Week 14: Principal Component Analysis (PCA)

Ekarat Rattagan

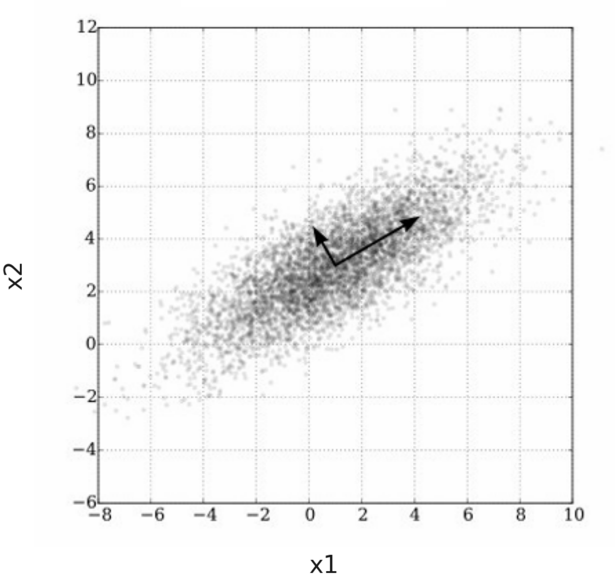
July 28, 2025

Principal Components Analysis (PCA)

- PCA: most popular instance of the second main class of unsupervised learning methods
- Projection methods, aka **dimensionality-reduction** methods
- Given dataset $\mathbf{X} \in \mathbb{R}^{N \times D}$
- D may be huge.
- We want to find dataset $\mathbf{Z} \in \mathbb{R}^{N \times K}$, where $K \ll D$

Principal Components Analysis (PCA)

- Aim: find a small number of directions in input space that explain variation in input data; re-represent data by projecting along those directions.
- Important assumption: variation contains information


x2
x1
12
10
8
6
4
2
0
−2
−4
−6
−8
−6
−4
−2
0
2
4
6
8
10

Principal Components Analysis (PCA)

- 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

Steps of PCA

1. Let $\bar{X}$ be the mean vector (mean of each column)
2. Adjust the original data: $X' = X - \bar{X}$
3. Compute the covariance matrix A of X'
4. Find the eigenvectors and eigenvalues of A

How does SVM works? (1/3)

X_1	X_2
1	3
2	3
3	4
3	5
4	4
4	6
5	6
5	7
6	8
7	8

Table: Sample data for variables X_1 and X_2

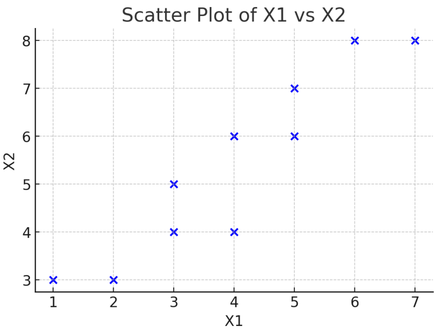


Figure: A scatter plot of X_1 and X_2

Step 1 and 2: Centering the Data

1. Mean of column $X_1 = 4$
2. Mean of column $X_2 = 5.4$
3. Subtract these means from each value in the respective columns
4. Resulting X_1', X_2' are centered data

X_1	X_2	X_1'	X_2'
1	3	-3	-2.4
2	3	-2	-2.4
3	4	-1	-1.4
3	5	-1	-0.4
4	4	0	-1.4
4	6	0	0.6
5	6	1	0.6
5	7	1	1.6
6	8	2	2.6
7	8	3	2.6
4	5.4		

Step 1 and 2: Centering the Data

X_1	X_2	X_1'	X_2'
1	3	-3	-2.4
2	3	-2	-2.4
3	4	-1	-1.4
3	5	-1	-0.4
4	4	0	-1.4
4	6	0	0.6
5	6	1	0.6
5	7	1	1.6
6	8	2	2.6
7	8	3	2.6
4	5.4		

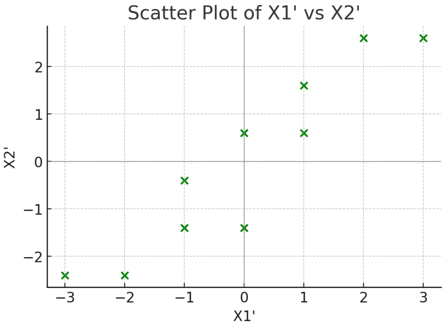


Figure: A scatter plot of X_1' and X_2'

Review: Covariance matrix

- Covariance measures the correlation between X_1' and X_2'

$$\text{cov}(X_1', X_2') = \frac{\sum_{i=1}^{n} (X_{1,i}' - \bar{X'_{1,i}})(X_{2,i}' - \bar{X'_{2,i}})}{n-1}$$

- $\text{Cov}(X_1', X_2') = 0$: independent
- $\text{Cov}(X_1', X_2') > 0$: move same direction
- $\text{Cov}(X_1', X_2') < 0$: move opposite direction
- What is a correlation matrix? How does it differ from a covariance matrix?

Step 3: Covariance Matrix Calculation

- Use the result from step 2 to calculate covariance matrix A.
- $A = \begin{bmatrix} \text{cov}(X_1', X_1') & \text{cov}(X_1', X_2') \\ \text{cov}(X_2', X_1') & \text{cov}(X_2', X_2') \end{bmatrix}$
- We obtain, $A = \begin{bmatrix} 3.33 & 3.22 \\ 3.22 & 3.60 \end{bmatrix}$
- Example for $\text{cov}(X_1', X_1')$:

$$\text{cov}(X_1', X_1') = \frac{1}{9}\sum_{i=1}^{10}(X_{1,i}' - \bar{X_{1,i}'})^2 = \frac{30}{9} = 3.33$$

Step 4: Compute Eigenvector and Eigenvalue

Review: Eigenvector and Eigenvalue

- An eigenvector of a square $n \times n$ matrix $\mathbf{A}$ is a non-zero vector $\mathbf{x}$ such that, when $\mathbf{x}$ is multiplied on the left by $\mathbf{A}$, it yields a constant multiple of $\mathbf{x}$. That is: $\mathbf{Ax} = \lambda\mathbf{x}$. The number λ is called the eigenvalue of $\mathbf{A}$ corresponding to the eigenvector $\mathbf{x}$. Reference [www.ncl.ac.uk]
- In $A\mathbf{x} = \lambda\mathbf{x}$.

$$\begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 2 \end{bmatrix} = \begin{bmatrix} 12 \\ 8 \end{bmatrix} = 4 \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

To find Eigenvector and Eigenvalue

- We first have, $A\mathbf{x} = \lambda\mathbf{x}$
- then, $A\mathbf{x} - \lambda\mathbf{x} = 0$
- next, $(A - \lambda I)\mathbf{x} = 0$, where I is the $n \times n$ identity matrix.
- For non-zero solutions to exist, the matrix $(A - \lambda I)$ must be singular (not invertible). Thus, the condition for a matrix to be singular is $\det(A - \lambda I) = 0$
- Example:

$$A = \begin{bmatrix} 3.33 & 3.22 \\ 3.22 & 3.60 \end{bmatrix}$$

$$\det(A - \lambda I) = (3.33 - \lambda)(3.60 - \lambda) - (3.22)^2 = 0$$

$$\Rightarrow \lambda_1 = 0.24, \quad \lambda_2 = 6.69$$

Step 4: Eigenvectors from Python

- Eigenvectors:

$$\mathbf{x}_1 = (-0.722, 0.692), \qquad \lambda_1 = 0.24$$
$$\mathbf{x}_2 = (0.6923, 0.722), \qquad \lambda_2 = 6.69$$

- Eigenvectors satisfy:

$$A \begin{bmatrix} x \\ y \end{bmatrix} = 6.69 \begin{bmatrix} x \\ y \end{bmatrix}$$

Reference

- Greenacre, M., Groenen, P. J., Hastie, T., d'Enza, A. I., Markos, A., and Tuzhilina, E. (2022). Principal component analysis. Nature Reviews Methods Primers, 2(1), 100.