Principal Components Analysis (PCA)

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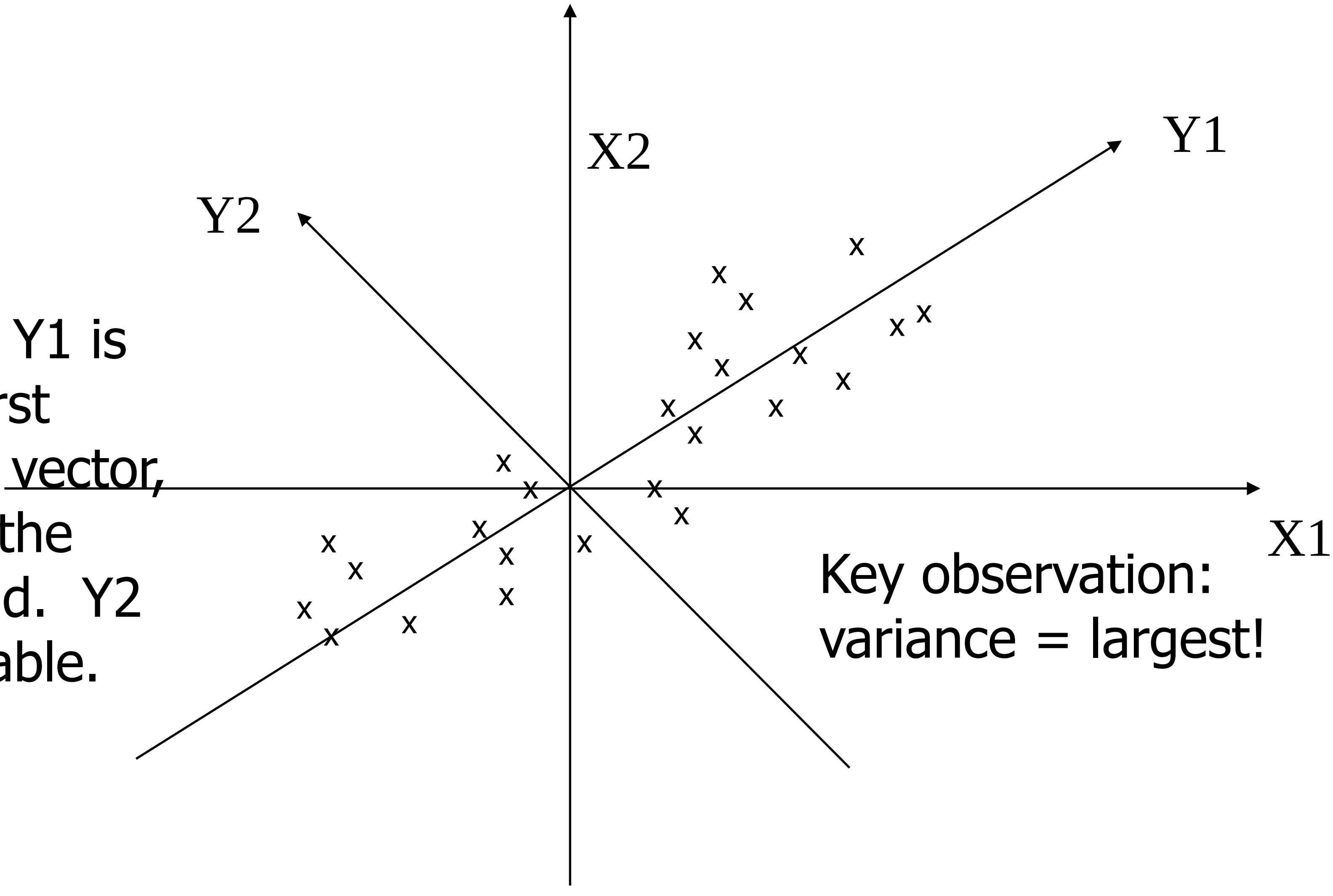
- An exploratory technique used to reduce the dimensionality of the data set
- Can be used to:
  - Reduce number of dimensions in data
  - Find patterns in high-dimensional data
  - Visualize data of high dimensionality
- Example applications:
  - Face recognition
  - Image compression
  - Gene expression analysis

Principal Components Analysis Ideas (PCA)

- Does the data set ‘span’ the whole of d dimensional space?
- For a matrix of *m* samples x *n* genes, create a new covariance matrix of size *n* x *n*.
- Transform some large number of variables into a smaller number of uncorrelated variables called principal components (PCs).
- developed to capture as much of the variation in data as possible

Principal Component Analysis



Note: Y1 is the first eigen vector, Y2 is the second. Y2 ignorable.

Key observation: variance = largest!

Two dimension attribute

Covariance: measures the correlation between X and Y

$$\operatorname{cov}(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y})}{(n-1)}$$

X=Temperature	Y=Humidity
40	90
40	90
40	90
30	90
15	70
15	70
15	70
30	90
15	70
30	70
30	70
30	90
40	70
30	90

More than two attributes: covariance matrix

- Contains covariance values between all possible dimensions (=attributes):

$$C^{nxn} = (c_{ij} \mid c_{ij} = \mathrm{cov}(Dim_i, Dim_j))$$

- Example for three attributes (x,y,z):

$$C = \begin{pmatrix} \mathrm{cov}(x,x) & \mathrm{cov}(x,y) & \mathrm{cov}(x,z) \\ \mathrm{cov}(y,x) & \mathrm{cov}(y,y) & \mathrm{cov}(y,z) \\ \mathrm{cov}(z,x) & \mathrm{cov}(z,y) & \mathrm{cov}(z,z) \end{pmatrix}$$

Principal components

1. principal component (PC1)
   – The eigenvalue with the largest absolute value will indicate that the data have the largest variance along its eigenvector, the direction along which there is greatest variation
2. principal component (PC2)
   – the direction with maximum variation left in data, orthogonal to the PC1

- In general, only few directions manage to capture most of the variability in the data.

Steps of PCA

- Step 1: Compute the Mean (Centering the Data)
- Step 2: Compute the Covariance Matrix
- Step 3: Compute Eigenvalues and Eigenvectors
- Step 4: Transform the Data into Principal Components
- Step 5: Interpretation

Example for PCA

Point	**X**	**y**
A	0.5	1.2
B	1.0	1.8
C	1.2	1.5
D	3.8	3.2
E	3.9	3.8
F	4.5	4.2
G	2.0	2.2
H	2.3	2.0

Solution

Step 1: Compute the Mean (Centering the Data)

Point	**X**	**y**
A	0.5	1.2
B	1.0	1.8
C	1.2	1.5
D	3.8	3.2
E	3.9	3.8
F	4.5	4.2
G	2.0	2.2
H	2.3	2.0

$$\bar{x} = \frac{0.5 + 1.0 + 1.2 + 3.8 + 3.9 + 4.5 + 2.0 + 2.3}{8} = \frac{19.2}{8} = 2.40$$

$$\bar{y} = \frac{1.2 + 1.8 + 1.5 + 3.2 + 3.8 + 4.2 + 2.2 + 2.0}{8} = \frac{19.9}{8} = 2.49$$

Solution

Step 2: Compute the Covariance Matrix

- Compute the Mean-Centered Data (Subtract the mean from each value)

Point	$X' = \mathbf{x} - \bar{x}$	$Y' = \mathbf{y} - \bar{y}$
A	-1.90	-1.29
B	-1.40	-0.69
C	-1.20	-0.99
D	1.40	0.71
E	1.50	1.31
F	2.10	1.71
G	-0.40	-0.29
H	-0.10	-0.49

Solution

Step 2: Compute the Covariance Matrix

$$\mathrm{Cov}(X', Y') = \frac{1}{n-1} \sum (X'_i \cdot Y'_i)$$

$$\mathrm{Var}(X') = \frac{1}{n-1} \sum (X'_i)^2$$

$$\mathrm{Var}(Y') = \frac{1}{n-1} \sum (Y'_i)^2$$

$$\mathrm{cov}(X, Y) = \frac{\sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

The covariance has the following properties:

Cov(X,X)=Var(X)

Solution

Step 2: Compute the Covariance Matrix

$$\sum(X')^2 = (-1.90)^2 + (-1.40)^2 + (-1.20)^2 + (1.40)^2 + (1.50)^2 + (2.10)^2 + (-0.40)^2 + (-0.10)^2$$

$$= 3.61 + 1.96 + 1.44 + 1.96 + 2.25 + 4.41 + 0.16 + 0.01 = 15.80$$

$$\text{Var}(X') = \frac{15.80}{7} = 2.257$$

$$\sum(Y')^2 = (-1.29)^2 + (-0.69)^2 + (-0.99)^2 + (0.71)^2 + (1.31)^2 + (1.71)^2 + (-0.29)^2 + (-0.49)^2$$

$$= 1.6641 + 0.4761 + 0.9801 + 0.5041 + 1.7161 + 2.9241 + 0.0841 + 0.2401 = 8.5888$$

$$\text{Var}(Y') = \frac{8.5888}{7} = 1.227$$

Solution

Step 2: Compute the Covariance Matrix

$$\sum(X' \cdot Y') = (-1.90)(-1.29) + (-1.40)(-0.69) + (-1.20)(-0.99) + (1.40)(0.71) + (1.50)(1.31) + (2.10)(1.71) + (-0.40)(-0.29) + (-0.10)(-0.49)$$

$$= 2.451 + 0.966 + 1.188 + 0.994 + 1.965 + 3.591 + 0.116 + 0.049 = 11.32$$

$$\mathrm{Cov}(X', Y') = \frac{11.32}{7} = 1.617$$

$$C = \begin{bmatrix} \mathrm{Var}(X') & \mathrm{Cov}(X', Y') \\ \mathrm{Cov}(Y', X') & \mathrm{Var}(Y') \end{bmatrix}$$

$$C = \begin{bmatrix} 2.257 & 1.617 \\ 1.617 & 1.227 \end{bmatrix}$$

Solution

Step 3: Compute Eigenvalues and Eigenvectors

Eigenvalues λ are found by solving the characteristic equation:

$$\det(C-\lambda I)=0$$

where I is the identity matrix:

$$\begin{bmatrix} 2.257 & 1.617 \\ 1.617 & 1.227 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2.257-\lambda & 1.617 \\ 1.617 & 1.227-\lambda \end{bmatrix}$$

The determinant of this matrix is:

$$(2.257-\lambda)(1.227-\lambda)-(1.617)(1.617)=0$$

Expanding:

$$(2.257-\lambda)(1.227-\lambda)-1.617^2=0$$

$$2.257\cdot 1.227-2.257\lambda-1.227\lambda+\lambda^2-2.616=0$$

$$2.772-3.484\lambda+\lambda^2-2.616=0$$

$$\lambda^2-3.484\lambda+0.156=0$$

Solution

Step 3: Compute Eigenvalues and Eigenvectors

Solving the quadratic equation:

$$\lambda = \frac{-(-3.484) \pm \sqrt{(-3.484)^2 - 4(1)(0.156)}}{2(1)}$$

$$\lambda = \frac{3.484 \pm \sqrt{12.147 - 0.624}}{2}$$

$$\lambda = \frac{3.484 \pm \sqrt{11.523}}{2}$$

Approximating:

$$\lambda = \frac{3.484 \pm 3.394}{2}$$

Thus, the two eigenvalues are:

$$\lambda_1 = \frac{3.484 + 3.394}{2} = \frac{6.878}{2}$$

=3.439

$$\lambda_2 = \frac{3.484 - 3.394}{2} = \frac{0.090}{2} = 0.045$$

Solution

Step 3: Compute Eigenvalues and Eigenvectors

To find the eigenvectors, we solve:

$$(C - \lambda I)v = 0$$

Eigenvector for $\lambda_1 = 3.439$:

$$\begin{bmatrix} 2.257 - 3.439 & 1.617 \\ 1.617 & 1.227 - 3.439 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} -1.182 & 1.617 \\ 1.617 & -2.212 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Solving for x and y:

$$-1.182x + 1.617y = 0 \quad \Rightarrow \quad x = \frac{1.617}{1.182}y$$

Approximating:

$$x = 1.37y$$

Solution

Step 3: Compute Eigenvalues and Eigenvectors

Choosing $y = 1$:

$$v_1 = \begin{bmatrix} 1.37 \\ 1 \end{bmatrix}$$

$$\boxed{\begin{gathered} y = \frac{0.6}{0.8} \cdot x \\ y = 0.75x \end{gathered}}$$

Normalizing:

$$\|v\| = \sqrt{x^2 + y^2}$$

$$v_{\text{normalized}} = \frac{1}{\|v\|} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$v_1 = \begin{bmatrix} 0.8 \\ 0.6 \end{bmatrix}$$

This means that for every 1 unit moved in the X-direction, we move 0.6/0.8 = 0.75 units in the Y-direction.

Eigenvector for $\lambda_2 = 0.045$:

$$\begin{bmatrix} 2.257 - 0.045 & 1.617 \\ 1.617 & 1.227 - 0.045 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 2.212 & 1.617 \\ 1.617 & 1.182 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Solution

Step 3: Compute Eigenvalues and Eigenvectors

Solving:

$$2.212x + 1.617y = 0 \quad \Rightarrow \quad x = -\frac{1.617}{2.212}y$$

Approximating:

$$x = -0.73y$$

Choosing $y = 1$:

$$v_2 = \begin{bmatrix} -0.73 \\ 1 \end{bmatrix}$$

Normalizing:

$$v_2 = \begin{bmatrix} -0.6 \\ 0.8 \end{bmatrix}$$

Solution

Step 4: Transform the Data into Principal Components

$$\text{New Data} = V^T \cdot X'$$

Where:

- X' is the **centered data matrix** (mean-subtracted original data).
- V is the matrix of **eigenvectors**.
- V^T is the **transpose** of the eigenvector matrix.
- **New Data** represents the **transformed data** in the new PCA coordinate system.

We obtained the **normalized eigenvectors** as:

$$V = \begin{bmatrix} 0.8 & -0.6 \\ 0.6 & 0.8 \end{bmatrix}$$

Each column represents a **principal component** (PC1 and PC2).

Solution

Step 4: Transform the Data into Principal Components

We compute:

$$\text{New Data} = V^T \cdot X'$$

1. **Transpose the eigenvector matrix V:**

$$V^T = \begin{bmatrix} 0.8 & 0.6 \\ -0.6 & 0.8 \end{bmatrix}$$

2. **Multiply V^T by the centered data X':**

For each data point (x', y'):

$$\begin{bmatrix} PC_1 \\ PC_2 \end{bmatrix} = \begin{bmatrix} 0.8 & 0.6 \\ -0.6 & 0.8 \end{bmatrix} \cdot \begin{bmatrix} x' \\ y' \end{bmatrix}$$

Which expands to:

$$PC_1 = 0.8x' + 0.6y'$$

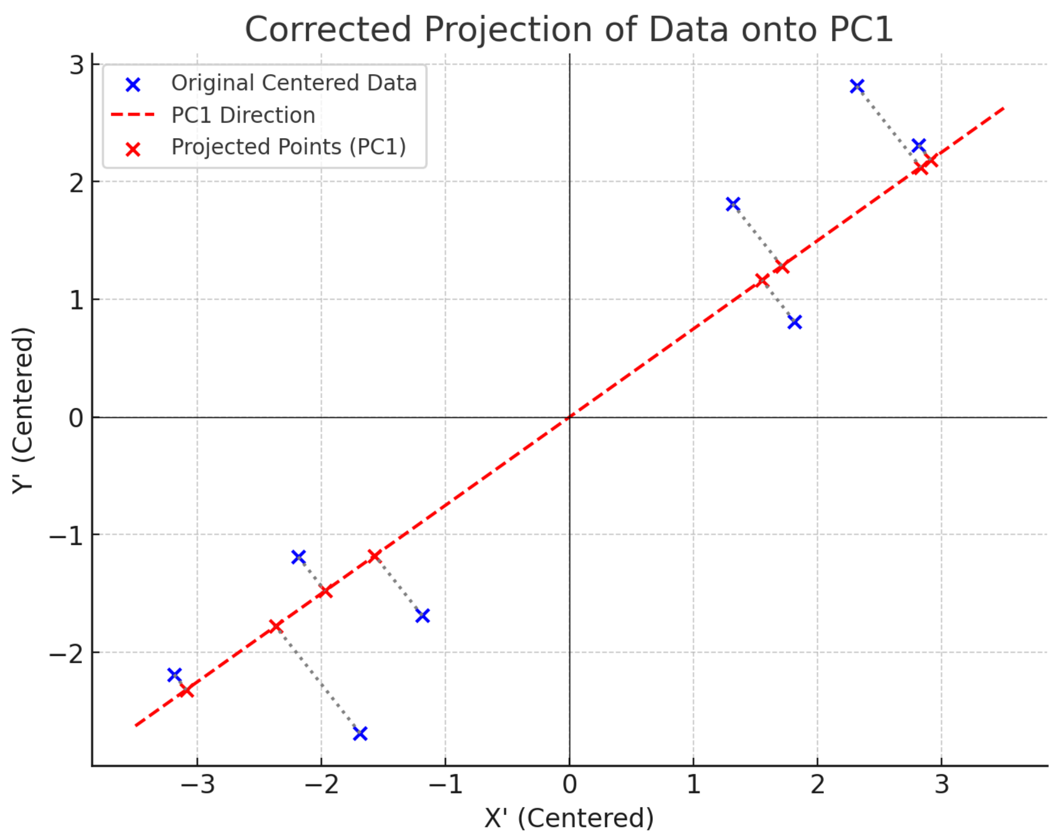
$$PC_2 = -0.6x' + 0.8y'$$

Point	X'**=x-**$\bar{x}$	Y'**=y-**$\bar{y}$
A	-1.90	-1.29
B	-1.40	-0.69
C	-1.20	-0.99
D	1.40	0.71
E	1.50	1.31
F	2.10	1.71
G	-0.40	-0.29
H	-0.10	-0.49

Solution

Step 4: Transform the Data into Principal Components

$$PC_1 = \begin{array}{c} -2.294 \\ \hline -1.536 \\ \hline -1.552 \\ \hline 1.551 \\ \hline 1.986 \\ \hline 2.706 \\ \hline -0.493 \\ \hline -0.368 \end{array}$$



Practice Problem

2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9