

Warm-up

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

First note that $AA^\top x = 0$ implies $\langle A^\top x, A^\top x \rangle = 0$ so that $A^\top x = 0$. The converse is obvious. Therefore, $\text{Ker}(AA^\top) = \text{Ker}(A^\top)$. And using that $\text{Ker}(B^\top) = (\text{Im}(B))^\perp$, we deduce that $\text{Im}(AA^\top)^\perp = \text{Im}(A)^\perp$, which concludes the proof.

2. Let $\{U_k\}_{1 \leq k \leq r}$ be a family of r orthonormal vectors of \mathbb{R}^n . Show that $\sum_{k=1}^r U_k U_k^\top$ 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,

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

Let $\pi_H(X)$ be the orthogonal projection of X onto H . Since $\{U_k\}_{1 \leq k \leq r}$ is an orthonormal basis of H ,

$$\pi_H(X) = \sum_{k=1}^r \langle X, U_k \rangle U_k = \left(\sum_{k=1}^r U_k U_k^\top \right) X.$$

This implies that for each $X \in H$, $X = (\sum_{k=1}^r U_k U_k^\top) X$. Since all the column vectors of A are in H , this yields $(\sum_{k=1}^r U_k U_k^\top) A = A$.

Kernel Principal Component Analysis

Principal Component Analysis

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^\top . 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:

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

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 $1 \leq i \leq n$, $U^\top X_i$ is a low dimensional representation of X_i . The original observation may then be partially recovered using $U \in \mathbb{R}^{d \times p}$. Principal Component Analysis computes U using the least squares approach:

$$U_\star \in \underset{U \in \mathbb{R}^{d \times p}}{\text{argmin}} \sum_{i=1}^n \|X_i - U U^\top X_i\|_2^2,$$

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

$$A = \sum_{k=1}^r \sigma_k u_k v_k^\top,$$

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 .

Since the matrix AA^\top is positive semidefinite, its spectral decomposition is given by

$$AA^\top = \sum_{k=1}^r \lambda_k u_k u_k^\top,$$

where $\lambda_1 \geq \dots \geq \lambda_r > 0$ are the nonzero eigenvalues of AA^\top and $\{u_1, \dots, u_r\}$ is an orthonormal family of \mathbb{R}^n . For all $1 \leq k \leq r$, define $v_k = \lambda_k^{-1/2} A^\top u_k$ so that

$$\begin{aligned} \|v_k\|^2 &= \lambda_k^{-1} \langle A^\top u_k; A^\top u_k \rangle = \lambda_k^{-1} u_k^\top A A^\top u_k = 1, \\ A^\top A v_k &= \lambda_k^{-1/2} A^\top A A^\top u_k = \lambda_k v_k. \end{aligned}$$

On the other hand, for all $1 \leq k \neq j \leq r$, $\langle v_k; v_j \rangle = \lambda_k^{-1/2} \lambda_j^{-1/2} u_k^\top A A^\top u_j = \lambda_k^{-1/2} \lambda_j^{1/2} u_k^\top u_j = 0$. Therefore, $\{v_1, \dots, v_r\}$ is an orthonormal family of eigenvectors of $A^\top A$ associated with the eigenvalues $\lambda_1 \geq \dots \geq \lambda_r > 0$. Define, for all $1 \leq k \leq r$, $\sigma_k = \lambda_k^{1/2}$ which yields

$$\sum_{k=1}^r \sigma_k u_k v_k^\top = \sum_{k=1}^r u_k u_k^\top A = \left(\sum_{k=1}^r u_k u_k^\top \right) A.$$

As $\{u_1, \dots, u_r\}$ is an orthonormal family, $UU^\top = \sum_{k=1}^r u_k u_k^\top$ is the orthogonal projection onto the range(AA^\top) = range(A) which implies

$$\sum_{k=1}^r \sigma_k u_k v_k^\top = \left(\sum_{k=1}^r u_k u_k^\top \right) A = A.$$

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

$$U_\star \in \operatorname{argmax}_{U \in \mathbb{R}^{d \times p}, U^\top U = I_p} \{\operatorname{trace}(U^\top \Sigma_n U)\}.$$

Let $U \in \mathbb{R}^{d \times p}$ be such that $U^\top U = I_p$. Then,

$$\begin{aligned} \sum_{i=1}^n \|X_i - UU^\top X_i\|_2^2 &= \sum_{i=1}^n \|X_i\|_2^2 + \sum_{i=1}^n \|UU^\top X_i\|_2^2 - 2 \sum_{i=1}^n \langle X_i; UU^\top X_i \rangle, \\ &= \sum_{i=1}^n \|X_i\|_2^2 + \sum_{i=1}^n X_i^\top UU^\top X_i - 2 \sum_{i=1}^n X_i^\top UU^\top X_i, \\ &= \sum_{i=1}^n \|X_i\|_2^2 - \sum_{i=1}^n X_i^\top UU^\top X_i, \\ &= \sum_{i=1}^n \|X_i\|_2^2 - \operatorname{trace}(U^\top X X^\top U). \end{aligned}$$

3. 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 this problem is given by the matrix U_\star with columns $\{\vartheta_1, \dots, \vartheta_p\}$.

Let $\Sigma_n = V D_n V^\top$ be the spectral decomposition of Σ_n where $D_n = \operatorname{Diag}(\lambda_1, \dots, \lambda_d)$ and $V \in \mathbb{R}^{d \times d}$ is a matrix with orthonormal columns $\{\vartheta_1, \dots, \vartheta_d\}$. For all $U \in \mathbb{R}^{d \times p}$ matrix with orthonormal columns define $B = V^\top U$ so that, as $V \in \mathbb{R}^{d \times d}$ is an orthogonal matrix,

$$VB = VV^\top U = U \quad \text{and} \quad U^\top \Sigma_n U = B^\top V^\top V D_n V^\top V B = B^\top D_n B.$$

Therefore,

$$\text{Trace}(U^\top \Sigma_n U) = \text{Trace}(B^\top D_n B) = \sum_{i=1}^d \lambda_i \sum_{j=1}^p b_{i,j}^2. \quad (1)$$

On the other hand,

$$B^\top B = U^\top V V^\top U = U^\top U = I_p,$$

so that the columns of B are orthonormal and

$$\sum_{i=1}^d \sum_{j=1}^p b_{i,j}^2 = p.$$

Hence, introducing for all $1 \leq i \leq d$, $\alpha_i = \sum_{j=1}^p b_{i,j}^2$, by (1),

$$\text{Trace}(U^\top \Sigma_n U) = \sum_{i=1}^d \alpha_i \lambda_i,$$

with, for all $1 \leq i \leq d$, $\alpha_i \in [0, 1]$ and $\sum_{i=1}^d \alpha_i = p$. As $\lambda_1 \geq \lambda_2 \geq \dots, \lambda_d$,

$$\text{Trace}(U^\top \Sigma_n U) \leq \sum_{i=1}^p \lambda_i.$$

Indeed, the function $f_d : (\alpha_1, \dots, \alpha_d) \mapsto \sum_{i=1}^d \alpha_i \lambda_i$ is maximized under the constraints $\alpha_i \in [0, 1]$ and $\sum_{i=1}^d \alpha_i = p$ by $(\alpha_i^*)_{1 \leq i \leq d}$ such that $\alpha_1^* = \dots = \alpha_p^* = 1$. Assume that $(\alpha_1, \dots, \alpha_d)$ is such that there exists $1 \leq j_0 \leq p$ such that $\alpha_{j_0} < 1$. Then, $\sum_{j=p+1}^d \alpha_j \geq 1 - \alpha_{j_0}$ and we may write, as $\lambda_{j_0} \geq \lambda_{p+1} \geq \dots \geq \lambda_d$,

$$f_d(\alpha_1, \dots, \alpha_d) \leq \sum_{i=1, i \neq j_0}^p \alpha_i \lambda_i + \lambda_{j_0} + \sum_{i=p+1}^d \tilde{\alpha}_i \lambda_i,$$

where $(\tilde{\alpha}_i)_{p+1 \leq i \leq d}$ are in $[0, 1]$ and such that $\sum_{i=1, i \neq j_0}^p \alpha_i + 1 + \sum_{i=p+1}^d \tilde{\alpha}_i = p$.

As the columns of U_\star are $\{\vartheta_1, \dots, \vartheta_p\}$, for all $1 \leq i \leq d$ and $1 \leq j \leq p$, $b_{i,j} = \langle \vartheta_i; \vartheta_j \rangle = \delta_{i,j}$. Therefore, for all $1 \leq i \leq p$, $\sum_{j=1}^p b_{i,j}^2 = 1$, for all $p < i$, $\sum_{j=1}^p b_{i,j}^2 = 0$ and

$$\text{Trace}(U_\star^\top \Sigma_n U_\star) = \sum_{i=1}^p \lambda_i,$$

which completes the proof.

4. 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_d defined as

$$V_p \in \underset{V \in \mathcal{F}_d^p}{\text{argmin}} \sum_{i=1}^n \|X_i - \pi_V(X_i)\|_2^2,$$

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

$$v_1 \in \underset{v \in \mathbb{R}^d; \|v\|_2=1}{\text{argmax}} \sum_{i=1}^n \langle X_i, v \rangle^2.$$

Write $V_1 = \text{span}\{v_1\}$ for $v_1 \in \mathbb{R}^d$ such that $\|v_1\|_2 = 1$. Then,

$$\begin{aligned} \sum_{i=1}^n \|X_i - \pi_{V_1}(X_i)\|_2^2 &= \sum_{i=1}^n \|X_i - \langle X_i; v_1 \rangle v_1\|_2^2, \\ &= \sum_{i=1}^n (\|X_i\|_2^2 - 2\langle X_i; \langle X_i; v_1 \rangle v_1 \rangle + \|\langle X_i; v_1 \rangle v_1\|_2^2), \\ &= \sum_{i=1}^n (\|X_i\|_2^2 - \langle X_i; v_1 \rangle^2). \end{aligned}$$

Consequently, V_1 is a solution if and only if v_1 is solution to:

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

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

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

Write $V_p = \text{span}\{v_1, \dots, v_p\}$ where $\{v_1, \dots, v_p\}$ is an orthonormal family. Then,

$$\sum_{i=1}^n \|X_i - \pi_{V_p}(X_i)\|^2 = \sum_{i=1}^n \|X_i - \sum_{k=1}^p \langle X_i; v_k \rangle v_k\|_2^2 = \sum_{i=1}^n \left(\|X_i\|_2^2 - \sum_{k=1}^p \langle X_i; v_k \rangle^2 \right).$$

(v_1, \dots, v_p) is therefore solution to

$$v = (v_1, \dots, v_p) \in \underset{v \in \mathbb{R}^d; \|v\|=1}{\operatorname{argmax}} \sum_{k=1}^p \sum_{i=1}^n \langle X_i; v_k \rangle^2.$$

The additive form of the function to be maximized allows to build the orthonormal basis of V_p sequentially as claimed.

6. Prove that the vectors $\{v_1, \dots, v_k\}$ defined by (2) can be chosen as the orthonormal eigenvectors associated with the k largest eigenvalues of the empirical covariance matrix Σ_n .

Note that for all $v \in \mathbb{R}^d$ such that $\|v\|_2 = 1$,

$$\frac{1}{n} \sum_{i=1}^n \langle X_i, v \rangle^2 = \frac{1}{n} \sum_{i=1}^n (v^\top X_i)(X_i^\top v) = v^\top \Sigma_n v.$$

As $(\vartheta_i)_{1 \leq i \leq d}$ are the orthonormal eigenvectors associated with the eigenvalues $\lambda_1 \geq \dots \geq \lambda_d \geq 0$ of Σ_n . Then,

$$\frac{1}{n} \sum_{i=1}^n \langle X_i, v \rangle^2 = v^\top \left(\sum_{i=1}^d \lambda_i \vartheta_i \vartheta_i^\top \right) v = \sum_{i=1}^d \lambda_i \langle v, \vartheta_i \rangle^2 \leq \lambda_1 \sum_{i=1}^d \langle v, \vartheta_i \rangle^2$$

and, as $(\vartheta_i)_{1 \leq i \leq d}$ is an orthonormal basis of \mathbb{R}^d , $\sum_{i=1}^d \langle v, \vartheta_i \rangle^2 = \|v\|_2^2 = 1$. Therefore,

$$\frac{1}{n} \sum_{i=1}^n \langle X_i, v \rangle^2 \leq \lambda_1.$$

On the other hand, for all $2 \leq i \leq d$, $\langle \vartheta_1, \vartheta_i \rangle = 0$ and $\langle \vartheta_1, \vartheta_1 \rangle = 1$ so that $\sum_{i=1}^d \lambda_i \langle \vartheta_1, \vartheta_i \rangle^2 = \lambda_1$ which proves that ϑ_1 is solution to (2).

Assume now that $v \in \mathbb{R}^d$ is such that $\|v\| = 1$ and for all $1 \leq j \leq k-1$, $\langle v, \vartheta_j \rangle = 0$ and write

$$\frac{1}{n} \sum_{i=1}^n \langle X_i, v \rangle^2 = \sum_{i=1}^d \lambda_i \langle v, \vartheta_i \rangle^2 \leq \lambda_k \sum_{i=k}^d \langle v, \vartheta_i \rangle^2 \leq \lambda_k,$$

since, as $(\vartheta_i)_{1 \leq i \leq d}$ is an orthonormal basis of \mathbb{R}^d , $\sum_{i=1}^d \langle v, \vartheta_i \rangle^2 = \sum_{i=k}^d \langle v, \vartheta_i \rangle^2 = \|v\|^2 = 1$. On the other hand, for all $1 \leq i \leq d$, $i \neq k$, $\langle \vartheta_k, \vartheta_i \rangle = 0$ and $\langle \vartheta_k, \vartheta_k \rangle = 1$ so that $\sum_{i=1}^d \lambda_i \langle \vartheta_k, \vartheta_i \rangle^2 = \lambda_k$ which proves that ϑ_k is solution to (2).

Therefore, $V_p = \text{span}\{\vartheta_1, \dots, \vartheta_p\}$ is a solution to (2) and, as $(\vartheta_i)_{1 \leq i \leq p}$ is an orthonormal family, the projection matrix onto V_p is given by $U_\star U_\star^\top$ where U_\star is a $\mathbb{R}^{d \times p}$ matrix with columns $\{\vartheta_1, \dots, \vartheta_p\}$.

7. 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 $1 \leq i \leq n$,

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

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.

The k -th principal component is the vector whose components are the coordinates of each X_i , $1 \leq i \leq n$, relative to the basis $\{\vartheta_1, \dots, \vartheta_d\}$ of V_d . For all $1 \leq i \neq j \leq d$,

$$\langle c_i, c_j \rangle = \vartheta_i^\top X^\top X \vartheta_j = \vartheta_i^\top (n \Sigma_n) \vartheta_j = n \lambda_j \vartheta_i^\top \vartheta_j = 0,$$

as $\{\vartheta_1, \dots, \vartheta_d\}$ is an orthonormal family.

Application to RKHS

Let $(X_i)_{1 \leq i \leq n}$ be n observations in a general space \mathcal{X} and $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ a positive function. We assume that k is symmetric and that for all $n \geq 1$, $(a_i)_{1 \leq i \leq n} \in \mathbb{R}^n$ and $(x_i)_{1 \leq i \leq n} \in \mathcal{X}^n$, $\sum_{1 \leq i, j \leq n} a_i a_j k(x_i, x_j) \geq 0$. For all $x \in \mathcal{X}$, $\phi(x)$ denotes the function $\phi(x) : y \rightarrow k(x, y)$.

Let \mathcal{W} be a Hilbert space of real-valued functions defined on \mathcal{X} , endowed with an inner product denoted by $\langle \cdot, \cdot \rangle_{\mathcal{W}}$, and such that for all $x \in \mathcal{X}$, $\phi(x) \in \mathcal{W}$ and for all $f \in \mathcal{W}$ and all $x \in \mathcal{X}$, $f(x) = \langle f, \phi(x) \rangle_{\mathcal{W}}$. The aim is now to perform a PCA on $(\phi(X_1), \dots, \phi(X_n))$. It is assumed that $\sum_{i=1}^n \phi(X_i) = 0$. Define

$$K = (k(X_i, X_j))_{1 \leq i, j \leq n}.$$

1. Prove that

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

may be written

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

Any solution to the optimization problem lies in the vectorial subspace $V = \text{span}\{\phi(X_1), \dots, \phi(X_n)\}$. Let $f = \sum_{i=1}^n \alpha(i) \phi(X_i)$ be such that $\|f\|_{\mathcal{W}} = 1$. Then,

$$\|f\|_{\mathcal{W}}^2 = \sum_{i,j=1}^n \alpha_i \alpha_j \langle \phi(X_i), \phi(X_j) \rangle_{\mathcal{W}} = \alpha^\top K \alpha.$$

On the other hand, $\langle \phi(X_i), f \rangle_{\mathcal{W}} = f(X_i) = [K\alpha](i)$ so that,

$$\sum_{i=1}^n \langle \phi(X_i), f \rangle_{\mathcal{W}}^2 = \sum_{i=1}^n f^2(X_i) = \sum_{i=1}^n ([K\alpha](i))^2 = (K\alpha_1)^\top K\alpha_1 = \alpha^\top K^2 \alpha .$$

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 K .

Let $\lambda_1 \geq \dots \geq \lambda_n \geq 0$ be the eigenvalues of K associated with the orthonormal basis of eigenvectors (b_1, \dots, b_n) . For any $\alpha \in \mathbb{R}^n$ such that $\alpha^\top K\alpha = 1$,

$$\alpha^\top K^2 \alpha = \alpha^\top \left(\sum_{i=1}^n \lambda_i b_i b_i^\top \right)^2 \alpha = \sum_{i=1}^n \lambda_i^2 \langle \alpha, b_i \rangle^2 \leq \lambda_1 \sum_{i=1}^n \lambda_i \langle \alpha, b_i \rangle^2 = \lambda_1 ,$$

as $\alpha^\top K\alpha = \sum_{i=1}^n \lambda_i \langle \alpha, b_i \rangle^2 = 1$. On the other hand,

$$\left(\lambda_1^{-1/2} b_1 \right)^\top K^2 \left(\lambda_1^{-1/2} b_1 \right) = \lambda_1^{-1} \sum_{i=1}^n \lambda_i^2 \langle b_1, b_i \rangle^2 = \lambda_1 .$$

Following the same steps, f_j may be written $f_j = \sum_{i=1}^n \alpha_j(i) \phi(x_i)$ with $\alpha_j = \lambda_j^{-1/2} b_j$.

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

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

Note first that the (f_1, \dots, f_d) is an orthonormal family. Therefore,

$$\pi_{H_d}(\phi(X_i)) = \sum_{j=1}^d \langle \phi(X_i), f_j \rangle_{\mathcal{W}} f_j = \sum_{j=1}^d \langle \phi(X_i), \sum_{\ell=1}^n \alpha_j(\ell) \phi(X_\ell) \rangle_{\mathcal{W}} f_j = \sum_{j=1}^d [K\alpha_j](i) f_j .$$

Therefore,

$$\pi_{H_d}(\phi(x_i)) = \sum_{j=1}^d \lambda_j^{-1/2} [Kb_j](i) f_j = \sum_{j=1}^d \lambda_j^{1/2} b_j(i) f_j = \sum_{j=1}^d \lambda_j \alpha_j(i) f_j .$$