Principal Component Analysis

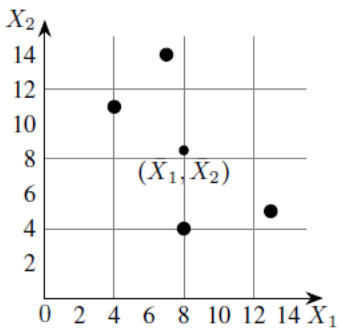
Problem definition

Given the data in Table, reduce the dimension from 2 to 1 using the Principal Component Analysis (PCA) algorithm.

Feature	Example 1	Example 2	Example 3	Example 4
X_1	4	8	13	7
X_2	11	4	5	14

Step 1: Calculate Mean

The figure shows the scatter plot of the given data points.



Calculate the mean of X_1 and X_2 as shown below.

$$\bar{X}_1 = \tfrac{1}{4}(4 + 8 + 13 + 7) = 8,$$
$$\bar{X}_2 = \tfrac{1}{4}(11 + 4 + 5 + 14) = 8.5.$$

Step 2: Calculation of the covariance matrix.

The covariances are calculated as follows:

$$\begin{aligned}
\operatorname{Cov}(X_1, X_2) &= \frac{1}{N-1}\sum_{k=1}^{N}(X_{1k} - \bar{X}_1)^2 \\
&= \tfrac{1}{3}\left((4-8)^2 + (8-8)^2 + (13-8)^2 + (7-8)^2\right) \\
&= 14 \\
\operatorname{Cov}(X_1, X_2) &= \frac{1}{N-1}\sum_{k=1}^{N}(X_{1k} - \bar{X}_1)(X_{2k} - \bar{X}_2) \\
&= \tfrac{1}{3}((4-8)(11-8.5) + (8-8)(4-8.5) \\
&\quad + (13-8)(5-8.5) + (7-8)(14-8.5) \\
&= -11 \\
\operatorname{Cov}(X_2, X_1) &= \operatorname{Cov}(X_1, X_2) \\
&= -11 \\
\operatorname{Cov}(X_2, X_2) &= \frac{1}{N-1}\sum_{k=1}^{N}(X_{2k} - \bar{X}_2)^2 \\
&= \tfrac{1}{3}\left((11-8.5)^2 + (4-8.5)^2 + (5-8.5)^2 + (14-8.5)^2\right) \\
&= 23
\end{aligned}$$

The covariance matrix is,

$$\begin{aligned}
S &= \begin{bmatrix} \operatorname{Cov}(X_1, X_1) & \operatorname{Cov}(X_1, X_2) \\ \operatorname{Cov}(X_2, X_1) & \operatorname{Cov}(X_2, X_2) \end{bmatrix} \\
&= \begin{bmatrix} 14 & -11 \\ -11 & 23 \end{bmatrix}
\end{aligned}$$

Step 3: Eigenvalues of the covariance matrix

The characteristic equation of the covariance matrix is,

$$\begin{aligned} 0 &= \det(S - \lambda I) \\ &= \begin{vmatrix} 14-\lambda & -11 \\ -11 & 23-\lambda \end{vmatrix} \\ &= (14-\lambda)(23-\lambda) - (-11) \times (-11) \\ &= \lambda^2 - 37\lambda + 201 \end{aligned}$$

Solving the characteristic equation we get,

$$\begin{aligned} \lambda &= \tfrac{1}{2}(37 \pm \sqrt{565}) \\ &= 30.3849,\ 6.6151 \\ &= \lambda_1,\ \lambda_2 \quad \text{(say)} \end{aligned}$$

Step 4: Computation of the eigenvectors

To find the first principal components, we need only compute the eigenvector corresponding to the largest eigenvalue. In the present example, the largest eigenvalue is λ_1 and so we compute the eigenvector corresponding to λ_1.

The eigenvector corresponding to $\lambda = \lambda_1$ is a vector

$$U = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

satisfying the following equation:

$$\begin{aligned} \begin{bmatrix} 0 \\ 0 \end{bmatrix} &= (S - \lambda_1 I)X \\ &= \begin{bmatrix} 14-\lambda_1 & -11 \\ -11 & 23-\lambda_1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \\ &= \begin{bmatrix} (14-\lambda_1)u_1 - 11u_2 \\ -11u_1 + (23-\lambda_1)u_2 \end{bmatrix} \end{aligned}$$

This is equivalent to the following two equations:

$$\begin{aligned} (14-\lambda_1)u_1 - 11u_2 &= 0 \\ -11u_1 + (23-\lambda_1)u_2 &= 0 \end{aligned}$$

Using the theory of systems of linear equations, we note that these equations are not independent and solutions are given by,

$$\frac{u_1}{11} = \frac{u_2}{14-\lambda_1} = t,$$

that is,

$$u_1 = 11t, \quad u_2 = (14-\lambda_1)t,$$

where `t` is any real number.

Taking `t = 1`, we get an eigenvector corresponding to λ_1 as

$$U_1 = \begin{bmatrix} 11 \\ 14-\lambda_1 \end{bmatrix}.$$

To find a unit eigenvector, we compute the length of X_1 which is given by,

$$\begin{aligned} ||U_1|| &= \sqrt{11^2 + (14-\lambda_1)^2} \\ &= \sqrt{11^2 + (14-30.3849)^2} \\ &= 19.7348 \end{aligned}$$

Therefore, a unit eigenvector corresponding to λ_1 is

$$e_1 = \begin{bmatrix} 11/||U_1|| \\ (14-\lambda_1)/||U_1|| \end{bmatrix} = \begin{bmatrix} 11/19.7348 \\ (14-30.3849)/19.7348 \end{bmatrix} = \begin{bmatrix} 0.5574 \\ -0.8303 \end{bmatrix}$$

By carrying out similar computations, the unit eigenvector e_2 corresponding to the eigenvalue $\lambda = \lambda_2$ can be shown to be,

$$e_2 = \begin{bmatrix} 0.8303 \\ 0.5574 \end{bmatrix}$$

Step 5: Computation of first principal components

let,

$$\begin{bmatrix} X_{1k} \\ X_{2k} \end{bmatrix}$$

be the k^{th} sample in the above Table (dataset). The first principal component of this example is given by (here "T" denotes the transpose of the matrix)

$$e_1^T \begin{bmatrix} X_{1k}-\bar{X}_1 \\ X_{2k}-\bar{X}_2 \end{bmatrix} = \begin{bmatrix} 0.5574 & -0.8303 \end{bmatrix} \begin{bmatrix} X_{1k}-\bar{X}_1 \\ X_{2k}-\bar{X}_2 \end{bmatrix} = 0.5574(X_{1k}-\bar{X}_1) - 0.8303(X_{2k}-\bar{X}_2).$$

For example, the first principal component corresponding to the first example

$$\begin{bmatrix} X_{11} \\ X_{21} \end{bmatrix} = \begin{bmatrix} 4 \\ 11 \end{bmatrix}$$

is calculated as follows:

$$\begin{bmatrix} 0.5574 & -0.8303 \end{bmatrix} \begin{bmatrix} X_{11}-\bar{X}_1 \\ X_{21}-\bar{X}_2 \end{bmatrix} = 0.5574(X_{11}-\bar{X}_1) - 0.8303(X_{21}-\bar{X}_2) = 0.5574(4-8) - 0.8303(11-8,5) = -4.30535$$

The results of the calculations are summarised in the below Table.

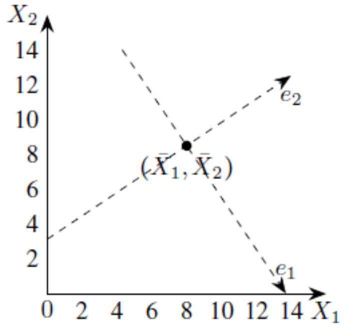
X_1	4	8	13	7
X_2	11	4	5	14
First Principle Components	-4.3052	3.7361	5.6928	-5.1238

Step 6: Geometrical meaning of first principal components

First, we shift the origin to the "center"

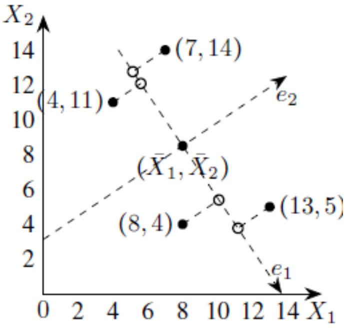
$$(\bar{X}_1, \bar{X}_2)$$

and then change the directions of coordinate axes to the directions of the eigenvectors e_1 and e_2.



The coordinate system for principal components

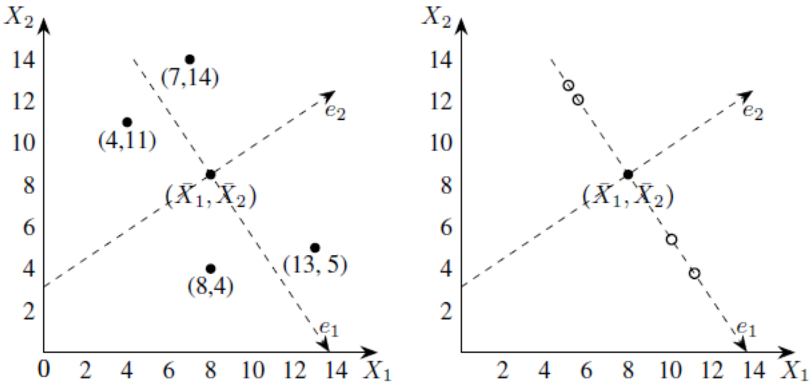
Next, we drop perpendiculars from the given data points to the e1-axis (see below Figure).



Projections of data points on the axis
of the first principal component

The first principal components are the e1-coordinates of the feet of perpendiculars, that is, the projections on the e1-axis. The projections of the data points on the e1-axis may be taken as approximations of the given data points hence we may replace the given data set with these points.

Now, each of these approximations can be unambiguously specified by a single number, namely, the e1-coordinate of approximation. Thus the two-dimensional data set can be represented approximately by the following one-dimensional data set.



Geometrical representation of one-dimensional approximation to the data set