

# (Linear) Principal Component Analysis

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A statistical technique used for dimensionality reduction that transforms data into a new coordinate system, maximizing variance along new axes (principal components).

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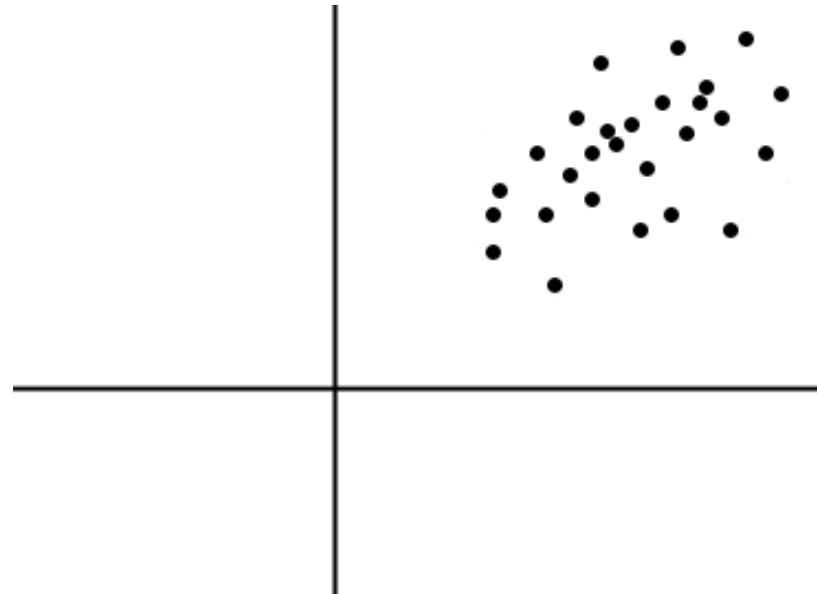
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## Applications

- Multivariate statistics
- Cluster analysis
- Data reduction
- Feature extraction
- Image processing



Source: [Ten07]

## What are we aiming for?

- **Structure identification** in the data
- **Extraction of meaningful features**
- **Data reduction** to most expressive information → Project into  $k$ -dimensional space ( $k < M$ ) with minimal information loss

# First step: Centering the Data in the Origin

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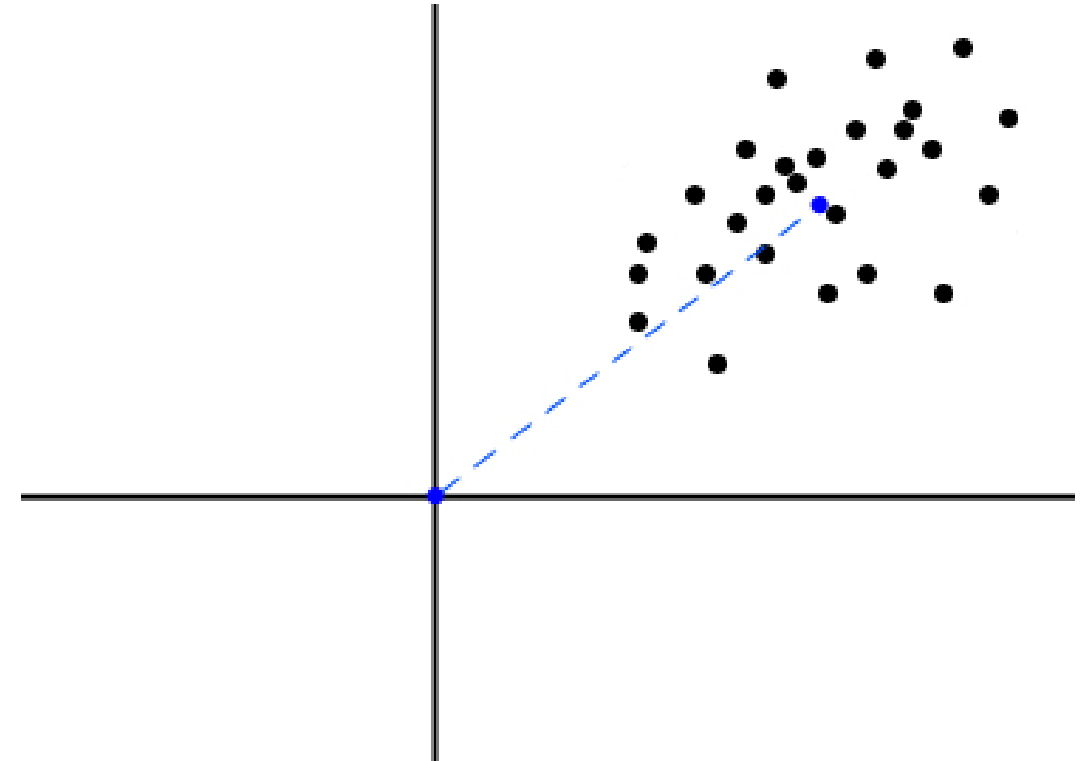
**Mean Value:**

$$\overline{X} = \frac{1}{N} \sum_{i=1}^N x^{(i)}$$

**Centering the Data:** For each data point, subtract the computed mean:

$$y^{(i)} = x^{(i)} - \overline{X}, \quad i = 1, \dots, N$$

- The resulting dataset centered around the origin
- Shows the **correlation** structure between variables



Source: [Ten07]

# Second Step:

## Covariance Matrix

### Covariance Matrix

The covariance matrix  $C \in \mathbb{R}^{M \times M}$  is defined as:

$$C := \frac{1}{N} \sum_{i=1}^N y^{(i)} y^{(i)T}$$

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### Interpretation:

- $\text{Cov}(X, Y) > 0$  : Dimensions increase together.
- $\text{Cov}(X, Y) < 0$  : One dimension increases, the other decreases.
- $\text{Cov}(X, Y) = 0$  : Dimensions are independent.

$$C(X) = \begin{bmatrix} \text{Cov}(X^{(1)}, X^{(1)}) & \text{Cov}(X^{(1)}, X^{(2)}) & \dots & \text{Cov}(X^{(1)}, X^{(n)}) \\ \text{Cov}(X^{(2)}, X^{(1)}) & \text{Cov}(X^{(2)}, X^{(2)}) & \dots & \text{Cov}(X^{(2)}, X^{(n)}) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(X^{(n)}, X^{(1)}) & \text{Cov}(X^{(n)}, X^{(2)}) & \dots & \text{Cov}(X^{(n)}, X^{(n)}) \end{bmatrix}$$

- **alternative data representation:**  $y^{(i)} \in \mathbb{R}^M \rightarrow z^{(i)} \in \mathbb{R}^k$
- Based on **orthogonal vectors** (principal components)
- Align vectors with directions of **highest variance**
- Ensure data representation is **uncorrelated**:
  - $\text{Cov}(z_j, z_l) = 0$  for  $j \neq l$
  - Diagonalize the covariance matrix  $C$

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- **Orthonormal Eigenvectors:** The eigenvectors of  $C$  are orthonormal, as  $C$  is symmetric.

## Spectral Theorem

- $C \in \mathbb{R}^{M \times M}$ : A real symmetric matrix.
- There exists an orthogonal matrix  $A$  such that:

$$A^T C A = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_M \end{pmatrix}$$

where  $\lambda_1, \dots, \lambda_M \in \mathbb{R}$  are the eigenvalues of  $C$ .

- The columns of  $A$  are the orthonormal eigenvectors of  $C$ .

[LK23]

# Third step:

## Solving Eigenvalue problem

### Eigenvalue equation

$$Cv = \lambda v$$

where:

- $v$  is the **eigenvector**.
- $\lambda$  is the **eigenvalue**.

Rearranging the equation:

$$Cv - \lambda Iv = 0 \quad \Rightarrow \quad (C - \lambda I)v = 0$$

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**solution can be found by methods:**

- Roots of characteristic polynomial
- QR algorithm
- Singular value decomposition

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## Transformation Matrix

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**Transformation Matrix:**

$$T := (v^{(1)}, \dots, v^{(k)}) \in \mathbb{R}^{M \times k}$$

where  $v^{(1)}, \dots, v^{(k)}$  are the eigenvectors corresponding to the largest eigenvalues  $k$ , with  $1 \leq k \leq M$ .

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## Principal Component Transformation

- Transform the data:

$$z^{(i)} := T^T y^{(i)}, \quad \text{for } i = 1, \dots, N$$

- $z^{(i)} \in \mathbb{R}^k$  : the transformed data containing the most relevant features of the input data.
- The components  $z_j^{(i)}, j = 1, \dots, k \rightarrow$  **principal components**.
- If  $T$  is quadratic ( $k = M$ ), PCA reduces to a simple rotation in  $\mathbb{R}^M$ .



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7. Compute the principal components for each centered input point  $y^{(i)}$  using:

$$T^T y^{(i)} = z^{(i)} \in \mathbb{R}^k$$

## Example Data:

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

**Task:** Reduce the dimension from 2D to 1D using the PCA algorithm.

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**Task:** Reduce the dimension from 2D to 1D using the PCA algorithm.

## Step 1: Calculate Mean

$$\bar{X} = \frac{1}{4} \begin{pmatrix} 4 + 8 + 13 + 7 \\ 11 + 4 + 5 + 14 \end{pmatrix} = \begin{pmatrix} 8 \\ 8.5 \end{pmatrix}$$

## Step 2: Center the Data

$$Y^{(1)} = \begin{pmatrix} 4 \\ 11 \end{pmatrix} - \begin{pmatrix} 8 \\ 8.5 \end{pmatrix} = \begin{pmatrix} -4 \\ 2.5 \end{pmatrix}$$

$$Y^{(2)} = \begin{pmatrix} 8 \\ 4 \end{pmatrix} - \begin{pmatrix} 8 \\ 8.5 \end{pmatrix} = \begin{pmatrix} 0 \\ -4.5 \end{pmatrix}$$

$$Y^{(3)} = \begin{pmatrix} 13 \\ 5 \end{pmatrix} - \begin{pmatrix} 8 \\ 8.5 \end{pmatrix} = \begin{pmatrix} 5 \\ -3.5 \end{pmatrix}$$

$$Y^{(4)} = \begin{pmatrix} 7 \\ 14 \end{pmatrix} - \begin{pmatrix} 8 \\ 8.5 \end{pmatrix} = \begin{pmatrix} -1 \\ 5.5 \end{pmatrix}$$

# Step 3: Compute the Covariance Matrix

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Compute the covariance matrix:

$$C = \frac{1}{3} \begin{bmatrix} -4 & 0 & 5 & -1 \\ 2.5 & -4.5 & -3.5 & 5.5 \end{bmatrix} \cdot \begin{bmatrix} -4 & 2.5 \\ 0 & -4.5 \\ 5 & -3.5 \\ -1 & 5.5 \end{bmatrix}.$$

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Simplify:

$$C = \begin{pmatrix} 14 & -11 \\ -11 & 23 \end{pmatrix}.$$

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The characteristic equation of  $C$ :

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

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Solving the quadratic equation:

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

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Eigenvectors corresponding to the eigenvalues:

$$v_1 = \begin{pmatrix} 0.5574 \\ -0.8303 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 0.8303 \\ 0.5574 \end{pmatrix}.$$

# Step 5: Select Eigenvectors

## Step 5: Select $k$ Eigenvectors:

After sorting eigenvalues, we select the eigenvectors corresponding to the largest eigenvalues:

$$\lambda_1 = 30.3849, \quad \lambda_2 = 6.6151.$$

Corresponding eigenvectors:

$$v_1 = \begin{pmatrix} 0.5574 \\ -0.8303 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 0.8303 \\ 0.5574 \end{pmatrix}.$$

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# Step 6: Compute Principal Components

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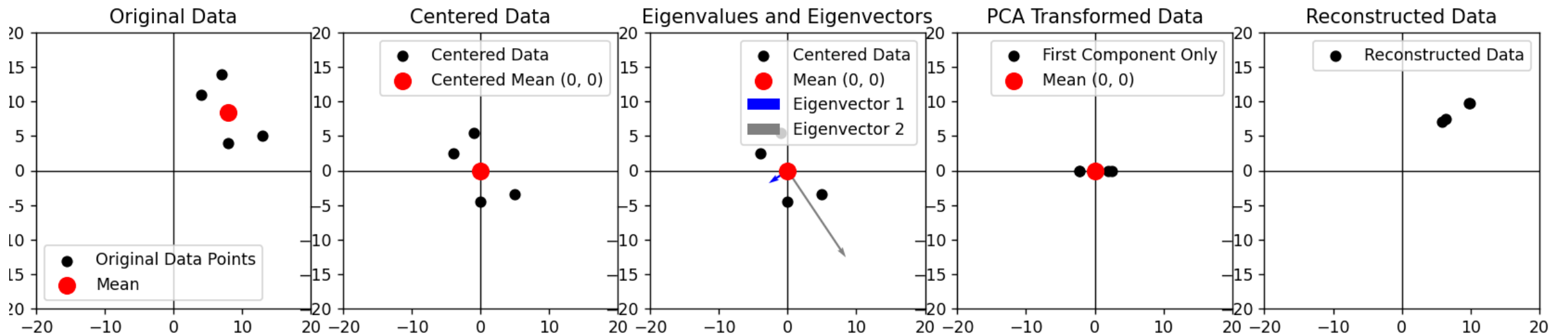
$$Z = T^T Y,$$

where:

$$T^T = (0.5574 \ -0.8303), \quad Y = \begin{pmatrix} -4 & 0 & 5 & -1 \\ 2.5 & -4.5 & -3.5 & 5.5 \end{pmatrix}.$$

**- first principal component for centered data :**

$$z_1 = (-4.31 \ 3.74 \ 5.69 \ -5.12).$$



## Data Reconstruction

Reconstructing the centered input data from its principal components is (partially) possible via:

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In our example:

$$T = \begin{pmatrix} 0.5574 & 0.8303 \end{pmatrix}^T, \quad Z = \begin{pmatrix} -4.31 & 3.74 & 5.69 & -5.12 \end{pmatrix}.$$

Full reconstruction uses all components:

$$Y = TZ.$$

Partial reconstruction (using fewer components) causes a **loss of information**.



- **Computational complexity:**

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If the variables were uncorrelated, PCA orders them according to their variance.

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- **Only Uses the Mean and Covariance**

## References

- [Far22] R. W. Farebrother. “Notes on the prehistory of principal components analysis”. In: *Journal of Multivariate Analysis* 188 (2022). 50th Anniversary Jubilee Edition, p. 104814. DOI: <https://doi.org/10.1016/j.jmva.2021.104814>.
- [LK23] M. Lachut and B. Keigwin. “Applications of the Spectral Theorem: Utilizing Eigenvalues and Eigenvectors”. In: *Journal of Student Research* 12.4 (2023).
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