

PCA Numerical Example

Let's understand steps of PCA with an example of two dimensional data.

We start with the following set of 5 points:

$$\mathbf{X} = \begin{bmatrix} 4 & 6 & -1 & -2 & -3 \\ 5 & 9 & -7 & -5 & -9 \end{bmatrix}$$

This is a more compact way of writing (using vectors & matrices); otherwise you will have many summations to deal with.

PCA Numerical Example

Calculate mean:

$$\bar{X} = \begin{bmatrix} 0.8 \\ -1.4 \end{bmatrix}$$

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Center the points by performing $(X - \bar{X})$

$$\begin{bmatrix} 3.2 & 5.2 & -1.8 & -2.8 & -3.8 \\ 6.4 & 10.4 & -5.6 & -3.6 & -7.6 \end{bmatrix}$$

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The covariance matrix A is: $1/n * (X - \bar{X})(X - \bar{X})^T$
where n is the number of points (=5).

$$A = \begin{bmatrix} 12.56 & 24.72 \\ 24.72 & 50.24 \end{bmatrix}$$

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Finding the eigenvalues:

$$\begin{bmatrix} 12.56 & 24.72 \\ 24.72 & 50.24 \end{bmatrix} - \lambda I$$

I is the identity matrix. $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

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Finding the eigenvalues:

$$\begin{bmatrix} 12.56 - \lambda & 24.72 \\ 24.72 & 50.24 - \lambda \end{bmatrix}$$

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Finding the eigenvalues:

$$\text{Determinant of } \begin{bmatrix} 12.56 - \lambda & 24.72 \\ 24.72 & 50.24 - \lambda \end{bmatrix} = 0$$

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Finding the eigenvalues:

$$(12.56 - \lambda) * (50.24 - \lambda) - 24.72^2 = 0$$

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Finding the eigenvalues:

$$(\lambda^2) - 62.8\lambda + 19.936 = 0$$

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Finding the eigenvalues:

Now, we find the roots of this quadratic equation as:

$$\frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

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Finding the eigenvalues:

This gives the roots as:

$$\lambda_1 = 62.4809$$

$$\lambda_2 = 0.3190$$

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Calculate the Eigenvector for the 1st Eigenvalue:

$$(A - \lambda_1 I) * X = 0$$

where $X = \begin{bmatrix} a_1 \\ b_1 \end{bmatrix}$

PCA Numerical Example

Calculate the Eigenvector for the 1st Eigenvalue:

$$(A - \lambda_1 I) = \begin{bmatrix} 12.56 & 24.72 \\ 24.72 & 50.24 \end{bmatrix} - \begin{bmatrix} 62.48 & 0 \\ 0 & 62.48 \end{bmatrix}$$

$$(A - \lambda_1 I) = \begin{bmatrix} -49.92 & 24.72 \\ 24.72 & -12.24 \end{bmatrix}$$

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Calculating the Eigenvector for the 1st Eigenvalue:

$$\begin{bmatrix} -49.92 & 24.72 \\ 24.72 & -12.24 \end{bmatrix} * \begin{bmatrix} a_1 \\ b_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$a_1^2 + b_1^2 = 1$$

From these equations, we can get the 1st eigenvector.

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Calculating the Eigenvector for the 1st Eigenvalue:

$$\begin{bmatrix} -49.92 & 24.72 \\ 24.72 & -12.24 \end{bmatrix} * \begin{bmatrix} a_1 \\ b_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow 24.72 a_1 = 12.24 b_1 \Rightarrow a_1 = 0.4951 b_1$$

$$a_1^2 + b_1^2 = 1 \Rightarrow 0.2452 b_1^2 + b_1^2 = 1 \Rightarrow 1.2452 b_1^2 = 1 \Rightarrow b_1^2 = 0.8031 \\ \Rightarrow b_1 = + \text{ or } - 0.8962 \Rightarrow a_1 = 0.4951 \times +/\text{- } 0.8962 = 0.4437$$

1st Eigen vector $\begin{pmatrix} 0.4437 \\ 0.8962 \end{pmatrix}$

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Calculate the Eigenvector for the 2nd Eigenvalue:

$$(A - \lambda_2 I) * X = 0$$

where $X = \begin{bmatrix} a_2 \\ b_2 \end{bmatrix}$

PCA Numerical Example

Calculate the Eigenvector for the 2nd Eigenvalue:

$$(A - \lambda_2 I) = \begin{bmatrix} 12.56 & 24.72 \\ 24.72 & 50.24 \end{bmatrix} - \begin{bmatrix} 0.03 & 0 \\ 0 & 0.03 \end{bmatrix}$$

$$(A - \lambda_2 I) = \begin{bmatrix} 12.53 & 24.72 \\ 24.72 & 50.21 \end{bmatrix}$$

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Calculate the Eigenvector for the 2nd Eigenvalue:

$$\begin{bmatrix} 12.53 & 24.72 \\ 24.72 & 50.21 \end{bmatrix} * \begin{bmatrix} a_2 \\ b_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$a_2^2 + b_2^2 = 1$$

From these equations, we can get the 2nd eigenvector.

PCA Numerical Example

Calculate the Eigenvector for the 2nd Eigenvalue:

$$\begin{bmatrix} 12.53 & 24.72 \\ 24.72 & 50.21 \end{bmatrix} * \begin{bmatrix} a_2 \\ b_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow 12.53 a_2 = -24.72 b_2 \Rightarrow a_2 = -1.97 b_2$$

$$a_2^2 + b_2^2 = 1 \Rightarrow 3.89 b_2^2 + b_2^2 = 1 \Rightarrow 4.89 b_2^2 = 1 \Rightarrow b_2^2 = 0.2045 \\ \Rightarrow b_2 = + \text{ or } - 0.4522 \Rightarrow a_2 = -1.97 \times +/ - 0.4522 = 0.8909$$

From these equations, we can get the 2nd eigenvector.

$$\text{2nd Eigen vector} \begin{pmatrix} 0.8909 \\ -0.4522 \end{pmatrix}$$

PCA Numerical Notes

The variance of projections in the line of the principal components is equal to the Eigenvalues of the principal components.

Sum of all the Eigenvalues is equal to the total variance of all the variance.

1st eigen value is bigger than 2nd, 2nd is bigger than 3rd and so on.