2.92 \\ 1.07 \\ 1.07 \end{pmatrix} \quad (28)$$

$$\|\hat{\mathbf{u}}\|_2 = \sqrt{8.53 + 1.14 + 1.14} = \sqrt{10.81} = 3.29 \quad (29)$$

$$\mathbf{u}_1 = \hat{\mathbf{u}}_1 / \|\hat{\mathbf{u}}\|_2 = \begin{pmatrix} 0.888 \\ 0.325 \\ 0.325 \end{pmatrix} \quad (30)$$

$$\begin{aligned} H_1 \mathbf{a}_2 &= \mathbf{a}_2 - 2(\mathbf{u}_1^T \mathbf{a}_2) \mathbf{u}_1 \\ &= \begin{pmatrix} 1.10 \\ 1.11 \\ 1.15 \end{pmatrix} - 2(0.977 + 0.374 + 0.374) \begin{pmatrix} 0.888 \\ 0.325 \\ 0.325 \end{pmatrix} \\ &= \begin{pmatrix} 1.10 \\ 1.11 \\ 1.15 \end{pmatrix} - 3.42 \begin{pmatrix} 0.888 \\ 0.325 \\ 0.325 \end{pmatrix} = \begin{pmatrix} -1.94 \\ 0 \\ 0.04 \end{pmatrix} \end{aligned} \quad (31)$$

Therefore we have:

$$H_1 A = \begin{pmatrix} -1.85 & -1.94 \\ 0 & 0 \\ 0 & 0.04 \end{pmatrix}. \quad (32)$$

Now we iterate the same procedure on A_1 , with

$$A_1 = [\mathbf{a}_2^{(1)}] = \begin{pmatrix} 0 \\ 0.04 \end{pmatrix}. \quad (33)$$

$$\hat{\mathbf{u}}_2^{(1)} = \mathbf{a}_2^{(1)} + \text{sgn}(a_{12}^{(1)}) \|\mathbf{a}_2^{(1)}\|_2 \mathbf{e}_2^{(1)} = \begin{pmatrix} 0 \\ 0.04 \end{pmatrix} + \text{sgn}(0) 0.04 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.04 \\ 0.04 \end{pmatrix} \quad (34)$$

$$\mathbf{u}_2^{(1)} = \hat{\mathbf{u}}_2^{(1)} / \|\hat{\mathbf{u}}_2^{(1)}\|_2 = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix}. \quad (35)$$

The complete vector \mathbf{u}_2 will be:

$$\mathbf{u}_2 = \begin{pmatrix} 0 \\ 0.707 \\ 0.707 \end{pmatrix} \quad (36)$$

and the element r_{22} will be

$$r_{22} = -\text{sgn}(a_{12}^{(1)}) \|\mathbf{a}_2^{(1)}\|_2 = -0.04 \quad (37)$$

so that, finally, we have

$$H_2 H_1 A = R = \begin{pmatrix} -1.85 & -1.94 \\ 0 & -0.04 \\ 0 & 0 \end{pmatrix}. \quad (38)$$

We can observe that the matrix R is full rank, therefore it is possible to use the QR factorization to solve the least square problem. It is important to stress that, as $A^T A$ is indefinite in 3 digit precision, using Cholesky is not possible.

Now we want to compute $Q = [\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3]$ and, in order to do it, we use the following relations:

$$\begin{aligned} \mathbf{q}_1 &= H_1 H_2 \mathbf{e}_1 = \mathbf{e}_1 - 2(\mathbf{u}_1^T \mathbf{e}_1) \mathbf{u}_1 \\ \mathbf{q}_2 &= H_1 H_2 \mathbf{e}_2 = H_1 (\mathbf{e}_2 - 2(\mathbf{u}_2^T \mathbf{e}_2) \mathbf{u}_2) \\ &= \mathbf{e}_2 - 2(\mathbf{u}_2^T \mathbf{e}_2) \mathbf{u}_2 - 2(\mathbf{u}_1^T \mathbf{e}_2) \mathbf{u}_1 + 4(\mathbf{u}_2^T \mathbf{e}_2)(\mathbf{u}_1^T \mathbf{u}_2) \mathbf{u}_1. \\ \mathbf{q}_3 &= H_1 H_2 \mathbf{e}_3 = H_1 (\mathbf{e}_3 - 2(\mathbf{u}_2^T \mathbf{e}_3) \mathbf{u}_2) \\ &= \mathbf{e}_3 - 2(\mathbf{u}_2^T \mathbf{e}_3) \mathbf{u}_2 - 2(\mathbf{u}_1^T \mathbf{e}_3) \mathbf{u}_1 + 4(\mathbf{u}_2^T \mathbf{e}_3)(\mathbf{u}_1^T \mathbf{u}_2) \mathbf{u}_1 \end{aligned} \quad (39)$$

Using these relations, we found the approximated matrix Q , that is:

$$Q = \begin{bmatrix} -0.578 & 0.572 & 0.572 \\ -0.578 & 0.212 & -0.788 \\ -0.578 & -0.788 & 0.212 \end{bmatrix}. \quad (40)$$

Finally, we can verify that, multiplying Q and R and approximating as before, we recover the original matrix A . It is important to point out that the columns of Q are not perfectly orthonormal.

(4) Let $A \in \mathbb{R}^{m \times n}$, with $\text{rank}(A) = n$, and let $\mathbf{b} \in \mathbb{R}^m$. Let $A = Q_1 R_1$ be a reduced QR decomposition of A , where $Q_1 \in \mathbb{R}^{m \times n}$ has orthonormal columns and $R_1 \in \mathbb{R}^{n \times n}$ is upper triangular and nonsingular. Show that a reduced QR factorization of the augmented matrix $A_+ = [A \ \mathbf{b}]$ is given by:

$$A_+ = [Q_1 \ \mathbf{q}_{n+1}] \begin{bmatrix} R_1 & \mathbf{z} \\ \mathbf{0}^T & \rho \end{bmatrix} \quad (41)$$

where $\mathbf{z} = Q_1^T \mathbf{b}$. Also, show that $|\rho| = \|\mathbf{b} - A\mathbf{x}^*\|_2$ where \mathbf{x}^* is the solution to the least squares problem $\|\mathbf{b} - A\mathbf{x}\|_2 = \min$.

We start recalling that any matrix has a QR factorization, therefore the matrix A_+ must have it. In particular we know that $A_+ = Q_+ R_+$, where Q_+ has orthonormal columns and R_+ is upper triangular. In order to find the value of \mathbf{z} and ρ , we compute the product $Q_+ R_+$ and impose that it is equal to A_+ :

$$[Q_1 \ \mathbf{q}_{n+1}] \begin{bmatrix} R_1 & \mathbf{z} \\ \mathbf{0}^T & \rho \end{bmatrix} = [Q_1 R_1 \ Q_1 \mathbf{z} + \rho \mathbf{q}_{n+1}] = [A \ \mathbf{b}], \quad (42)$$

therefore we must have

$$\mathbf{b} = Q_1 \mathbf{z} + \rho \mathbf{q}_{n+1}. \quad (43)$$

Multiplying both members of the last equation for Q_1^T we find that:

$$Q_1^T \mathbf{b} = Q_1^T Q_1 \mathbf{z} + \rho Q_1^T \mathbf{q}_{n+1} = \mathbf{z} \quad (44)$$

where we used that the columns of Q_1 are orthonormal and \mathbf{q}_{n+1} is orthogonal to all the columns of Q_1 .

Now we consider the complete QR factorization of A_+ :

$$A_+ = QR = [Q_1 \ Q_2] \begin{bmatrix} R_1 & \mathbf{z} \\ \mathbf{0}^T & \rho \\ \mathbf{0} & \end{bmatrix} = [Q_1 R_1 \ Q_1 \mathbf{z} + Q_2(\rho, 0, \dots, 0)^T] \quad (45)$$

obtaining the relation

$$\mathbf{b} = Q_1 \mathbf{z} + Q_2(\rho, 0, \dots, 0)^T \quad (46)$$

and, therefore, multiplying both sides for Q_2^T :

$$Q_2^T \mathbf{b} = \rho(1, 0, \dots, 0)^T. \quad (47)$$

Now we define the residual \mathbf{r} as

$$\mathbf{r} = \mathbf{b} - A\mathbf{x}^* \quad (48)$$

where \mathbf{x}^* is the solution to the least square problem, and compute:

$$\|\mathbf{r}\|_2^2 = \|Q^T \mathbf{r}\|_2^2 = \left\| \begin{bmatrix} Q_1^T \mathbf{b} \\ Q_2^T \mathbf{b} \end{bmatrix} - \begin{bmatrix} Q_1^T A\mathbf{x}^* \\ Q_2^T A\mathbf{x}^* \end{bmatrix} \right\|_2^2 = \|Q_1^T \mathbf{b} - R_1 \mathbf{x}^*\|_2^2 + \|Q_2^T \mathbf{b}\|_2^2 \quad (49)$$

where we used the invariance of the 2-norm with respect to unitary transformations. Knowing that $\mathbf{x}^* = R_1^{-1} Q_1^T \mathbf{b}$ we obtain:

$$\|\mathbf{r}\|_2 = \|Q_2^T \mathbf{b}\|_2 = \|\rho(1, 0, \dots, 0)^T\|_2 = |\rho| \quad (50)$$

that concludes the proof. \square

Problem 3

(1) Let $A \in \mathbb{R}^{m \times n}$, with singular value decomposition $A = U\Sigma V^T = \sum_{i=1}^n \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n$ and $\text{rank}(A) = n$. Express the singular values and singular vectors of the following matrices in terms of those of A .

(a) $(A^T A)^{-1}$

$$(A^T A)^{-1} = (V^T)^{-1} \Sigma^{-2} V^{-1} = V \Sigma^{-2} V^{-1}$$

- Both left and right singular vectors of $(A^T A)^{-1}$ are equal to the right singular vectors of A ;
- Singular values of $(A^T A)^{-1}$ are equal to singular values of A raised to the -2 power.

(b) $(A^T A)^{-1} A^T$

$$(A^T A)^{-1} A^T = V \Sigma^{-2} V^T V \Sigma U^T = V \Sigma^{-1} U^{-1}$$

- Left singular vectors of $(A^T A)^{-1} A^T$ are equal to the right singular vectors of A ;
- Right singular vectors of $(A^T A)^{-1}$ are equal to the left singular vectors of A ;
- Singular values of $(A^T A)^{-1}$ are equal to the inverse of singular values of A .

(c) $A(A^T A)^{-1}$

$$A(A^T A)^{-1} = U \Sigma V^T V \Sigma^{-2} V^{-T} = U \Sigma^{-1} V^T$$

- Left and right singular vectors of $(A^T A)^{-1}$ coincide with that of A ;
- Singular values of $(A^T A)^{-1}$ are equal to the inverse of singular values of A .

(d) $A(A^T A)^{-1} A^T$

$$A(A^T A)^{-1} A^T = U \Sigma (V^T) V \Sigma^{-2} V^T V \Sigma U^T = \mathbb{1}$$

(2)

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 2 \end{bmatrix} \tag{51}$$

$$A^T A = \begin{bmatrix} 1 & 2 \\ 2 & 8 \end{bmatrix} \tag{52}$$

$$\det(A^T A - \lambda \mathbb{1}) = 0 \tag{53}$$

$$\lambda_{1,2} = \frac{9 \pm \sqrt{65}}{2} \tag{54}$$

$$k_2(A) = \frac{\sigma_{\max}}{\sigma_{\min}} = \sqrt{\frac{9 + \sqrt{65}}{9 - \sqrt{65}}} \tag{55}$$