Lab 12

Machine Learning 2021-2022 - UMONS
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1

Consider the following design matrix X:

X_1	X_2
4	1
2	3
5	4
1	0

We want to represent the data in only one dimension using principal components analysis (PCA). To this end :

- Center the data.
- Compute the sample covariance matrix C.
- Compute the eigenvalues and eigenvectors of the covariance matrix C.
- Plot the dataset, and draw the first principal component direction (as a line) and the projections of all four sample points onto the principal direction.
- Label each data point with its principal component score.
- Compute the proportion of variance explained by the first principal component.
- Add the projections of the data points onto the second principal component, compute the second principal component scores, and show that the sum of the variance explained by each component is equal to the total variance of the data.

Recall that the eigenvalues of a square matrix A are obtained by resolving the characteristic equation $\det(A - \lambda I) = 0$. If $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, then $\det(A) = ad - bc$. Finally, an eigenvector v of A must satisfy $Av = \lambda v$. The sample covariance matrix is equal to $\frac{1}{n}X^\top X$.
The sample means are $\bar{X}_1 = 3$ and $\bar{X}_2 = 2$, which gives :

X_1	X_2
1	-1
-1	1
2	2
-2	-2

The sample covariance matrix is obtained as :

$$C = \frac{1}{4}X^T X = \frac{1}{4}\begin{pmatrix} 10 & 6 \\ 6 & 10 \end{pmatrix}.$$

The eigenvalues of C are obtained by solving the characteristic equation :

$$
\begin{aligned}
&\det(C-\lambda I)=0\\
\iff &\begin{vmatrix} \frac{5}{2}-\lambda & \frac{3}{2} \\ \frac{3}{2} & \frac{5}{2}-\lambda \end{vmatrix}=0\\
\iff &(\frac{5}{2}-\lambda)^2-\frac{9}{4}=0\\
\iff &\lambda_1=4 \quad \lambda_2=1
\end{aligned}
$$

The eigenvector v_1 associated to the first eigenvalue $\lambda_1=4$ must verify :

$$
\begin{aligned}
&(C-\lambda_1 I)v_1=0\\
\iff &\begin{pmatrix} -3/2 & 3/2 \\ 3/2 & -3/2 \end{pmatrix}\begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix}=0\\
\iff &\begin{cases} -\frac{3}{2}v_{11}+\frac{3}{2}v_{12}=0 \\ \frac{3}{2}v_{11}-\frac{3}{2}v_{12}=0 \end{cases}
\end{aligned}
$$

An arbitrary choice can be $v_1=\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, which once normalized, gives $\phi_1=\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

The eigenvector v_2 associated to the eigenvalue $\lambda_2=1$ must verify :

$$
\begin{aligned}
&(C-\lambda_2 I)v_2=0\\
\iff &\begin{pmatrix} 3/2 & 3/2 \\ 3/2 & 3/2 \end{pmatrix}\begin{pmatrix} v_{21} \\ v_{22} \end{pmatrix}=0\\
\iff &\begin{cases} -\frac{3}{2}v_{21}+\frac{3}{2}v_{22}=0 \\ \frac{3}{2}v_{21}-\frac{3}{2}v_{22}=0 \end{cases}
\end{aligned}
$$

An arbitrary choice can be $v_2=\begin{pmatrix} 1 \\ -1 \end{pmatrix}$, which once normalized, gives $\phi_2=\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$

Figure [1] displays the plot of the centered dataset (Left), and their projection onto the first principal component direction (Right). The first component scores are given as:

$$
Z_1=X\phi_1=\begin{pmatrix} 0 \\ 0 \\ \frac{4}{\sqrt{2}} \\ \frac{4}{\sqrt{2}} \end{pmatrix}
$$

The total variance in the data is obtained as :

$$
\begin{aligned}
\mathrm{TV}&=\sum_{j}^{p}\mathrm{Var}(X_j)\\
&=\sum_{j}^{p}\frac{1}{n}\sum_{i}^{n}x_{ij}^2\\
&=5
\end{aligned}
$$

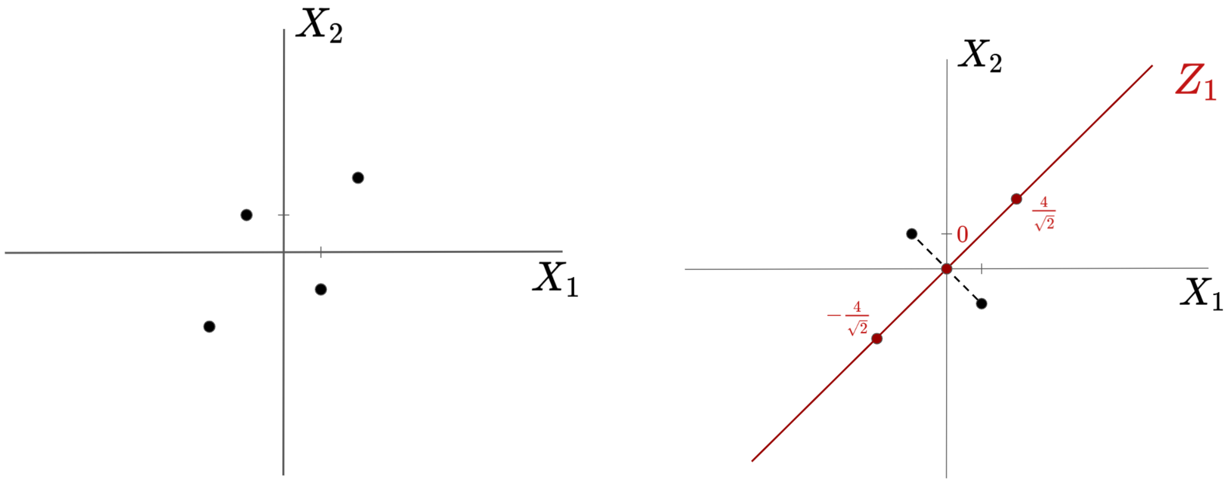

Figure 1: Plots of the centered data points (Left) and of their projections onto the direction of the first principal component.

The variance explained by the first principal component is given by :

$$\begin{aligned}\mathrm{Var}(Z_1) &= \frac{1}{n}\sum_i^n z_{1i}^2 \\ &= \frac{1}{4}(0+0+8+8) = 4\end{aligned}$$

And finally, the proportion of the variance explained by the first principal component is obtained as $\mathrm{TV}_1 = \frac{\mathrm{Var}(Z_1)}{TV} = \frac{4}{5}$.

The second principal components scores are obtained as:

$$Z_2 = X\phi_2 = \begin{pmatrix} \frac{2}{\sqrt{2}} \\ -\frac{2}{\sqrt{2}} \\ 0 \\ 0 \end{pmatrix}$$

And thus, the coordinates of the data points in the principal components space are

$$Z = \begin{pmatrix} 0 & \frac{2}{\sqrt{2}} \\ 0 & -\frac{2}{\sqrt{2}} \\ \frac{4}{\sqrt{2}} & 0 \\ \frac{4}{\sqrt{2}} & 0 \end{pmatrix}$$

leading to Figure [2]. The variance explained by the second principal component is obtained as:

$$\mathrm{Var}(Z_2) = \frac{1}{n}\sum_i^n z_{2i}^2 = 1$$

From which we have:

$$\mathrm{Var}(Z_1) + \mathrm{Var}(Z_2) = 5 = \mathrm{TV}$$

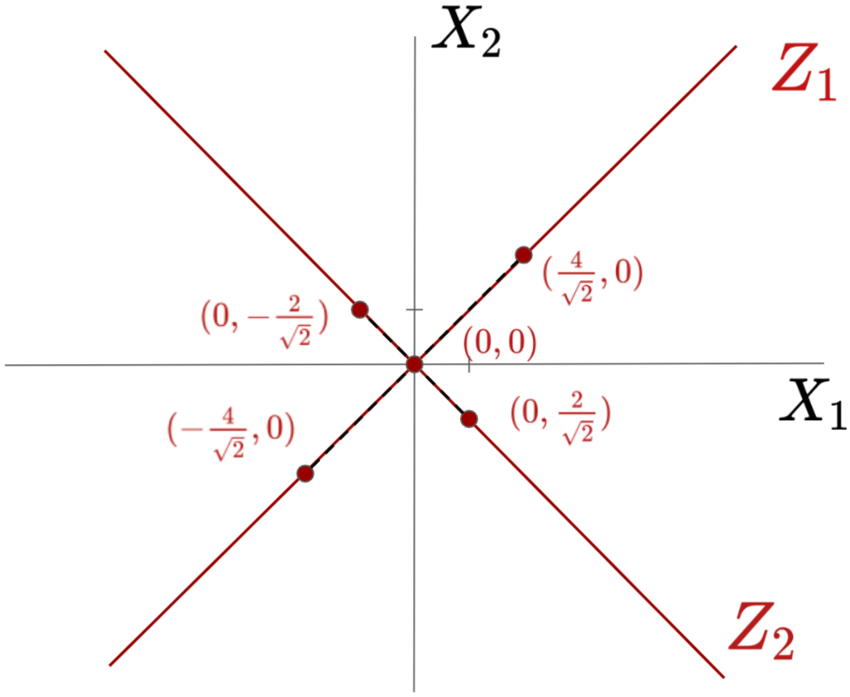

Figure 2: Projection of the centered data points onto the principal components.

2

Suppose that the columns of $X \in \mathbb{R}^{n\times p}$ have been centered (i.e. they have sample mean zero). The total sample variance of X is defined as $\frac{1}{n}\text{Trace}(X^\intercal X)$.

Let $X = UDV^\intercal$ be the singular value decomposition of X where the columns of $U \in \mathbb{R}^{n\times p}$ and $V \in \mathbb{R}^{p\times p}$ are orthonormal and the matrix $D \in \mathbb{R}^{p\times p}$ is diagonal with positive real entries, $D = \text{diag}(d_1,...,d_n)$, with $d_1 \geq d_2 \geq ... \geq d_n \geq 0$.

Prove that the total variance of X is given by $\frac{1}{n}\sum_i^n d_j^2$. How do you link this result to the eigenvalues of covariance matrix C ?

(Hint : Use the fact that $\text{Trace}(AB) = \text{Trace}(BA)$)

$(AB)^\intercal = B^\intercal A^\intercal$

If V is orthonormal, then $V^\intercal V = I$

If A is diagonal, then $A^\intercal A = A^2$

$$
\begin{aligned}
\text{TV} &= \frac{1}{n}\text{Trace}(X^\intercal X) \\
&= \frac{1}{n}\text{Trace}\Big((UDV^\intercal)^\intercal UDV^\intercal\Big) \\
&= \frac{1}{n}\text{Trace}(VD^\intercal U^\intercal UDV^\intercal) \qquad (AB)^\intercal = B^\intercal A^\intercal \\
&= \frac{1}{n}\text{Trace}(VD^\intercal DV^\intercal) \qquad U^\intercal U = I \text{ as the columns of } U \text{ are orthonormal} \\
&= \frac{1}{n}\text{Trace}(VD^2V^\intercal) \qquad D^\intercal D = D^2 \text{ as } D \text{ is diagonal} \\
&= \frac{1}{n}\text{Trace}(D^2V^\intercal V) \qquad \text{Trace}(AB) = \text{Trace}(BA) \\
&= \frac{1}{n}\text{Trace}(D^2) \qquad V^\intercal V = I \text{ as the columns of } V \text{ are orthonormal} \\
&= \frac{1}{n}\sum_{j=1}^{p} d_j^2
\end{aligned}
$$

We have that $C = X^\intercal X = VDU^\intercal UDV^\intercal = VD^2V^\intercal$, where D^2 is the matrix of eigenvalues of C. This means that the total variance of X is equal to the sum of the eigenvalues of the covariance matrix C.

3

If again $X = UDV^\intercal$, with centered columns, and $V_k \in \mathbb{R}^{p\times k}$ denotes the first k columns of V, prove that $XV_kV_k^\intercal$ has total sample variance $\frac{1}{n}\sum_{j=1}^k d_j^2$

Prove that XV_k has also total variance $\frac{1}{n}\sum_{j=1}^k d_j^2$. How do you relate this result to the eigenvalues of the covariance matrix C ?

(Hint : Use the fact that $V_k^\intercal V = [I_k\ 0] \in \mathbb{R}^{k\times p}$ where I_k is a $k\times k$ identity matrix and where the $p-k$ remaining entries are filled with 0's).

$$
\begin{aligned}
&\frac{1}{n}\text{Trace}\Big((XV_kV_k^\intercal)^\intercal XV_kV_k^\intercal\Big)\\
&= \frac{1}{n}\text{Trace}(V_kV_k^\intercal X^\intercal XV_kV_k^\intercal) \qquad (ABC)^\intercal = C^\intercal B^\intercal C^\intercal\\
&= \frac{1}{n}\text{Trace}(V_kV_k^\intercal VD^2V^\intercal V_kV_k^\intercal)\\
&= \frac{1}{n}\text{Trace}(V_k\begin{bmatrix} I_k & 0\end{bmatrix} D^2 \begin{bmatrix} I_k \\ 0\end{bmatrix} V_k^\intercal)\\
&= \frac{1}{n}\text{Trace}(\begin{bmatrix} V_k & 0\end{bmatrix} D^2 \begin{bmatrix} V_k^\intercal \\ 0\end{bmatrix})\\
&= \frac{1}{n}\text{Trace}(D^2 \begin{bmatrix} I_k & 0 \\ 0 & 0\end{bmatrix}) \qquad \text{Trace}(AB) = \text{Trace}(BA) \text{ and } \begin{bmatrix} I_k & 0 \\ 0 & 0\end{bmatrix} \in \mathbb{R}^{p\times p}\\
&= \frac{1}{n}\sum_{j=1}^k d_j^2
\end{aligned}
$$

$$
\begin{aligned}
&\frac{1}{n}\text{Trace}\Big((XV_k)^\intercal XV_k\Big)\\
&= \frac{1}{n}\text{Trace}(V_k^\intercal X^\intercal XV_k) \qquad (AB)^\intercal = B^\intercal A^\intercal\\
&= \frac{1}{n}\text{Trace}(V_k^\intercal VD^2V^\intercal V_k)\\
&= \frac{1}{n}\text{Trace}(\begin{bmatrix} I_k & 0\end{bmatrix} D^2 \begin{bmatrix} I_k \\ 0\end{bmatrix})\\
&= \frac{1}{n}\text{Trace}(D^2 \begin{bmatrix} I_k & 0 \\ 0 & 0\end{bmatrix})\\
&= \frac{1}{n}\sum_{j=1}^k d_j^2
\end{aligned}
$$

The total variance explained by the k first principal components $Z_k = XV_k$ is given by the sum of the k first eigenvalues of C, the sample covariance matrix of X.