Principal Component Analysis (PCA)

Definition: PCA is an unsupervised technique to project high-dimensional data into a lower-dimensional space by maximizing variance.

Steps:

1. **Standardize Data:** Ensure all features have zero mean and unit variance.
2. **Compute Covariance Matrix**: Measures feature relationships.
3. **Perform EVD**: Find eigenvalues and eigenvectors of the covariance matrix.
4. **Select Top Components:** Select eigenvectors with the largest eigenvalues.
5. **Transform Data**: Project original data onto selected components.

Applications:

- Noise reduction
- Image compression
- Visualization of high-dimensional data.

PCA

Computation of the principal component vectors (PCA algorithm)

The following is an outline of the procedure for performing a principal component analysis on a given data. The procedure is heavily dependent on mathematical concepts. A knowledge of these concepts is essential to carry out this procedure.

Step 1. Data

We consider a dataset having n features or variables denoted by $X_1, X_2, \ldots, X_n$. Let there be N examples. Let the values of the i-th feature X_i be $X_{i1}, X_{i2}, \ldots, X_{iN}$ (see Table 4.1).

Features	Example 1	Example 2	$\cdots$	Example N
X_1	X_{11}	X_{12}	$\cdots$	X_{1N}
X_2	X_{21}	X_{22}	$\cdots$	X_{2N}
$\vdots$				
X_i	X_{i1}	X_{i2}	$\cdots$	X_{iN}
$\vdots$				
X_n	X_{n1}	X_{n2}	$\cdots$	X_{nN}

Table 4.1: Data for PCA algorithm

Step 2. Compute the means of the variables

We compute the mean $\bar{X}_i$ of the variable X_i:

$$\bar{X}_i = \frac{1}{N}(X_{i1} + X_{i2} + \cdots + X_{iN}).$$

Step 3. Calculate the covariance matrix

Consider the variables X_i and X_j (i and j need not be different). The covariance of the ordered pair (X_i, X_j) is defined as[1]

$$\operatorname{Cov}(X_i, X_j) = \frac{1}{N-1}\sum_{k=1}^{N}(X_{ik} - \bar{X}_i)(X_{jk} - \bar{X}_j). \tag{4.1}$$

We calculate the following $n \times n$ matrix S called the covariance matrix of the data. The element in the i-th row j-th column is the covariance $\operatorname{Cov}(X_i, X_j)$:

$$S = \begin{bmatrix} \operatorname{Cov}(X_1, X_1) & \operatorname{Cov}(X_1, X_2) & \cdots & \operatorname{Cov}(X_1, X_n) \\ \operatorname{Cov}(X_2, X_1) & \operatorname{Cov}(X_2, X_2) & \cdots & \operatorname{Cov}(X_2, X_n) \\ \vdots & & & \\ \operatorname{Cov}(X_n, X_1) & \operatorname{Cov}(X_n, X_2) & \cdots & \operatorname{Cov}(X_n, X_n) \end{bmatrix}$$

Step 4. Calculate the eigenvalues and eigenvectors of the covariance matrix

Let S be the covariance matrix and let I be the identity matrix having the same dimension as the dimension of S.

i) Set up the equation:

$$\det(S - \lambda I) = 0. \tag{4.2}$$

This is a polynomial equation of degree n in λ. It has n real roots (some of the roots may be repeated) and these roots are the eigenvalues of S. We find the n roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of Eq. (4.2).

ii) If $\lambda = \lambda'$ is an eigenvalue, then the corresponding eigenvector is a vector

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

such that

$$(S - \lambda' I)U = 0.$$

(This is a system of n homogeneous linear equations in u_1, u_2, …, u_n and it always has a nontrivial solution.) We next find a set of n orthogonal eigenvectors $U_1, U_2, \ldots, U_n$ such that U_i is an eigenvector corresponding to λ_i.[2]

iii) We now normalise the eigenvectors. Given any vector X we normalise it by dividing X by its length. The length (or, the norm) of the vector

$$X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

is defined as

$$||X|| = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}.$$

Given any eigenvector U, the corresponding normalised eigenvector is computed as

$$\frac{1}{||U||}U.$$

We compute the n normalised eigenvectors $e_1, e_2, \ldots, e_n$ by

$$e_i = \frac{1}{||U_i||}U_i, \quad i = 1, 2, \ldots, n.$$

Step 5. Derive new data set

Order the eigenvalues from highest to lowest. The unit eigenvector corresponding to the largest eigenvalue is the first principal component. The unit eigenvector corresponding to the next highest eigenvalue is the second principal component, and so on.

i) Let the eigenvalues in descending order be $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ and let the corresponding unit eigenvectors be $e_1, e_2, \ldots, e_n$.

ii) Choose a positive integer p such that $1 \leq p \leq n$.

iii) Choose the eigenvectors corresponding to the eigenvalues λ_1, λ_2, ..., λ_p and form the following $p \times n$ matrix (we write the eigenvectors as row vectors):

$$F = \begin{bmatrix} e_1^T \\ e_2^T \\ \vdots \\ e_p^T \end{bmatrix},$$

where T in the superscript denotes the transpose.

iv) We form the following $n \times N$ matrix:

$$X = \begin{bmatrix} X_{11} - \bar{X}_1 & X_{12} - \bar{X}_1 & \cdots & X_{1N} - \bar{X}_1 \\ X_{21} - \bar{X}_2 & X_{22} - \bar{X}_2 & \cdots & X_{2N} - \bar{X}_2 \\ \vdots & & & \\ X_{n1} - \bar{X}_n & X_{n2} - \bar{X}_n & \cdots & X_{nN} - \bar{X}_n \end{bmatrix}$$

v) Next compute the matrix:

$$X_{\text{new}} = FX.$$

Note that this is a $p \times N$ matrix. This gives us a dataset of N samples having p features.

Step 6. New dataset

The matrix X_{new} is the new dataset. Each row of this matrix represents the values of a feature. Since there are only p rows, the new dataset has only features.

Step 7. Conclusion

This is how the principal component analysis helps us in dimensional reduction of the dataset. Note that it is not possible to get back the original n-dimensional dataset from the new dataset.

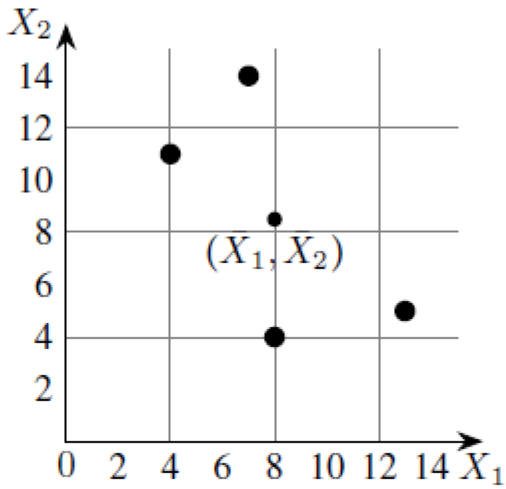
Problem definition

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:

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

The covariance matrix is,

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

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

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

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)

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

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.

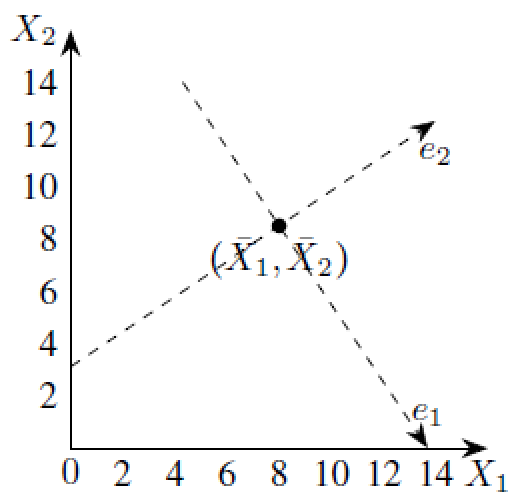
X_1	4	8	13	7
X_2	11	4	5	14
First Principle Components	-4.3052	3.7361	5.6928	-5.1238

Step 6: Geometrical meaning of first principal components

First, we shift the origin to the "center"

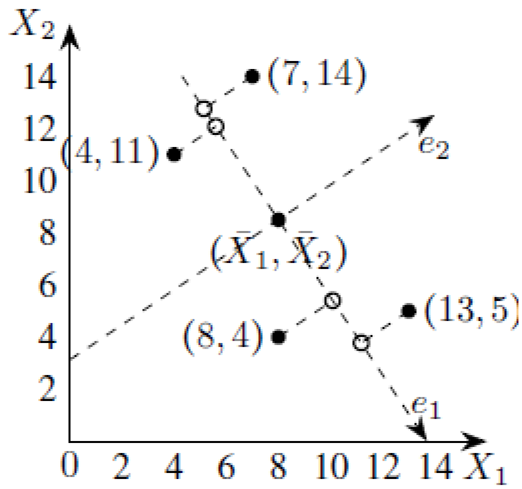
$$(\bar{X}_1, \bar{X}_2)$$

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

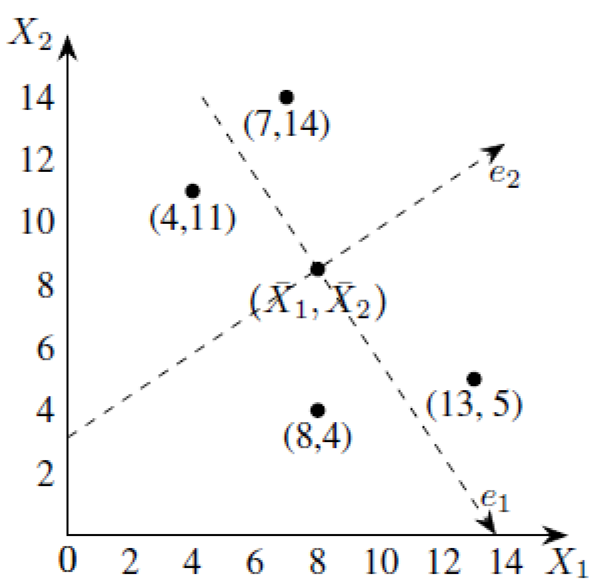
Next, we drop perpendiculars from the given data points to the e1-axis (see below Figure).

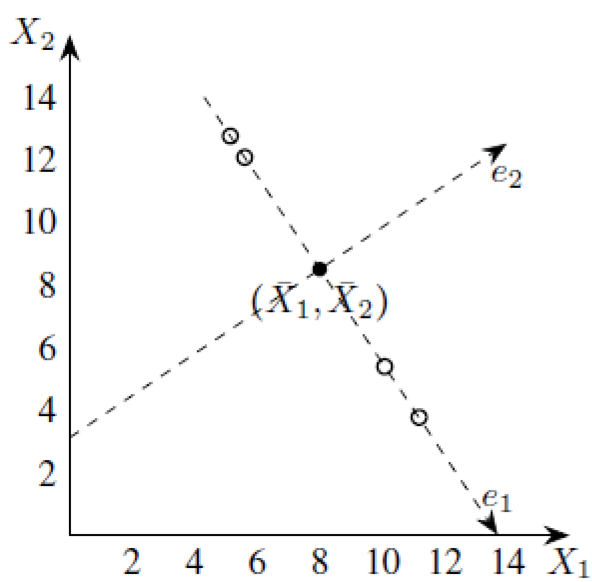


Projections of data points on the axis of the first principal component

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