Principal Component Analysis

Tutorial

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Principal Component Analysis (PCA)

- Step-1: Data matrix X has n data points, each data point consists of m features

  $X = \begin{bmatrix} x_i & x_2 & x_3 & \dots & x_n \end{bmatrix}$ where each $x_i = \begin{bmatrix} feature_1 \\ feature_2 \\ \vdots \\ feature_m \end{bmatrix}$

- Step-2: Find the mean vector of data points
  $\bar{X} = \Sigma_{i=1}^{n} \frac{1}{n} x_i$
- Step-3: Subtract mean vector from the given data points
  $X - \bar{X} = \begin{bmatrix} x_i - \bar{x} & x_2 - \bar{x} & x_3 - \bar{x} & \dots & x_n - \bar{x} \end{bmatrix}$
- Step-4: Find the covariance matrix C (A symmetric mxm matrix)
  $C = \frac{1}{n} \Sigma_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})^T$

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Principal Component Analysis (PCA)

- Step-5: Write the characteristic equation
  $(C - \lambda I)\ u_j = 0$
- Step-6: Find the eigen vectors and eigen values of matrix C
  Eigen value matrix: $\Lambda = \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \dots & \lambda_n \end{bmatrix}$, Corresponding eigen vector matrix: $U = \begin{bmatrix} u_1 & u_2 & \dots & u_n \end{bmatrix}$ where each $u_j = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix}$
- Step-7: Choose eigen vectors corresponding to top k eigen values and derive the transformed data points
  $\tilde{x}_i = \Sigma_{j=1}^{k} \alpha_j u_j$ where $\alpha_j = (x_i^T u_j)$
- Step-8: Calculate the reconstruction error and projected variance
  Reconstruction Error $= J = \frac{1}{n}\Sigma_{i=1}^{n}||x_i - \tilde{x}_i||^2$,
  Projected Variance $= \lambda_1 + \lambda_2 + \dots + \lambda_k$

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Example 1

- Step-1: Data points: $x_1 = \begin{bmatrix} 3 \\ 6 \\ 9 \end{bmatrix}$, $x_2 = \begin{bmatrix} 2 \\ 4 \\ 6 \end{bmatrix}$, $x_3 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$
- Step-2: Mean vector: $\bar{X} = \begin{bmatrix} 2 \\ 4 \\ 6 \end{bmatrix}$
- Step-3: Symmetric matrix, C =

$$\frac{1}{3}\left(\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} -1 \\ -2 \\ -3 \end{bmatrix} \begin{bmatrix} -1 & -2 & -3 \end{bmatrix} \right) =$$

$$\frac{2}{3} \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 9 \end{bmatrix}$$

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Example 1

- Step-4: Characteristic equation: $(\frac{2}{3}\begin{bmatrix}1-\lambda & 2 & 3\\ 2 & 4-\lambda & 6\\ 3 & 6 & 9-\lambda\end{bmatrix})u_j = 0$
- Step-5: Eigen values: $\lambda_1 = 14, \lambda_2 = 0, \lambda_3 = 0$
  Eigen vectors:

$$\lambda_1 = 14, a_1 = \frac{1}{3}, a_2 = \frac{2}{3}, a_3 = 1 => u_1 = \frac{1}{\sqrt{14}}\begin{bmatrix}1\\2\\3\end{bmatrix},$$

$$\lambda_2 = 0, a_1 = -2, a_2 = 1, a_3 = 0 => u_1 = \frac{1}{\sqrt{5}}\begin{bmatrix}-2\\1\\0\end{bmatrix}$$

$$\lambda_3 = 0, a_1 = -3, a_2 = 0, a_3 = 1 => u_2 = \frac{1}{\sqrt{10}}\begin{bmatrix}-3\\0\\1\end{bmatrix}$$

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Example 1

- Step 6: Projecting data points

  Projecting x_1 on u_1

  - Projection on $u_1 = \alpha_1 = \frac{1}{\sqrt{14}}\left(\begin{bmatrix} 3 & 6 & 9 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}\right) = \frac{42}{\sqrt{14}}$

  Projecting x_2 on u_1

  - Projection on $u_1 = \alpha_1 = \frac{1}{\sqrt{14}}\left(\begin{bmatrix} 2 & 4 & 6 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}\right) = \frac{28}{\sqrt{14}}$

  Projecting x_3 on u_1

  - Projection on $u_1 = \alpha_1 = \frac{1}{\sqrt{14}}\left(\begin{bmatrix} 1 & 2 & 3 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}\right) = \frac{14}{\sqrt{14}}$

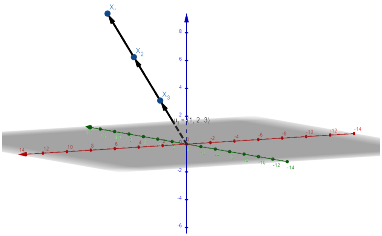

Figure: PCA using one component

https://www.geogebra.org/calculator/dj8pkvwk

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Example 1

- Step 7: Choose eigen vectors corresponding to top k eigen values (k=1 here)
  Derive the transformed data points:

  $$\tilde{x_1} = 3 \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}, \tilde{x_2} = 2 \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix},$$

  $$\tilde{x_3} = 1 \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

- Step-8:
  Reconstruction Error $=$
  $J = \frac{1}{n}\Sigma_{i=1}^{n}||x_i - \tilde{x_i}||^2 = \frac{1}{3}[0^2 + 0^2 + 0^2] = 0,$
  Projected Variance $= \lambda_1 = 14$

Original	Transformed
$x_1 = \begin{bmatrix} 3 \\ 6 \\ 9 \end{bmatrix}$	$\tilde{x_1} = 3 \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$
$x_2 = \begin{bmatrix} 2 \\ 4 \\ 6 \end{bmatrix}$	$\tilde{x_2} = 2 \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$
$x_3 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$	$\tilde{x_3} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$

Table: Data points

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Example 2

- Step-1: Data points: $x_1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$, $x_2 = \begin{bmatrix} 0 \\ 2 \end{bmatrix}$, $x_3 = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$, $x_4 = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$
- Step-2: Mean vector: $\bar{X} = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$
- Step-3: Symmetric matrix, C =
  $\frac{1}{4}(\begin{bmatrix} 0 \\ -2 \end{bmatrix} \begin{bmatrix} 0 & -2 \end{bmatrix} + \begin{bmatrix} -2 \\ 0 \end{bmatrix} \begin{bmatrix} -2 & 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 2 \end{bmatrix} \begin{bmatrix} 0 & 2 \end{bmatrix} + + \begin{bmatrix} 2 \\ 0 \end{bmatrix} \begin{bmatrix} 2 & 0 \end{bmatrix}) =$
  $\frac{2}{3} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$
- Step-4: Characteristic equation: $(\begin{bmatrix} 2-\lambda & 0 \\ 0 & 2-\lambda \end{bmatrix})u_j = 0$
- Step-5: Eigen values: $\lambda_1 = 2, \lambda_2 = 2$
  Eigen vectors:
  $\lambda_1 = 2, a_1 = 1, a_2 = 0 => u_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$,
  $\lambda_2 = 2, a_1 = 0, a_2 = 1 => u_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

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Example 2

- Step 6: Projecting data points

  Projecting x_1 on u_1

  - Projection on $u_1 = \alpha_1 = \left(\begin{bmatrix} 2 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = 2$

  Projecting x_2 on u_1

  - Projection on $u_1 = \alpha_1 = \left(\begin{bmatrix} 0 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = 0$

  Projecting x_3 on u_1

  - Projection on $u_1 = \alpha_1 = \left(\begin{bmatrix} 2 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = 2$

  Projecting x_4 on u_1

  - Projection on $u_1 = \alpha_1 = \left(\begin{bmatrix} 4 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = 4$

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Example 2

- Step 7: Choose eigen vectors corresponding to top k eigen values (k=1 here)
  Derive the transformed data points:
  $\tilde{x_1} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}, \tilde{x_2} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tilde{x_3} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$
  $\tilde{x_4} = \begin{bmatrix} 4 \\ 0 \end{bmatrix}$
- Step-8:
  Reconstruction Error =
  $J = \frac{1}{n}\Sigma_{i=1}^{n}||x_i - \tilde{x_i}||^2 =$
  $\frac{1}{4}[0^2 + 2^2 + 4^2 + 2^2] = 24,$
  Projected Variance $= \lambda_1 = 2$

Original	Transformed
$x_1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$	$\tilde{x_1} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$
$x_2 = \begin{bmatrix} 0 \\ 2 \end{bmatrix}$	$\tilde{x_2} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
$x_3 = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$	$\tilde{x_3} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$
$x_4 = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$	$\tilde{x_4} = \begin{bmatrix} 4 \\ 1 \end{bmatrix}$

Table: Data points

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Thank you

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