Introduction to Machine Learning

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University of Science and Technology of China

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Notice, to get the full credits, please show your solutions step by step.

Exercise 1: 10pts

Show that $(1-\epsilon)^m \leq e^{-m\epsilon}$, where $m \in \mathbb{N}^+$ and $0 \leq \epsilon < 1$.

Solution: Let $f(x) = e^{-x}$. The first-order Taylor expansion of f at 0 with lagrangian remainder is

$$e^{-x} = 1 - x + \frac{1}{2!}e^{-\xi}x^2 \,(\text{assume } x \geq 0)$$

for some $\xi \in [0, x]$. Then for all $\epsilon \in [0, 1)$,

$$e^{-\epsilon} \geq 1 - \epsilon > 0.$$

Therefore, for all $m \in \mathbb{N}^+$, $\epsilon \in [0, 1)$,

$$(1-\epsilon)^m \leq e^{-m\epsilon}.$$

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Exercise 2: Markov inequality 10pts

Let X be a nonnegative random variable on $\mathbb{R}$. Then, for all $t > 0$, show that

$$\mathbf{P}(X \geq t) \leq \frac{\mathbf{E}[X]}{t}.$$

You can assume that X is a continuous random variable.

Solution: Let $f_X(x)$ be the probability density function of X. We have

$$\begin{aligned}
\mathbf{E}[X] &= \int_{-\infty}^{+\infty} x f_X(x) dx \\
&= \int_{0}^{+\infty} x f_X(x) dx \\
&= \int_{0}^{t} x f_X(x) dx + \int_{t}^{+\infty} x f_X(x) dx \\
&\geq \int_{t}^{+\infty} x f_X(x) dx \\
&\geq t \int_{t}^{+\infty} f_X(x) dx \\
&= t\, \mathbf{P}(X \geq t).
\end{aligned}$$

Thus,

$$\mathbf{P}(X \geq t) \leq \frac{\mathbf{E}[X]}{t}.$$

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Exercise 3: VC-dimension 10pts

Assume that the instance space $X = \mathbb{R}^2$ and the hypothesis space H be the set of all linear threshold functions defined on $\mathbb{R}^2$. Find $VC(H)$ and prove it.

Solution: We show that $VC(H) = 3$.

For convenience, we assume that the labels are -1 and 1, and $\text{sign}(0) \triangleq 1$.

Suppose that x is a sample, y is the corresponding label, and $\hat{y}$ is the predicted label. WLOG, we assume that x is a column vector in $\mathbb{R}^2$.

A linear classifier can be formulated as $\hat{y} = \text{sign}(w^T x + b)$, where $w \in \mathbb{R}^{2\times 1}$ and $b \in \mathbb{R}$. We can rewrite it as $\hat{y} = \text{sign}(\tilde{w}^T \tilde{x})$, where $\tilde{w} = [w; b]$ and $\tilde{x} = [x; 1]$.

Let x_1, x_2, x_3 be three different samples, then we can get the predicted labels

$$[\hat{y}_1, \hat{y}_1, \hat{y}_3] = \text{sign}(\tilde{w}^T [\tilde{x}_1, \tilde{x}_2, \tilde{x}_3]).$$

Since $X_1 \triangleq [\tilde{x}_1, \tilde{x}_2, \tilde{x}_3]$ is a 3×3 matrix, if $\mathbf{rank}(X_1) = 3$, then for any possible labels $[y_1, y_2, y_3]$, there exists a $\tilde{w}_0$, such that

$$[y_1, y_2, y_3] = \text{sign}(\tilde{w}_0^T [\tilde{x}_1, \tilde{x}_2, \tilde{x}_3]) = [\hat{y}_1, \hat{y}_2, \hat{y}_3].$$

That is, $VC(H) \geq 3$.

Let x_1, x_2, x_3, x_4 be four (not necessarily different) samples , then we can get the predicted labels

$$[\hat{y}_1, \hat{y}_2, \hat{y}_3, \hat{y}_4] = \text{sign}(\tilde{w}^T [\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \tilde{x}_4]).$$

Let $X_2 \triangleq [\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \tilde{x}_4]$. Since X_2 is a 3×4 matrix, $\mathbf{rank}(X_2) \leq 3 < 4$. We can write at least one of $\tilde{x}_i$ ($1 \leq i \leq 4$) as a linear combination of the other vectors. WLOG, we assume that $\tilde{x}_4 = \alpha_1 \tilde{x}_1 + \alpha_2 \tilde{x}_2 + \alpha_3 \tilde{x}_3$, where not all of α_i are zero. Then we have

$$\begin{aligned} \tilde{w}^T \tilde{x}_4 &= \tilde{w}^T (\alpha_1 \tilde{x}_1 + \alpha_2 \tilde{x}_2 + \alpha_3 \tilde{x}_3) \\ &= \alpha_1 (\tilde{w}^T \tilde{x}_1) + \alpha_2 (\tilde{w}^T \tilde{x}_2) + \alpha_3 (\tilde{w}^T \tilde{x}_3). \end{aligned}$$

Let the true labels

$$[y_1, y_2, y_3] \triangleq [\text{sign}(\alpha_1), \text{sign}(\alpha_2), \text{sign}(\alpha_3)].$$

If the classifier can correctly classify x_1, x_2 and x_3, then

$$[\text{sign}(\tilde{w}^T \tilde{x}_1), \text{sign}(\tilde{w}^T \tilde{x}_2), \text{sign}(\tilde{w}^T \tilde{x}_3)] = [\text{sign}(\alpha_1), \text{sign}(\alpha_2), \text{sign}(\alpha_3)].$$

Thus,

$$\alpha_i (\tilde{w}^T \tilde{x}_i) \geq 0,\ i = 1, 2, 3,$$

which implies that

$$\hat{y}_4 = [\text{sign}(\tilde{w}^T \tilde{x}_4)] = 1.$$

Now if we let the true label $y_4 = -1$, then there is a contradictory.

Thus, $VC(H) < 4$.

From the above all, we know that $VC(H) = 3$.

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Exercise 4: Learning intervals 20pts

Let the target concept class be $C = \{[a,b] : a < b, a, b \in \mathbb{R}\}$ and the hypotheses class $H = C$, and the version space be $VS_{H,D}$. Each $c \in C$ labels the points inside the interval positive and the others negative. A consistent learner will pick a consistent hypothesis—if any—$h \in H$ according to a set of i.i.d. samples $\{(x_1, c(x_1)), (x_2, c(x_2)), \ldots, (x_m, c(x_m))\}$ that obey an unknown absolute continuous distribution $\mathcal{D}$. $\mathcal{D}$'s p.d.f. is $p(x)$. Please find

$$\mathbf{P}[\exists\, h \in VS_{H,D} \text{ and } error_{\mathcal{D}}(h) > \epsilon],$$

and the corresponding sample complexity.

Solution: Let $\hat{a}$ and $\hat{b}$ be the estimation of a and b.

We define ϵ_1, ϵ_2 in the following way:

$$\epsilon_1 = \begin{cases} \int_a^{\hat{a}} p(x)\mathrm{d}x, \hat{a} \geq a \\ \int_{\hat{a}}^{a} p(x)\mathrm{d}x, \hat{a} < a \end{cases}$$

$$\epsilon_2 = \begin{cases} \int_b^{\hat{b}} p(x)\mathrm{d}x, \hat{b} \geq b \\ \int_{\hat{b}}^{b} p(x)\mathrm{d}x, \hat{b} < b \end{cases}$$

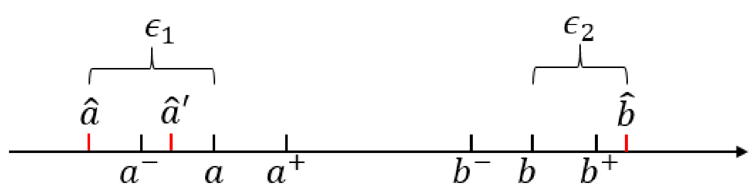
The event "$\exists\, h \in VS_{H,D}$ and $error_{\mathcal{D}}(h) > \epsilon$" is equivalent to the event "$\epsilon_1 + \epsilon_2 > \epsilon$". Note that "$\epsilon_1 + \epsilon_2 > \epsilon$" $\subset$ "$(\epsilon_1 > \frac{\epsilon}{2}) \vee (\epsilon_2 > \frac{\epsilon}{2})$" since "$(\epsilon_1 \leq \frac{\epsilon}{2}) \wedge (\epsilon_2 \leq \frac{\epsilon}{2})$" $\Rightarrow$ "$\epsilon_1 + \epsilon_2 \leq \epsilon$"
We have the following inequality:

$$\begin{aligned} \mathbf{P}[\exists\, h \in VS_{H,D} \text{ and } error_{\mathcal{D}}(h) > \epsilon] &= \mathbf{P}[\epsilon_1 + \epsilon_2 > \epsilon] \\ &\leq \mathbf{P}[\epsilon_1 > \tfrac{\epsilon}{2}] + \mathbf{P}[\epsilon_2 > \tfrac{\epsilon}{2}] \end{aligned}$$

We also define the a^+, a^-, b^+, b^- in the following way:

$$a^+ = \inf\{x \geq a : \int_a^x p(t)\mathrm{d}t \geq \frac{\epsilon}{2}\}; \quad a^- = \sup\{x \leq a : \int_x^a p(t)\mathrm{d}t \geq \frac{\epsilon}{2}\};$$

$$b^+ = \inf\{x \geq b : \int_b^x p(t)\mathrm{d}t \geq \frac{\epsilon}{2}\}; \quad b^- = \sup\{x \leq b : \int_x^b p(t)\mathrm{d}t \geq \frac{\epsilon}{2}\};$$



We also have the following conclusions, and the picture above may help you understand:

$$\text{“}\epsilon_1 > \frac{\epsilon}{2}\text{”} \subset \text{“}\textit{all samples} \notin [a^-, a^+]\text{”}$$

$$\text{“}\epsilon_2 > \frac{\epsilon}{2}\text{”} \subset \text{“}\textit{all samples} \notin [b^-, b^+]\text{”}$$

Thus we have the following inequalities:

$$\mathbf{P}[\epsilon_1 > \tfrac{\epsilon}{2}] \leq \mathbf{P}\left[\textit{all samples} \notin [a^-, a^+]\right]$$

$$\mathbf{P}[\epsilon_2 > \tfrac{\epsilon}{2}] \leq \mathbf{P}\left[\textit{all samples} \notin [b^-, b^+]\right]$$

Then according to the above inequalities, we will have:

$$\begin{aligned}
\mathbf{P}[\exists\, h \in VS_{H,D} \text{ and } error_{\mathcal{D}}(h) > \epsilon] &= \mathbf{P}[\epsilon_1 + \epsilon_2 > \epsilon] \\
&\leq \mathbf{P}[\epsilon_1 > \frac{\epsilon}{2}] + \mathbf{P}[\epsilon_2 > \frac{\epsilon}{2}] \\
&\leq \mathbf{P}\left[\textit{all samples} \notin [a^-, a^+]\right] + \mathbf{P}\left[\textit{all samples} \notin [b^-, b^+]\right] \\
&\leq 2e^{-m\frac{\epsilon}{2}} + 2e^{-m\frac{\epsilon}{2}} \\
&= 4e^{-m\frac{\epsilon}{2}}.
\end{aligned}$$

If let $4e^{-m\epsilon/2} \leq \delta$, then we have

$$m \geq \frac{2}{\epsilon} \ln \frac{4}{\delta}.$$

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Exercise 5: Basic Matrix Manipulations 20pts

For an arbitrary matrix M, we denote its i^{th} row, j^{th} column, and $(i,j)^{th}$ entry by $\mathbf{m}_{i,*}$, $\mathbf{m}_{*,j}$, and $m_{i,j}$, respectively.

1. Suppose that $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times d}$, $C \in \mathbb{R}^{d\times n}$, and $A = BC$. Show that

$$A = \sum_{\ell=1}^{d} \mathbf{b}_{*,\ell}\mathbf{c}_{\ell,*}.$$

2. Suppose that $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{m\times p}$, $C \in \mathbb{R}^{p\times q}$, $D \in \mathbb{R}^{q\times n}$, and $A = BCD$. Show that

$$A = \sum_{i=1}^{p}\sum_{j=1}^{q} c_{i,j}\mathbf{b}_{*,i}\mathbf{d}_{j,*}.$$

Solution:

1. Suppose that

$$\begin{aligned} B &= (\mathbf{b}_{*,1}, \mathbf{b}_{*,2}, \dots, \mathbf{b}_{*,d}), \\ C &= (\mathbf{c}_{1,*}^\top, \mathbf{c}_{2,*}^\top, \dots, \mathbf{c}_{d,*}^\top)^\top. \end{aligned}$$

Suppose that

$$\begin{aligned} A &= BC \\ &= \sum_{\ell=1}^{d} \mathbf{b}_{*,\ell}\mathbf{c}_{\ell,*}. \end{aligned}$$

2. Suppose that

$$\begin{aligned} B &= (\mathbf{b}_{*,1}, \mathbf{b}_{*,2}, \dots, \mathbf{b}_{*,p}), \\ D &= (\mathbf{d}_{1,*}^\top, \mathbf{d}_{2,*}^\top, \dots, \mathbf{d}_{q,*}^\top)^\top. \end{aligned}$$

Then

$$
\begin{aligned}
A &= BCD \\
&= (\mathbf{b}_{*,1}, \mathbf{b}_{*,2}, \ldots, \mathbf{b}_{*,p}) \begin{bmatrix} c_{1,1} & \ldots & c_{1,q} \\ \ldots & \ldots & \ldots \\ c_{p,1} & \ldots & c_{p,q} \end{bmatrix} (\mathbf{d}_{1,*}^\top, \mathbf{d}_{2,*}^\top, \ldots, \mathbf{d}_{q,*}^\top)^\top \\
&= (\sum_{i=1}^{p} \mathbf{b}_{*,i} c_{i,1}, \ldots, \sum_{i=1}^{p} \mathbf{b}_{*,i} c_{i,q})(\mathbf{d}_{1,*}^\top, \mathbf{d}_{2,*}^\top, \ldots, \mathbf{d}_{q,*}^\top)^\top \\
&= \sum_{j=1}^{q} \sum_{i=1}^{p} \mathbf{b}_{*,i} c_{i,j} \mathbf{d}_{j,*} \\
&= \sum_{i=1}^{p} \sum_{j=1}^{q} c_{i,j} \mathbf{b}_{*,i} \mathbf{d}_{j,*}.
\end{aligned}
$$

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Exercise 6: Subspace 90pts

The column space of a matrix $A \in \mathbb{R}^{m\times n}$ is the set

$$\mathcal{C}(A) = \{\mathbf{y} \in \mathbb{R}^m : \mathbf{y} = A\mathbf{x}, \mathbf{x} \in \mathbb{R}^n\}. \tag{1}$$

1. Let $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{n\times p}$, and $C = AB$.
   (a) Show that $\mathcal{C}(C) \subseteq \mathcal{C}(A)$.
   (b) Suppose that B is nonsingular, that is, B is invertible. Show that $\mathcal{C}(C) = \mathcal{C}(A)$.
2. Suppose that $A \in \mathbb{R}^{m\times n}$ has full column rank, that is, the column vectors in A are linearly independent. Let $\mathbf{x} \in \mathbb{R}^m$ and

$$P_{\mathcal{C}(A)}(\mathbf{x}) := \mathop{\mathbf{argmin}}_{\mathbf{z}\in\mathbb{R}^m} \{\|\mathbf{x}-\mathbf{z}\|_2 : \mathbf{z} \in \mathcal{C}(A)\}. \tag{2}$$

   (a) Is $P_{\mathcal{C}(A)}$ unique? If so, please justify your answer and find $P_{\mathcal{C}(A)}$; otherwise, please find all the projections.
   (b) What are the coordinates of $P_{\mathcal{C}(A)}$ with respect to the column vectors in A? Are the coordinates unique?
3. Suppose that the column vectors in $A \in \mathbb{R}^{m\times n}$ are orthonormal.
   (a) Please answer the questions in 2.
   (b) Suppose that the column vectors in $\widetilde{A} \in \mathbb{R}^{m\times n}$ are also orthonormal, and $\mathcal{C}(A) = \mathcal{C}(\widetilde{A})$. Show that $P_{\mathcal{C}(A)}(\mathbf{x}) = P_{\mathcal{C}(\widetilde{A})}(\mathbf{x})$ for any $\mathbf{x} \in \mathbb{R}^m$.
4. Suppose that the column vectors in $A \in \mathbb{R}^{m\times n}$ are linearly dependent.
   (a) Is $P_{\mathcal{C}(A)}$ unique? If so, please justify your answer; otherwise, please find all the projections.
   (b) Are the coordinates of $P_{\mathcal{C}(A)}$ with respect to the column vectors in A unique? If so, please justify your answer; otherwise, please find all the possible coordinates.

   Hint: you may assume that the first r column vectors with $r < n$ are a basis of $\mathcal{C}(A)$.

Solution: 1. (a) Suppose that $A = (\mathbf{a}_1, \dots, \mathbf{a}_n)$ and

$$B = \begin{bmatrix} b_{11} & \dots & b_{1p} \\ \dots & \dots & \dots \\ b_{n1} & \dots & b_{np} \end{bmatrix}.$$

Then

$$\begin{aligned} C &= AB \\ &= (\sum_{i=1}^n b_{i1}\mathbf{a}_i, \dots, \sum_{i=1}^n b_{ip}\mathbf{a}_i). \end{aligned}$$

For all $\mathbf{v} \in \mathcal{C}(C)$, there exist $d_1, \ldots, d_p$ such that

$$\begin{aligned}\mathbf{v} &= \sum_{j=1}^{p} d_j (\sum_{i=1}^{n} b_{ij} \mathbf{a}_i) \\ &= \sum_{i=1}^{n} (\sum_{j=1}^{p} d_j b_{ij}) \mathbf{a}_i.\end{aligned}$$

Thus, $\mathbf{v} \in \mathcal{C}(A)$, i.e. $\mathcal{C}(C) \subseteq \mathcal{C}(A)$.

(b) We have proven that $\mathcal{C}(C) \subseteq \mathcal{C}(A)$.
We next show that $\mathcal{C}(A) \subseteq \mathcal{C}(C)$. As $C = AB$ and B is invertible,

$$A = CB^{-1}.$$

Then it is easy to show that

$$\mathcal{C}(A) \subseteq \mathcal{C}(C).$$

Therefore, $\mathcal{C}(C) = \mathcal{C}(A)$.

2. (a) $P_{\mathcal{C}(A)}$ is unique.
We first show that $P_{\mathcal{C}(A)}$ is unique. Suppose that there exist two different points $\mathbf{z}_1, \mathbf{z}_2 \in \mathcal{C}(A)$ such that

$$\|\mathbf{x} - \mathbf{z}_1\|_2 = \|\mathbf{x} - \mathbf{z}_2\|_2 = \min_{\mathbf{z} \in \mathcal{C}(A)} \|\mathbf{x} - \mathbf{z}\|_2$$

Let $\mathbf{z_0} = \frac{\mathbf{z}_1 + \mathbf{z}_2}{2}$, then

$$\begin{aligned}\|\mathbf{x} - \frac{\mathbf{z}_1 + \mathbf{z}_2}{2}\|_2^2 &< \|\mathbf{x} - \mathbf{z}_1\|_2^2 \\ \text{and } \frac{\mathbf{z}_1 + \mathbf{z}_2}{2} &\in \mathcal{C}(A).\end{aligned}$$

which leads to a contradiction. Thus, $P_{\mathcal{C}(A)}$ is unique.
We next find $P_{\mathcal{C}(A)}$.
Assume that $\{\mathbf{a}_1, \ldots, \mathbf{a}_n, \mathbf{a}_{n+1}, \ldots, \mathbf{a}_m\}$ is a basis of $\mathbb{R}^m$, where $\langle \mathbf{a}_i, \mathbf{a}_j \rangle = 0$ for all $1 \leq i \leq n$ and $n+1 \leq j \leq m$. For all $\mathbf{y} \in \mathcal{C}(\mathbf{A})$, there exist $\lambda_y^i \in \mathbb{R}$, such that $\mathbf{y} = \sum_{i=1}^{n} \lambda_y^i \mathbf{a}_i$. For all $\mathbf{x} \in \mathbb{R}^m$, there exist $\lambda_x^i \in \mathbb{R}$, such that $\mathbf{x} = \sum_{i=1}^{m} \lambda_x^i \mathbf{a}_i$. Let $\boldsymbol{\lambda}_x = \left(\lambda_x^1, \ldots, \lambda_x^m\right)^\top$. Then, $\mathbf{x} = A\boldsymbol{\lambda}_x$ and $\boldsymbol{\lambda}_x = \left(A^T A\right)^{-1} A^T \mathbf{x}$.

Suppose that $\mathbf{z} = P_{\mathcal{C}(A)}(\mathbf{x})$, then

$$\begin{aligned}\|\mathbf{x}-\mathbf{z}\|_2^2 &= \|\sum_{i=1}^{m}\lambda_x^i\mathbf{a}_i - \sum_{i=1}^{n}\lambda_z^i\mathbf{a}_i\|_2^2\\ &= \min_{\lambda_y^i\in\mathbb{R}}\|\sum_{i=1}^{m}\lambda_x^i\mathbf{a}_i - \sum_{i=1}^{n}\lambda_y^i\mathbf{a}_i\|_2^2\\ &= \min_{\lambda_y^i\in\mathbb{R}}\|\sum_{i=1}^{n}(\lambda_x^i-\lambda_y^i)\mathbf{a}_i + \sum_{i=n+1}^{m}\lambda_x^i\mathbf{a}_i\|_2^2\\ &= \min_{\lambda_y^i\in\mathbb{R}}\|\sum_{i=1}^{n}(\lambda_x^i-\lambda_y^i)\mathbf{a}_i\|_2^2 + \|\sum_{i=n+1}^{m}\lambda_x^i\mathbf{a}_i\|_2^2\end{aligned}$$

where the last equality holds for $\langle\mathbf{a}_i,\mathbf{a}_j\rangle = 0$, $1\le i\le n$ and $n+1\le j\le m$. It's clear that $\lambda_z^i = \lambda_x^i$, $i=1,...,n$, i.e.,

$$\begin{aligned}\mathbf{z} &= A\boldsymbol{\lambda}_z\\ &= A\boldsymbol{\lambda}_x\\ &= A(A^TA)^{-1}A^T\mathbf{x}\end{aligned}$$

Hence we know that $P_{\mathcal{C}(A)} = A(A^TA)^{-1}A^T$.

(b) The coordinates are unique.
For all $\mathbf{x}\in\mathbb{R}^m$,

$$P_{\mathcal{C}(A)}(\mathbf{x}) = A(A^\top A)^{-1}A^\top\mathbf{x},$$

which is a vector in $\mathbb{R}^m$. Suppose that $\alpha = (\alpha_1,\ldots,\alpha_n)^\top$ are the coordinates of $P_{\mathcal{C}(A)}(\mathbf{x})$ with respect to the column vectors in A, then

$$\begin{aligned}&A\alpha = A(A^\top A)^{-1}A^\top\mathbf{x}\\ \Rightarrow &A(\alpha-(A^\top A)^{-1}A^\top\mathbf{x}) = \mathbf{0}\end{aligned}$$

Since A has full column rank,

$$\alpha = (A^\top A)^{-1}A^\top\mathbf{x}.$$

3. (a) It follows from Exercise 6.2 that

$$P_{\mathcal{C}(A)} = A(A^\top A)^{-1}A^\top$$

and

$$\alpha = (A^\top A)^{-1}A^\top\mathbf{x}.$$

Since the column vectors in A are orthonormal,

$$A^\top A = I.$$

Thus,

$$P_{\mathcal{C}(A)} = AA^\top$$

and

$$\alpha = A^\top \mathbf{x}$$

(b) We can prove that $P_{\mathcal{C}(A)}(x) = P_{\mathcal{C}(\tilde{A})}(x)$ in the same way as 2.(a).
Suppose that there exist two different points $\mathbf{z}_1, \mathbf{z}_2 \in \mathcal{C}(A)$ such that

$$\|\mathbf{x} - \mathbf{z}_1\|_2 = \|\mathbf{x} - \mathbf{z}_2\|_2 = \min_{\mathbf{z} \in \mathcal{C}(A)} \|\mathbf{x} - \mathbf{z}\|_2$$

Let $\mathbf{z_0} = \frac{\mathbf{z}_1+\mathbf{z}_2}{2}$, then

$$\|\mathbf{x} - \frac{\mathbf{z}_1 + \mathbf{z}_2}{2}\|_2^2 < \|\mathbf{x} - \mathbf{z}_1\|_2^2$$
$$\text{and } \frac{\mathbf{w}_1 + \mathbf{w}_2}{2} \in \mathcal{C}(A).$$

This is a contradiction. Thus, $P_{\mathcal{C}(A)}(x) = P_{\mathcal{C}(\tilde{A})}(x)$.

4. (a) The uniqueness comes from Exercise 6.2.
We next find the projection. Suppose that $\mathbf{rank}(A) = r$ and the first r columns of A are linearly independent. Let $A = (\mathbf{a}_1, \dots, \mathbf{a}_n)$ and $A_r = (\mathbf{a}_1, \dots, \mathbf{a}_r)$. Then

$$\mathcal{C}(A) = \mathcal{C}(A_r)$$

and $A_r \in \mathbb{R}^{m \times r}$ has full column rank. Then

$$\begin{aligned} P_{\mathcal{C}(A)} &= P_{\mathcal{C}(A_r)} \\ &= A_r (A_r^\top A_r)^{-1} A_r^\top. \end{aligned}$$

(b) They may not be unique.
For example, if $A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}$, then for $\mathbf{x} = (3, 3)^T$, we know that $(3, 3, 0)^T$ and $(0, 0, 3)^T$ are two possible coordinates.

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Exercise 7: SVD 80pts

Let $A \in \mathbb{R}^{m\times n}$, $\mathbf{rank}(A) = r$, its SVD be $A = U\Sigma V^\top$, where we sort the diagonal entries of Σ in the descending order $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$, and

$$U_1 = (\mathbf{u}_{*,1}, \mathbf{u}_{*,2}, \ldots, \mathbf{u}_{*,r}), U_2 = (\mathbf{u}_{*,r+1}, \ldots, \mathbf{u}_{*,m}),$$
$$V_1 = (\mathbf{v}_{*,1}, \mathbf{v}_{*,2}, \ldots, \mathbf{v}_{*,r}), V_2 = (\mathbf{v}_{*,r+1}, \ldots, \mathbf{u}_{*,n}).$$

We define the column space of a matrix A in (3). The null space of A is the set

$$\mathcal{N}(A) = \{\mathbf{y} \in \mathbb{R}^n : A\mathbf{y} = 0\}. \tag{3}$$

1. Show that
   (a) $P_{\mathcal{C}(A)}(\mathbf{x}) = U_1 U_1^\top \mathbf{x}$;
   (b) $P_{\mathcal{N}(A)}(\mathbf{x}) = V_2 V_2^\top \mathbf{x}$;
   (c) $P_{\mathcal{C}(A^\top)}(\mathbf{x}) = V_1 V_1^\top \mathbf{x}$;
   (d) $P_{\mathcal{N}(A^\top)}(\mathbf{x}) = U_2 U_2^\top \mathbf{x}$.
2. The Frobenius norm of A is
$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} a_{i,j}^2}.$$
   (a) Show that $\|A\|_F^2 = \mathbf{tr}\,(A^\top A)$.
   (b) Let $B \in \mathbb{R}^{m\times n}$. Suppose that $\mathcal{C}(A) \perp \mathcal{C}(B)$, that is,
$$\langle \mathbf{a}, \mathbf{b}\rangle = 0, \forall\, \mathbf{a} \in \mathcal{C}(A),\, \mathbf{b} \in \mathcal{C}(B).$$
   Show that
$$\|A + B\|_F^2 = \|A\|_F^2 + \|B\|_F^2.$$
3. Please solve the problem as follows.
$$\min_{X\in\mathbb{R}^{m\times n}} \{\|A - X\|_F : \mathbf{rank}(X) \leq K\}. \tag{4}$$
   For simplicity, you can assume that all singular values of A are different.
4. **Programming Exercise** We provide you a grayscale image ("Alan_Turing.jpg"). Suppose that A is the data matrix of the image. We have $A \in \mathbb{R}^{512\times 512}$ and $r = \mathbf{rank}(A) = 512$. In this exercise, you are expected to implement an image compression algorithm following the steps below. You can use your favorite programming language.
   (a) Compute the SVD $A = U\Sigma V^\top = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$, where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ are the diagonal entries of Σ, $\mathbf{u}_i$ is the ith column of U, and $\mathbf{v}_i$ is the ith column of V.

(b) Use the first k ($k < r$) terms of SVD to approximate the original image A. Then, we get the compressed images, of which the data matrices are $A_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$. Compute A_k for $k = 2, 4, 8, 16, 32, 64, 128, 256$.

(c) Plot A_k as images for all k.

Please put the compressed images and their corresponding k in this file.

Solution: 1. (a) We first show that

$$\mathcal{C}(A) = \mathcal{C}(U_1).$$

Let $\Sigma_r = \operatorname{diag}(\sigma_1, \ldots, \sigma_r)$, then we have

$$\begin{aligned} A &= U\Sigma V^\top \\ &= U_1 \Sigma_r V_1^\top \\ \Rightarrow U_1 &= AV_1\Sigma_r^{-1}. \end{aligned}$$

It follows from $A = U_1\Sigma_r V_1^\top$ that $\mathcal{C}(A) \subseteq \mathcal{C}(U_1)$. And it follows from $U_1 = AV_1\Sigma_r^{-1}$ that $\mathcal{C}(U_1) \subseteq \mathcal{C}(A)$.
Thus, $\mathcal{C}(A) = \mathcal{C}(U_1)$. Therefore,

$$\begin{aligned} P_{\mathcal{C}(A)}(\mathbf{x}) &= P_{\mathcal{C}(U_1)}(\mathbf{x}) \\ &= U_1(U_1^\top U_1)^{-1}U_1^\top \mathbf{x} \\ &= U_1 U_1^\top \mathbf{x}. \end{aligned}$$

(b) Similarly, we show that

$$\mathcal{N}(A) = \mathcal{C}(V_2).$$

As

$$\begin{aligned} AV &= U\Sigma \\ \Rightarrow AV_2 &= \mathbf{0}, \end{aligned}$$

$\mathbf{v}_{*,i} \in \mathcal{N}(A)$, $i = r+1, \ldots, n$. Since $\dim(\mathcal{N}(A)) = n - \mathbf{rank}(A) = n - r$ and $(\mathbf{v}_{*,r+1}, \mathbf{v}_{*,r+2}, \ldots, \mathbf{v}_{*,n})$ are linearly independent, $(\mathbf{v}_{*,r+1}, \mathbf{v}_{*,r+2}, \ldots, \mathbf{v}_{*,n})$ is a basis of $\mathcal{N}(A)$, i.e. $\mathcal{C}(V_2) = \mathcal{N}(A)$. Thus, it follows from Exercise 6.2 that

$$\begin{aligned} P_{\mathcal{N}(A)}(\mathbf{x}) &= P_{\mathcal{C}(V_2)}(\mathbf{x}) \\ &= V_2(V_2^\top V_2)^{-1}V_2^\top \mathbf{x} \\ &= V_2 V_2^\top \mathbf{x}. \end{aligned}$$

(c) Similarly, we can prove that

$$\mathcal{C}(A^\top) = \mathcal{C}(V_1).$$

Thus,

$$\begin{aligned}P_{\mathcal{C}(A^\top)}(\mathbf{x}) &= P_{\mathcal{C}(V_1)}(\mathbf{x})\\ &= V_1V_1^\top\mathbf{x}.\end{aligned}$$

(d) Similarly, we can prove that

$$\mathcal{N}(A^\top) = \mathcal{C}(U_2).$$

Thus,

$$\begin{aligned}P_{\mathcal{N}(A^\top)}(\mathbf{x}) &= P_{\mathcal{C}(U_2)}(\mathbf{x})\\ &= U_2U_2^\top\mathbf{x}.\end{aligned}$$

2. (a) Letting $A = (\mathbf{a}_{*,1}, \dots, \mathbf{a}_{*,n})$, we have

$$A^\top A = \begin{bmatrix} \mathbf{a}_{*,1}^\top\mathbf{a}_{*,1} & \dots & \mathbf{a}_{*,1}^\top\mathbf{a}_{*,n}\\ \dots & \dots & \dots\\ \mathbf{a}_{*,n}^\top\mathbf{a}_{*,1} & \dots & \mathbf{a}_{*,n}^\top\mathbf{a}_{*,n}\end{bmatrix}.$$

Thus,

$$\begin{aligned}\mathbf{tr}\,(A^\top A) &= \sum_{j=1}^n \mathbf{a}_{*,j}^\top\mathbf{a}_{*,j}\\ &= \sum_{j=1}^n\sum_{i=1}^m a_{i,j}^2\\ &= \|A\|_F^2.\end{aligned}$$

(b) As $\mathcal{C}(A)\perp\mathcal{C}(B)$,

$$A^\top B = 0 \text{ and } B^\top A = 0.$$

Thus,

$$\begin{aligned}\|A+B\|_F^2 &= \mathbf{tr}\,((A+B)^\top(A+B))\\ &= \mathbf{tr}\,(A^\top A) + \mathbf{tr}\,(B^\top B) + \mathbf{tr}\,(A^\top B) + \mathbf{tr}\,(B^\top A)\\ &= \mathbf{tr}\,(A^\top A) + \mathbf{tr}\,(B^\top B)\\ &= \|A\|_F^2 + \|B\|_F^2.\end{aligned}$$

3. (a) **Solution 1:** Assume that all singular values of A are different. Note that $\mathbf{rank}(A) = r$. Suppose $A^* \in \mathbb{R}^{m\times n}$ is an optimal solution to the problem (4).
If $K \geq r$, it is trival that $A^* = A$.
If $K < r$, suppose $X = WY$, where $W \in \mathbb{R}^{m\times K}$, $W^\top W = I$,and $Y = (\mathbf{y}_1, \dots, \mathbf{y}_n) \in \mathbb{R}^{K\times n}$. Clearly, $\mathcal{C}(X) \subset \mathcal{C}(W)$.

Let $A = (\mathbf{a}_1, \dots, \mathbf{a}_n)$. The problem (4) can be formulated as

$$\begin{aligned}
&\min_{W,Y} \{\|A - WY\|_F^2 : W^\top W = I, W \in \mathbb{R}^{m \times K}\} \\
= &\min_{W \in \mathbb{R}^{m \times K}} \min_{Y \in \mathbb{R}^{K \times n}} \{\|A - WY\|_F^2 : W^\top W = I\} \\
= &\min_{W \in \mathbb{R}^{m \times K}} \min_{\mathbf{y}_1, \dots, \mathbf{y}_n \in \mathbb{R}^K} \{\sum_{i=1}^n \|\mathbf{a}_i - W\mathbf{y}_i\|_2^2 : W^\top W = I\} \\
= &\min_{W \in \mathbb{R}^{m \times K}} \sum_{i=1}^n \min_{\mathbf{y}_i \in \mathbb{R}^K} \{\|\mathbf{a}_i - W\mathbf{y}_i\|_2^2 : W^\top W = I\}
\end{aligned}$$

Let $\mathbf{z}_i = W\mathbf{y}_i$. Note that the solution to the subproblem $\min_{\mathbf{z}_i \in \mathbb{R}^m} \{\|\mathbf{a}_i - \mathbf{z}_i\|_2^2 : \mathbf{z}_i \in \mathcal{C}(W), W^\top W = I\}$ is the projection of the point $\mathbf{a}_i$ onto $\mathcal{C}(W)$. It follows from Exercise 6.3 that

$$P_{\mathcal{C}(W)}(\mathbf{a}_i) = WW^\top \mathbf{a}_i.$$

Hence the problem (4) becomes

$$\min_{W} \{\|A - WW^\top A\|_F^2 : W^\top W = I, W \in \mathbb{R}^{m \times K}\} \tag{5}$$

Note that

$$\begin{aligned}
\|A - WW^\top A\|_F^2 &= \mathbf{tr}\,((A - WW^\top A)^\top (A - WW^\top A)) \\
&= 2\,\mathbf{tr}\,(A^\top A) - 2\,\mathbf{tr}\,(A^\top WW^\top A) \\
&= 2\,\mathbf{tr}\,(V\Sigma^\top \Sigma V^\top) - 2\,\mathbf{tr}\,(W^\top U\Sigma\Sigma^\top U^\top W).
\end{aligned}$$

Letting $Q = U^\top W = (\mathbf{q}_1, \dots, \mathbf{q}_K)$, the problem (5) becomes

$$\begin{aligned}
\max_{Q \in \mathbb{R}^{m \times K}} \quad & \mathbf{tr}\,(Q^\top \Sigma\Sigma^\top Q) \\
\text{s.t.} \quad & Q^\top Q = I.
\end{aligned} \tag{6}$$

We have

$$\begin{aligned}
\mathbf{tr}\,(Q^\top \Sigma\Sigma^\top Q) &= \sum_{j=1}^K \mathbf{q}_j^\top \Sigma\Sigma^\top \mathbf{q}_j \\
&= \sum_{j=1}^K \sum_{i=1}^r \sigma_i^2 q_{i,j}^2 \\
&= \sum_{i=1}^r \sigma_i^2 \sum_{j=1}^K q_{i,j}^2,
\end{aligned}$$

where $q_{i,j}$ is the entry in the i^{th} row, j^{th} column of Q. Denote

$$\alpha_i = \sum_{j=1}^{K} q_{i,j}^2, i = 1, \ldots, m.$$

We can see that

$$\begin{aligned} &\alpha_i \in [0, 1], i = 1, \ldots, m, \\ &\sum_{i=1}^{m} \alpha_i = K. \end{aligned} \tag{7}$$

Thus, we consider the following problem

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^m} \ &\sum_{i=1}^{r} \alpha_i \sigma_i^2 \\ \text{s.t.} \ \ &\alpha_i \in [0, 1], i = 1, \ldots, m, \\ &\sum_{i=1}^{m} \alpha_i = K. \end{aligned} \tag{8}$$

Let Q^* be a solution to problem (6) and α^* be a solution to problem (8) respectively. Notice that $\mathbf{tr}\left((Q^*)^\top \Sigma\Sigma^\top Q^*\right) \leq (\alpha^*)^\top \Sigma\Sigma^\top \alpha^*)$.
Since $\sigma_1^2 \geq \sigma_2^2 \geq \ldots, \geq \sigma_r^2$, $\alpha^* = (\alpha_1^*, \ldots, \alpha_m^*)^\top$ is a solution to problem (8) with

$$\alpha_i^* = \begin{cases} 1 & i = 1, \ldots, K, \\ 0 & i = K+1, \ldots, m. \end{cases} \tag{9}$$

In view of Eq. (7) and (9), we can see that the last $m - K$ entries of $\mathbf{q}_i^*$ are 0 for all $i = 1, \ldots, K$, that is

$$Q^* = \begin{pmatrix} \tilde{Q}^* \\ 0 \end{pmatrix}_{m \times K},$$

where

$$\tilde{Q}^* \in \mathbb{R}^{K \times K} \ \text{ and } \ (\tilde{Q}^*)^\top \tilde{Q}^* = I.$$

We can see that $\mathbf{tr}\left((Q^*)^\top \Sigma\Sigma^\top Q^*\right) = (\alpha^*)^\top \Sigma\Sigma^\top \alpha^*)$.
Therefore, the solution to problem (4) is

$$\begin{aligned} A^* &= W^*(W^*)^\top A \\ &= UQ^*(Q^*)^\top U^\top A \\ &= U\Sigma_k V^\top, \end{aligned}$$

where $\Sigma_k = \text{diag}(\sigma_1, \ldots, \sigma_K, 0, \ldots, 0)$

(b) **Solution 2:** Assume that all singular values of A are different, and suppose $S \in \mathbb{R}^{m\times n}$ is an optimal solution. Note that $\mathbf{rank}(A) = r$.

If $K \geq r$, it is trival that $S = A$.

If $K < r$, let $A' = U\Sigma' V^T$, where $\Sigma' = \begin{bmatrix} \Sigma_K & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{m\times n}$, $\Sigma_K = \text{diag}(\sigma_1, ..., \sigma_K)$. Then we have

$$\|A - A'\|_F = (\sigma_{K+1}^2 + ... + \sigma_r^2)^{\frac{1}{2}} \geq \|A - S\|_F$$

Now we prove that $\|A - S\|_F \geq \|A - A'\|_F$:

Suppose that

$$X = Q\Omega P^T,$$

where $QQ^\top = I$, $PP^\top = I$, $\Omega = \begin{bmatrix} \Omega_K & 0 \\ 0 & 0 \end{bmatrix}$, and $\Omega_K = \text{diag}(\omega_1, ..., \omega_K)$. Let $B = Q^T AP$. Then $A = QBP^T$. Thus,

$$\|A - S\|_F = \|Q(B - \Omega)P^T\|_F = \|B - \Omega\|_F.$$

Block the matrix

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix},$$

where $B_{11} \in \mathbb{R}^{K\times K}$, $B_{12} \in \mathbb{R}^{K\times(n-K)}$, $B_{21} \in \mathbb{R}^{(m-K)\times K}$, $B_{22} \in \mathbb{R}^{(m-K)\times(n-K)}$. Then by the definition of Frobenius norm, we have

$$\|A - S\|_F^2 = \|B_{11} - \Omega_K\|_F^2 + \|B_{12}\|_F^2 + \|B_{21}\|_F^2 + \|B_{22}\|_F^2.$$

Firstly, we prove that $B_{12} = 0$ and $B_{21} = 0$ by contradiction.

Suppose that $B_{12} \neq 0$, then let

$$Y = Q \begin{bmatrix} B_{11} & B_{12} \\ 0 & 0 \end{bmatrix} P^T.$$

Note that $\mathbf{rank}(Y) \leq K$. And

$$\|A - Y\|_F^2 = \|B_{21}\|_F^2 + \|B_{22}\|_F^2 < \|A - S\|_F^2,$$

which leads to a contradiction. Similarly, $B_{21} = 0$.

Next, we show $B_{11} = \Omega_K$. Suppose that $B_{11} \neq \Omega_K$. Let

$$Z = Q \begin{bmatrix} B_{11} & 0 \\ 0 & 0 \end{bmatrix} P^T$$

and note that $\mathbf{rank}(Z) \leq K$. Then

$$\begin{aligned}\|A - Z\|_F^2 = \|B_{22}\|_F^2 \leq \|B_{11} - \Omega_K\|_F^2 + \|B_{22}\|_F^2 = \|A - S\|_F^2 \\ \Rightarrow B_{11} = \Omega_K.\end{aligned}$$

Finally, we find B_{22}. Take SVD for B_{22}, i.e.

$$B_{22} = U_1 \Lambda V_1^T.$$

Now we prove the diagonal entries of Λ are A's singular values. Let

$$\begin{aligned}U_2 &= \begin{bmatrix} I_K & 0 \\ 0 & U_1 \end{bmatrix}, \\ V_2 &= \begin{bmatrix} I_K & 0 \\ 0 & V_1 \end{bmatrix}.\end{aligned}$$

Note that

$$\begin{aligned}U_2^T Q^T A P V_2 = \begin{bmatrix} \Omega_K & 0 \\ 0 & \Lambda \end{bmatrix}, \\ \Rightarrow A = (QU_2) \begin{bmatrix} \Omega_K & 0 \\ 0 & \Lambda \end{bmatrix} (PV_2)^T.\end{aligned}$$

which implies that the diagonal entries of Λ are A's singular values. Hence

$$\|A - S\|_F = \|\Lambda\|_F \geq (\sigma_{K+1}^2 + ... + \sigma_r^2)^{\frac{1}{2}}$$

which completes the proof.
Therefore,

$$\min_{X \in \mathbb{R}^{m \times n}} \{\|A - X\|_F : \mathbf{rank}(X) \leq K\} = \begin{cases} 0, & K \geq r \\ (\sigma_{K+1}^2 + \cdots + \sigma_r^2)^{\frac{1}{2}}, & K < r. \end{cases}$$

4.

■

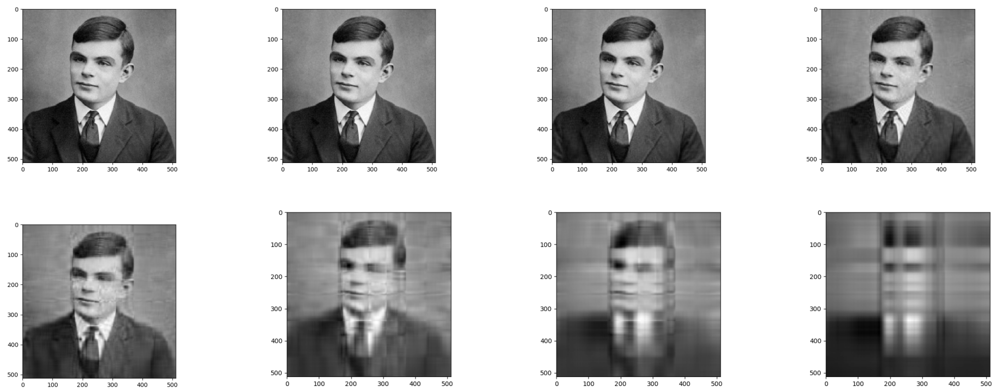

Figure 1: Grayscale images. The number of K decreases from left to right.

Exercise 8: PCA 60pts

Suppose that we have a set of data instances $\{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^d$. Let $\widetilde{X} \in \mathbb{R}^{d\times n}$ be the matrix whose i^{th} column is $\mathbf{x}_i - \bar{\mathbf{x}}$, where $\bar{\mathbf{x}}$ is the sample mean, and S be the sample variance matrix.

1. For $G \in \mathbb{R}^{d\times K}$, let us define

$$f(G) = \mathbf{tr}\,(G^\top S G). \tag{10}$$

   Show that $f(GQ) = f(G)$ for any orthogonal matrix $Q \in \mathbb{R}^{K\times K}$.

2. Please find $\mathbf{g}_1$ defined as follows by the Lagrange multiplier method.

$$\mathbf{g}_1 := \underset{\mathbf{g}\in\mathbb{R}^d}{\mathbf{argmax}}\{f(\mathbf{g}) : \|\mathbf{g}\|_2 = 1\}, \tag{11}$$

   where f is defined by (10). Notice that, the vector $\mathbf{g}_1$ is the first principle component vector of the data.

3. Please find $\mathbf{g}_2$ defined as follows by the Lagrange multiplier method.

$$\mathbf{g}_2 := \underset{\mathbf{g}\in\mathbb{R}^d}{\mathbf{argmax}}\{f(\mathbf{g}) : \|\mathbf{g}\|_2 = 1, \langle \mathbf{g}, \mathbf{g}_1\rangle = 0\}, \tag{12}$$

   where $\mathbf{g}_1$ is given by (11). Similar to $\mathbf{g}_1$, the vector $\mathbf{g}_2$ is the second principle component vector of the data.

4. Please derive the first K principle component vectors by repeating the above process.

5. What is $f(\mathbf{g}_k)$, $k = 1, \ldots, K$? What about their meaning?

6. When the first K principle component vectors are unique?

Solution: 1. Since $\mathbf{tr}\ (AB) = \mathbf{tr}\ (BA)$, we have

$$\begin{aligned} f(GQ) &= \mathbf{tr}\,(Q^\top G^\top SGQ) \\ &= \mathbf{tr}\,(QQ^\top G^\top SG) \\ &= \mathbf{tr}\,(G^\top SG) \\ &= f(G), \end{aligned}$$

which completes the proof.

2. Suppose $\tilde{X} = U\Sigma V^\top$, where $\Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \sigma_r & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{d\times n}$, assume $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_r > 0$. Thus

$$S = \frac{1}{n-1}\tilde{X}\tilde{X}^\top = \frac{1}{n-1}U\Sigma\Sigma^\top U^\top = \frac{1}{n-1}U\Sigma_d^2 U^\top,$$

where $\Sigma_d = \mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_r, 0, \cdots, 0) \in \mathbb{R}^{d\times d}$.

We have

$$f(G) = \mathbf{tr}\ (\frac{1}{n-1}G^\top U\Sigma_d^2 U^\top G).$$

Let $Q = U^\top G$, and we have $Q^\top Q = I$. Hence the problem becomes

$$\begin{aligned} &\max_{\mathbf{q}\in\mathbb{R}^d} \mathbf{tr}\ (\mathbf{q}^\top \Sigma_d^2 \mathbf{q}), \\ &\text{s.t. } \|\mathbf{q}\|^2 = 1. \end{aligned} \tag{13}$$

Since $\mathbf{tr}\ (\mathbf{q}^\top \Sigma_d^2 \mathbf{q}) = \mathbf{q}^\top \Sigma_d^2 \mathbf{q}$, the Lagrangian is

$$L(\mathbf{q}, \lambda) = \mathbf{q}^\top \Sigma_d^2 \mathbf{q} - \lambda(\mathbf{q}^\top \mathbf{q} - 1).$$

We have

$$\nabla_{\mathbf{q}} L(\mathbf{q}, \lambda)|_{\mathbf{q}=\mathbf{q}_1} = 2\Sigma_d^2 \mathbf{q}_1 - 2\lambda \mathbf{q}_1 = 0,$$

i.e., $\Sigma_d^2 \mathbf{q}_1 = \lambda \mathbf{q}_1$, which implies that λ is an eigenvalue of Σ_d^2 and $\mathbf{q}_1$ is the corresponding unit eigenvector.

Then the objective function is $f(\mathbf{q}_1) = \frac{1}{n-1}\mathbf{q}_1^\top \Sigma_d^2 \mathbf{q}_1 = \frac{1}{n-1}\mathbf{q}_1^\top \lambda \mathbf{q}_1 = \frac{1}{n-1}\lambda$. The optimality of $f(\mathbf{q}_1)$ implies that λ is the largest eigenvalue of Σ_d^2, i.e., $\lambda = \max_i \sigma_i^2$ and $\mathbf{q}_1$ is the corresponding unit eigenvector.

Since $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_r > 0$, $\mathbf{q}_1 = (1, 0, ..., 0)^\top \in \mathbb{R}^d$ is a solution to problem (13). And $\mathbf{g}_1 = U\mathbf{q}_1 \in \mathbf{argmax}_{\mathbf{g}\in\mathbb{R}^d}\{f(\mathbf{g}) : \|\mathbf{g}\|_2 = 1\}$, where $U = (\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d)$, i.e., $\mathbf{u}_1$ is a solution to problem (11).

3. Since $\mathbf{q} = U^\top \mathbf{g}$, we have $\mathbf{q}_i^\top \mathbf{q}_j = 0$ if $\mathbf{g}_i^\top \mathbf{g}_j = 0$. Thus the problem becomes

$$\max_{\mathbf{q} \in \mathbb{R}^d} \mathbf{q}^\top \Sigma_d^2 \mathbf{q}, \tag{14}$$
$$\text{s.t. } \|\mathbf{q}\|^2 = 1,,$$
$$\mathbf{q}^\top \mathbf{q}_1 = 0.$$

The Lagrangian is

$$L(\mathbf{q}, \lambda, \mu) = \mathbf{q}^\top \Sigma_d^2 \mathbf{q} - \lambda(\mathbf{q}^\top \mathbf{q} - 1) - \mu(\mathbf{q}^\top \mathbf{q}_1).$$

We have

$$\nabla_{\mathbf{q}} L(\mathbf{q}, \lambda, \mu)|_{\mathbf{q}=\mathbf{q}_2} = 2\Sigma_d^2 \mathbf{q}_2 - 2\lambda \mathbf{q}_2 - \mu \mathbf{q}_1 = 0. \tag{15}$$

Note that $\mathbf{q}_2^\top \mathbf{q}_1 = 0$ and $\mathbf{q}_1^\top \Sigma_d^2 \mathbf{q}_2 = \mathbf{q}_2^\top (\Sigma_d^2 \mathbf{q}_1) = \mathbf{q}_2^\top (\sigma_1^2 \mathbf{q}_1) = 0$.
Left-multiplying (15) by $\mathbf{q}_1^\top$, we have

$$0 = 2\mathbf{q}_1^\top \Sigma_d^2 \mathbf{q}_2 - 2\lambda \mathbf{q}_1^\top \mathbf{q}_2 - \mu \mathbf{q}_1^\top \mathbf{q}_1 = -\mu.$$

Thus $\Sigma_d^2 \mathbf{q}_2 = \lambda \mathbf{q}_2$. Similarly, we derive that $\mathbf{q}_2 = (0, 1, 0, ..., 0)^\top \in \mathbb{R}^d$ is a solution to problem (14). Thus $\mathbf{g}_2 = U\mathbf{q}_2 = \mathbf{u}_2$ is a solution to problem (12).

4. Let $\mathbf{e}_i \in \mathbb{R}^d$ denote the one-hot vector with i^{th} entry 1 and all other entries 0. Repeating the above process, we derive that $\mathbf{q}_k = \mathbf{e}_k$, $k = 1, ..., K$. Therefore, $\mathbf{g}_k = \mathbf{u}_k$, $k = 1, ..., K$ are the first K principle component vectors.

5. Assume $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_r > 0$ and $K \leq r \leq d$. For any $k \in [K]$,

$$f(\mathbf{g}_k) = \mathbf{tr}\ (\frac{1}{n-1} \mathbf{g}_k^\top U \Sigma_d^2 U^\top \mathbf{g}_k) = \frac{1}{n-1} \sigma_k^2$$

That is, $f(\mathbf{g}_k)$ corresponds to the square of the k^{th} largest singular value of $\tilde{X}$.

6. Assume $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_r > 0$ and $r \leq d$. If $K < r$

$$\sigma_1 > \sigma_2 > \ldots > \sigma_K > \sigma_{K+1},$$

then the first K principle component vectors $\{\mathbf{g}_i\}_{j=1}^K$ are unique.
If $K = r$

$$\sigma_1 > \sigma_2 > \ldots > \sigma_K,$$

then the first K principle component vectors $\{\mathbf{g}_i\}_{j=1}^K$ are unique.

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