

EXERCISE 1 (REFRESHER ON MATRICES)

1. Let A be a $n \times d$ matrix with real entries. Show that $\text{range}(A) = \text{range}(AA^T)$.

or $\begin{matrix} d \\ \leftarrow \\ A \end{matrix}$? $\text{range}(A) = \text{range}(AA^T)$.

$\text{Ker}(AA^T) \supseteq \text{Ker}(A^T)$.

if $x \in \text{Ker}(A^T)$, then: $AA^T x = 0$ hence $x \in \text{Ker}(AA^T)$.

$\pi \subset \rho \iff$ if $x \in \text{Ker}(AA^T)$, then, $x^T \underbrace{AA^T}_{0} x = 0 = \|[A^T x]\|^2$

$\Rightarrow A^T x = 0 \Rightarrow x \in \text{Ker} A^T$.

Thus: $\text{Ker}(AA^T) = \text{Ker}(A^T)$.

$\text{rng}(\text{Ker}(A^T))^\perp = \text{Range}(A)$

Eq. of ρ : $\text{Range}(A)^\perp = \text{Ker}(A^T)$.

$A = [A_1, \dots, A_d]$
 $x \in \text{Range}(A)^\perp \iff \begin{bmatrix} A_1^T x \\ \vdots \\ A_d^T x \end{bmatrix} = 0 = A^T x \iff x \in \text{Ker}(A^T)$

Ainsi: $\text{Range}(A) = \left[\text{Ker}(A^T) \right]^\perp = \left[\text{Ker}(AA^T) \right]^\perp = \text{Range}(AA^T)$.

2. Let $\{U_k\}_{1 \leq k \leq r}$ be a family of r orthonormal vectors of \mathbb{R}^n . Show that $\sum_{k=1}^r U_k U_k^T$ is the matrix associated with the orthogonal projection onto $H = \{\sum_{k=1}^r \alpha_k U_k; \alpha_1, \dots, \alpha_r \in \mathbb{R}\}$. Deduce that if A is a $n \times d$ matrix with real entries such that each column of A is in H , then,

$\left(\sum_{k=1}^r U_k U_k^T \right) A = A$.

$P_H^\perp(x) = \sum_{k=1}^r \underbrace{\langle x, U_k \rangle}_{U_k^T x} U_k = \left(\sum_{k=1}^r U_k U_k^T \right) x$.

$A = [A_1, \dots, A_d]$.

$\left(\sum_{k=1}^r U_k U_k^T \right) ([A_1, \dots, A_d]) = \left(\underbrace{\sum_{k=1}^r U_k U_k^T A_1}_{A_1}, \dots, \underbrace{\sum_{k=1}^r U_k U_k^T A_d}_{A_d} \right)$

$\sum_{k=1}^r U_k U_k^T A = A$

3. Let $p < d$ and $B \in \mathbb{R}^{d \times p}$ such that $B^T B = I_p$. Let us denote $B = (b_{ij})_{\substack{1 \leq i \leq d \\ 1 \leq j \leq p}}$ the components of B and for all $i \in [1, d]$, $\alpha_i = \sum_{j=1}^p b_{ij}^2$. Show that $\sum_{i=1}^d \alpha_i = p$ and $\alpha_i \leq 1$.

$$B \in M'_{d,p} \Leftrightarrow B \in \mathbb{R}^{d \times p}. \quad B = [B_1, \dots, B_p] \downarrow d, \quad B^T B = I_p.$$

$$\tilde{B} = [B_{p+1}, \dots, B_d]$$

Eq: $[B, \tilde{B}] : B$: BON de \mathbb{R}^d .

$$\sum_{i=1}^d \alpha_i = \sum_{i=1}^d \sum_{j=1}^p b_{ij}^2 = \text{tr} \left(\underbrace{B^T B}_{I_p} \right) = p.$$

$$= \sum_{j=1}^p \left(\sum_{i=1}^d b_{ij}^2 \right) = \sum_{j=1}^p \|B_j\|^2 = p.$$

$$B = (B_1, \dots, B_p) \leftarrow i$$

$$\alpha_i = \sum_{j=1}^p b_{ij}^2 \leq \sum_{j=1}^d b_{ij}^2 = 1.$$

$$\underline{\underline{B \tilde{B}^T = I}} \Leftrightarrow \underline{\underline{\tilde{B} = B^{-1}}} \Leftrightarrow \underline{\underline{\tilde{B}^T B = I}}$$

EXERCISE 2 (PRINCIPAL COMPONENT ANALYSIS) Principal component analysis is a multivariate technique which aims at analyzing the statistical structure of high dimensional dependent observations by representing data using orthogonal variables called *principal components*. Reducing the dimensionality of the data is motivated by several practical reasons such as improving computational complexity. Let $(X_i)_{1 \leq i \leq n}$ be i.i.d. random variables in \mathbb{R}^d and consider the matrix $X \in \mathbb{R}^{n \times d}$ such that the i -th row of X is the observation X_i^T . In this exercise, it is assumed that data are preprocessed so that the columns of X are centered. This means that for all $1 \leq k \leq d$, $\sum_{i=1}^n X_{i,k} = 0$. Let Σ_n be the empirical covariance matrix:

$$\Sigma_n = n^{-1} \sum_{i=1}^n X_i X_i^T.$$

Principal Component Analysis aims at reducing the dimensionality of the observations $(X_i)_{1 \leq i \leq n}$ using a *compression* matrix $U \in \mathbb{R}^{d \times p}$ with orthonormal columns with $p \leq d$ so that for each $1 \leq i \leq n$, $U^T X_i$ is a low dimensional representation of X_i . The original observation may then be partially recovered using U . Principal Component Analysis computes U using the least squares approach:

$$U_* \in \operatorname{argmin}_{\substack{U \in \mathbb{R}^{d \times p} \\ U^T U = I_p}} \sum_{i=1}^n \|X_i - \underbrace{U U^T}_{P_H} X_i\|^2, \quad U = [u_1, \dots, u_p]$$

$H = \operatorname{Range}(U)$

1. Prove that for all matrix $A \in \mathbb{R}^{n \times d}$ with rank r , there exist $\sigma_1 \geq \dots \geq \sigma_r > 0$ such that

$$A = \sum_{k=1}^r \sigma_k u_k v_k^T \in \mathbb{R}^d.$$

$u_k \in \mathbb{R}^n, v_k \in \mathbb{R}^d$

where $\{u_1, \dots, u_r\} \subset \mathbb{R}^n$ and $\{v_1, \dots, v_r\} \subset \mathbb{R}^d$ are two families of orthonormal vectors. The vectors $\{u_1, \dots, u_r\}$ (resp. $\{v_1, \dots, v_r\}$) are the left-singular (resp. right-singular) vectors associated with $\{\sigma_1, \dots, \sigma_r\}$, the singular values of A . If U denotes the $\mathbb{R}^{n \times r}$ matrix with columns given by $\{u_1, \dots, u_r\}$ and V denotes the $\mathbb{R}^{d \times r}$ matrix with columns given by $\{v_1, \dots, v_r\}$, then the singular value decomposition of A may also be written as

$$A = U D_r V^T$$

where $D_r = \operatorname{diag}(\sigma_1, \dots, \sigma_r)$. Then, $A^T A$ and $A A^T$ are positive semidefinite such that

$$A^T A = V D_r^2 V^T \quad \text{and} \quad A A^T = U D_r^2 U^T.$$

In the framework of this exercise, $n \Sigma_n = X^T X$ so that diagonalizing $n \Sigma_n$ is equivalent to computing the singular value decomposition of X .

$$A = \sum_{k=1}^r \sigma_k u_k v_k^T = \underbrace{[u_1, \dots, u_r]}_U \underbrace{\begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_r \end{pmatrix}}_{D_r} \underbrace{\begin{pmatrix} v_1^T \\ \vdots \\ v_r^T \end{pmatrix}}_{V^T}$$

$$= [\sigma_1 u_1, \sigma_2 u_2, \dots, \sigma_r u_r] \begin{pmatrix} v_1^T \\ \vdots \\ v_r^T \end{pmatrix} = \sum_{i=1}^r \sigma_i u_i v_i^T$$

Soit $A \in M_{m,d}(\mathbb{R})$, $A A^T$ est symétrique, réel, $\oplus \left(u^T A A^T u = \|A^T u\|^2 \geq 0 \right)$

$$A A^T = U \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} U^T = \sum_{i=1}^n \lambda_i u_i u_i^T \quad \text{avec } u = (u_1, \dots, u_n)$$

$\lambda_1 \geq \dots \geq \lambda_n$ $(u_i)_{1 \leq i \leq n}$ BON de vecteurs propres de $A A^T$.

or : $\operatorname{rang}(A) = r = \operatorname{rang}(A A^T)$. donc : $\lambda_1 > \dots > \lambda_r > \lambda_{r+1} = 0 = \dots = \lambda_n$.

$$A A^T = \sum_{i=1}^r \lambda_i u_i u_i^T, \quad \underbrace{A A^T u_i = \lambda_i u_i}_{\forall i \in \{1, \dots, r\}}$$

$$A^T A \overline{A^T u_i} = \lambda_i \overline{A^T u_i}$$

$$v_i = \gamma_i A^T u_i$$

En posant $v_i = \frac{A^T u_i}{\sqrt{\lambda_i}}$

$$v_i^T v_i = \gamma_i^2 \underbrace{u_i^T A A^T u_i}_{\lambda_i} = \gamma_i^2 \lambda_i = 1 \implies \gamma_i = 1/\sqrt{\lambda_i}$$

On a : $A^T A v_i = \lambda_i v_i$, v_i BON de vect. propres associé à (λ_i) pour $A^T A$.

Polyn : $\sigma_i = \sqrt{\lambda_i}$

$$\sum_{i=1}^n \sigma_i u_i v_i^T = \sum_{i=1}^n \sqrt{\lambda_i} u_i \left(\frac{A^T u_i}{\sqrt{\lambda_i}} \right)^T = \underbrace{\left(\sum_{i=1}^n u_i u_i^T \right)}_{\substack{P \perp \\ \text{Range}(A^T A) \\ \text{Range}(A)}} A = \underbrace{A}_{\substack{P \perp \\ \text{In}(A)}} = A$$

2. Prove that solving the PCA least squares optimization problem boils down to computing

$$U_* \in \operatorname{argmax}_{U \in \mathbb{R}^{d \times p}, U^T U = I_p} \{ \operatorname{Trace}(U^T \Sigma_n U) \}$$

$$U_* \in \operatorname{argmin}_{\substack{U \in \mathbb{R}^{d \times p} \\ U^T U = I_p}} \sum_{i=1}^n \|x_i - \overbrace{U U^T x_i}^{I_p}\|^2 = \sum_{i=1}^n \left(\|x_i\|^2 - 2 \underbrace{\langle x_i, U U^T x_i \rangle}_{x_i^T U U^T x_i} + \underbrace{x_i^T U U^T x_i}_{x_i^T U U^T x_i} \right)$$

$$= \operatorname{argmax}_{\substack{U^T U = I_p \\ U \in \mathbb{R}^{d \times p}}} \sum_{i=1}^n \underbrace{x_i^T U U^T x_i}_{= \operatorname{tr}(x_i^T U U^T x_i)} = \operatorname{tr}(U^T \left(\sum_{i=1}^n x_i x_i^T \right) U)$$

$$= \operatorname{argmax}_{\substack{U^T U = I_p \\ U \in \mathbb{R}^{d \times p}}} \operatorname{tr} \left(U^T \left(\sum_{i=1}^n x_i x_i^T \right) U \right) = \operatorname{argmax}_{\substack{U \in \mathbb{R}^{d \times p} \\ U^T U = I_p}} \operatorname{tr}(U^T \Sigma_n U)$$

3. Let $\lambda_1 \geq \dots \geq \lambda_d$ be real numbers and denote $f : \alpha \in \mathbb{R}^d \mapsto \sum_{i=1}^d \alpha_i \lambda_i$. Show that

$$\sup \left\{ f(\alpha) : \alpha \in [0, 1]^d, \sum_{i=1}^d \alpha_i = p \right\}$$

is attained for $\alpha^* = (\mathbb{1}_{i \leq p})_{1 \leq i \leq d}$.

4. Let $\{\vartheta_1, \dots, \vartheta_d\}$ be orthonormal eigenvectors associated with the eigenvalues $\lambda_1 \geq \dots \geq \lambda_d$ of Σ_n . Prove that a solution to the PCA least squares optimization problem is given by the matrix U_* with columns $\{\vartheta_1, \dots, \vartheta_p\}$.

3). $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$.

$$\sum_{i=1}^d \alpha_i \lambda_i \leq \sum_{i=1}^p \alpha_i \lambda_i + \lambda_p \left(\sum_{i=p+1}^d \alpha_i \right) = \sum_{i=1}^p \left(\alpha_i \lambda_i + \underbrace{\lambda_p (1 - \alpha_i)}_{\leq \lambda_i} \right) \leq \sum_{i=1}^p \lambda_i$$

4) $\Pi_f : \begin{matrix} U^* \in \text{Argmax.} \\ U \in \mathbb{R}^{d \times p} \\ U^T U = I_p \end{matrix} \quad h(U^T \Sigma_n U)$

où : v_i : vect propre de Σ_n associé à λ_i (avec $\lambda_1 \geq \dots \geq \lambda_d$).

$$\Sigma_n = \underbrace{V D_n V^T}_{= \sum_{i=1}^d \lambda_i v_i v_i^T} \quad \text{où : } \begin{cases} D_n = \text{diag}(\lambda_1, \dots, \lambda_d) \\ V = (v_1, \dots, v_d) \end{cases} \quad \text{où : } (v_i)_{1 \leq i \leq d} : \text{BON de vecteurs propres de } \Sigma_n$$

$$\begin{aligned} h(U^T \Sigma_n U) &= h \left(\underbrace{U^T V}_{B^T} \underbrace{D_n}_{D_n} \underbrace{V^T U}_{B} \right) = \sum_{i=1}^p \sum_{k=1}^d (B^T)_{ik} \lambda_k B_{ki} \\ &= \sum_{i=1}^p \sum_{k=1}^d B_{ki}^2 \lambda_k \\ &= \sum_{k=1}^d \underbrace{\left(\sum_{i=1}^p B_{ki}^2 \right)}_{\leq 1} \lambda_k \end{aligned} \quad \underbrace{B^T B}_{= U^T V V^T U = I_p}$$

Par Ex 1, Q3. $\sum_{i=1}^d \alpha_i = p, \alpha_i \in [0, 1]$
 Par Ex 2, Q3. $\sum_{k=1}^d \alpha_k \lambda_k \leq \sum_{k=1}^p \lambda_k = \sum_{k=1}^d \alpha_k^* \lambda_k$ où $\alpha_k^* = \begin{cases} 1 & k \in [1, p] \\ 0 & \text{sinon} \end{cases}$

En prenant $U_* = (v_1, \dots, v_p)$. $V = (U_*, \tilde{V})$ où $\tilde{V} = (v_{p+1}, \dots, v_d)$.

$$\begin{aligned} h(U_*^T \Sigma_n U_*) &= h \left(U_*^T (U_*, \tilde{V}) D_n \begin{pmatrix} U_*^T \\ \tilde{V}^T \end{pmatrix} U_* \right) \\ &= h \left((I_p, 0) D_n \begin{pmatrix} I_p \\ 0 \end{pmatrix} \right) = \sum_{i=1}^p \lambda_i \end{aligned}$$

5. For any dimension $1 \leq p \leq d$, let \mathcal{F}_d^p be the set of all vector subspaces of \mathbb{R}^d with dimension p . Consider the linear span V_p defined as

$$V_p \in \operatorname{argmin}_{V \in \mathcal{F}_d^p} \sum_{i=1}^n \|X_i - \pi_V(X_i)\|^2,$$

where π_V is the orthogonal projection onto the linear span V . Prove that $V_1 = \operatorname{span}\{v_1\}$ where

$$v_1 \in \operatorname{argmax}_{v \in \mathbb{R}^d; \|v\|=1} \sum_{i=1}^n \langle X_i, v \rangle^2.$$

6. For all $2 \leq p \leq d$, following the same steps, prove that a solution to the optimization problem is given by $V_p = \operatorname{span}\{v_1, \dots, v_p\}$ where

$$v_1 \in \operatorname{argmax}_{v \in \mathbb{R}^d; \|v\|=1} \sum_{i=1}^n \langle X_i, v \rangle^2 \quad \text{and for all } 2 \leq k \leq p, \quad v_k \in \operatorname{argmax}_{\substack{v \in \mathbb{R}^d; \|v\|=1; \\ v \perp v_1, \dots, v \perp v_{k-1}}} \sum_{i=1}^n \langle X_i, v \rangle^2. \quad (1)$$

7. Prove that the vectors $\{v_1, \dots, v_k\}$ defined by (1) can be chosen as the orthonormal eigenvectors associated with the k largest eigenvalues of the empirical covariance matrix Σ_n .

(5, 6, 7). (v_1, \dots, v_p) p vect proprii maximi $\lambda_1, \dots, \lambda_p$ de la matrice Σ_n .

(v_1, \dots, v_d) : BON de vect proprii de Σ_n .

$$v = \sum_{i=1}^d \beta_i v_i$$

$$\begin{aligned} \Rightarrow v^T \Sigma_n v &= v^T \left[\sum_{i=1}^d \beta_i \underbrace{\sum_n r_i}_{\lambda_i v_i} \right] = \left(\sum_{k=1}^d \beta_k v_k \right)^T \left(\sum_{i=1}^d \beta_i \lambda_i v_i \right) \\ &= \sum_{i=1}^d \beta_i^2 \lambda_i \leq \lambda_1 \underbrace{\sum_{i=1}^d \beta_i^2}_{\|v\|^2 = 1} = \lambda_1. \end{aligned}$$

or: $v_1^T \Sigma_n v_1 = \lambda_1, v_1^T v_1 = 1$

Dmc: $v_1 \in \operatorname{argmax}_{\substack{v \in \mathbb{R}^d \\ \|v\|=1}} v^T \Sigma_n v$

$\forall v \in \operatorname{Span}(v_1, \dots, v_{p-1})^\perp$
 $v = \sum_{i=p}^d \beta_i v_i$

$$\left| \begin{aligned} v^T \Sigma_n v &= \sum_{i=p}^d \beta_i^2 \lambda_i \leq \lambda_p \underbrace{\left(\sum_{i=p}^d \beta_i^2 \right)}_{=1} = \lambda_p \\ v_p^T \Sigma_n v_p &= \lambda_p v_p^T v_p = \lambda_p. \end{aligned} \right.$$

Dmc: $v_p \in \operatorname{argmax}_{v \in \operatorname{Span}(v_1, \dots, v_{p-1})^\perp} v^T \Sigma_n v$

8. The orthonormal eigenvectors associated with the eigenvalues of Σ_n allow to define the principal components as follows. Then, as $V_d = \text{span}\{\vartheta_1, \dots, \vartheta_d\}$, for all $1 \leq i \leq n$,

$$\pi_{V_d}(X_i) = \sum_{k=1}^d \langle X_i, \vartheta_k \rangle \vartheta_k = \sum_{k=1}^d (X_i^T \vartheta_k) \vartheta_k = \sum_{k=1}^d c_k(i) \vartheta_k,$$

where for all $1 \leq k \leq d$, the k -th principal component is defined as $c_k = \mathbf{X} \vartheta_k$. Prove that (c_1, \dots, c_d) are orthogonal vectors.

$$\pi_{V_d}(X_i) = P_{V_d}^\perp(X_i) = \sum_{k=1}^d \underbrace{\langle X_i, \vartheta_k \rangle}_{\substack{X_i^T \vartheta_k \\ c_k(i)}} \vartheta_k.$$

$$c_k(i) = X_i^T \vartheta_k.$$

$$\forall k \in \{1, \dots, d\}$$

$$n \Sigma_n.$$

$$c_k = \begin{pmatrix} c_k(1) \\ \vdots \\ c_k(n) \end{pmatrix} = \begin{pmatrix} X_1^T \\ \vdots \\ X_n^T \end{pmatrix} \vartheta_k = \underbrace{\mathbf{X}^T}_{\mathbf{X}} \vartheta_k.$$

$$\langle c_h, c_l \rangle = 0 = \underbrace{\vartheta_h^T \mathbf{X}^T \mathbf{X} \vartheta_l}_{n \lambda_l \vartheta_h^T \vartheta_l} = n \lambda_l \underbrace{\vartheta_h^T \vartheta_l}_{=0 \text{ if } h \neq l}.$$

EXERCISE 3 (KERNEL PRINCIPAL COMPONENT ANALYSIS) Let $(X_i)_{1 \leq i \leq n}$ be n observations in a general space \mathcal{X} , $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ a positive kernel and $\mathbf{K} = (k(X_i, X_j))_{1 \leq i, j \leq n}$. \mathcal{W} denotes the Reproducing Kernel Hilbert Space associated with k and for all $x \in \mathcal{X}$, $\phi(x)$ denotes the function $\phi(x) : y \rightarrow k(x, y)$. The aim is now to perform a PCA on $(\phi(X_1), \dots, \phi(X_n))$. It is assumed that $\sum_{i=1}^n \phi(X_i) = 0$.

1. Prove that

$$f_1 = \operatorname{argmax}_{f \in \mathcal{W}; \|f\|_{\mathcal{W}}=1} \sum_{i=1}^n \langle \phi(X_i), f \rangle_{\mathcal{W}}^2$$

may be written

$$f_1 = \sum_{i=1}^n \alpha_1(i) \phi(X_i), \quad \text{where } \alpha_1 = \operatorname{argmax}_{\alpha \in \mathbb{R}^n; \alpha^\top \mathbf{K} \alpha = 1} \alpha^\top \mathbf{K}^2 \alpha.$$

2. Prove that $\alpha_1 = \lambda_1^{-1/2} b_1$ where b_1 is the unit eigenvector associated with the largest eigenvalue λ_1 of \mathbf{K} . What about (f_2, \dots, f_p) defined iteratively as in (1)?

3. Write $H_p = \text{span}\{f_1, \dots, f_p\}$. Prove that, for all $1 \leq i \leq n$,

$$\pi_{H_p}(\phi(X_i)) = \sum_{j=1}^p \lambda_j \alpha_j(i) f_j .$$