PCA

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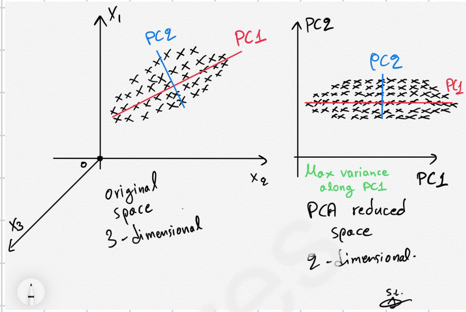
- PCA is a linear dimensionality reduction technique that can be used to simplify a dataset by reducing the number of dimensions



- Dimensions: Number of features
- Why reduce the dimensionality?
  - Too many features
  - Correlated features
  - Plotting

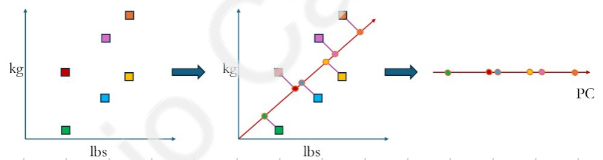
The idea of PCA is to find directions in the data where variance is maximized

- PCA transform the original data into principal components
- Principal components: New dimensions that my data are projected, they are chosen to capture the most important patterns in the data
- How can we measure "the most important patterns"? Using the variance.

Futhermore, PC is a linear combination of the original features (each PC is a weighted sum of my original features)

$$PC1 = w_1x_1 + w_2x_2 + \dots w_nx_n = w^TX$$

w^T → Come from eigenvectors of the covariance matrix



Variance means how much our data spread out or varies from its own mean

$$\text{Variance} = \frac{\Sigma(X-\mu)^2}{N}$$

- High variance direction: My data are more spread out, which usually means there's more information in that direction
- Low variance direction: Is flat or compressed, it likely contains less useful information (noise, redundancy...)

Covariance means whether two variables moves in the same direction. We calculate the covariance matrix to identify relations between features so the algorithm can rotate the data and drop unimportant dimensions

Covariance matrix: $\frac{1}{N}X^TX$

We find from the covariance matrix
- Eigenvectors: Are principal components
- Eigenvalues: Are how much variance is in that direction

Therefore, we select the highest eigenvector with the highest eigenvalues

$$\text{Covariance} = \frac{1}{N}\sum_{n=1}^{N}(x_n-\bar{x})(y_n-\bar{y})$$

Covariance
- >0 Positive relationship ↑x ↑y
- $=0$ No linear relationship ↑x ↑↓y
- <0 Negative relationship ↑x ↓y

$$\begin{array}{c|cc} & x & y \\ \hline x & & \\ y & & \end{array}\begin{bmatrix} var(x) & cov(x,y) \\ cov(x,y) & var(y) \end{bmatrix} \qquad \begin{array}{c} \\ x \\ y \\ z \end{array}\begin{array}{c} \begin{array}{ccc} x & y & z \end{array} \\ \begin{bmatrix} var(x) & cov(x,y) & cov(x,z) \\ cov(x,y) & var(y) & cov(y,z) \\ cov(x,z) & cov(y,z) & var(z) \end{bmatrix} \end{array}$$

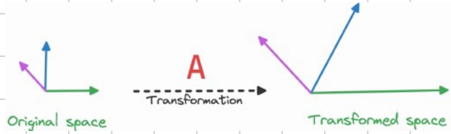
Properties of covariance matrix
- Symmetric
- Real and non-negatives elements (variance ≥ 0)
- Diagonal elements: Variance of each feature
- Off-diagonal elements: Covariances between pairs

- How can we get eigenvalues and eigenvectors?

In math terms:

$$\boxed{A\vec{v} = \lambda\vec{v}}$$

This means: multiply a matrix A by a vector $\vec{v}$, it gives you the same vector $\vec{v}$, just scaled by λ



A: covariance matrix (in PCA)
$\vec{v}$: eigenvectors
λ: eigenvalues

- Rearrange the eigenvalue equation

$$A\vec{v} = \lambda\vec{v}$$
$$A\vec{v} - \lambda\vec{v} = 0$$
$$(A - \lambda I)\vec{v} = 0 \longrightarrow \text{To solve it for a non-zero "v" the } \boxed{\det(A - \lambda I) = 0} \longrightarrow$$

Solving this would give us the eigenvalues and them we can calculate the eigenvectors

- Example:

① Covariance matrix

$$A = \begin{bmatrix} 4 & 2 \\ 2 & 3 \end{bmatrix}$$

② Solve the equation

$$A\vec{v} = \lambda\vec{v} \longrightarrow (A - \lambda I)\vec{v} = 0$$
$$\vdots$$
$$\det(A - \lambda I) = 0 \longrightarrow \det\left(\begin{bmatrix} 4-\lambda & 2 \\ 2 & 3-\lambda \end{bmatrix}\right) = 0 \longrightarrow (4-\lambda)\cdot(3-\lambda) - 2\cdot 2 = 0$$
$$12 - 4\lambda - 3\lambda + \lambda^2 - 4 = 0$$
$$\lambda^2 - 7\lambda + 8 = 0 \qquad x = \frac{-b \pm \sqrt{b^2 - 2ac}}{2a} \longrightarrow x = \frac{7 \pm \sqrt{(-7)^2 - 2\cdot 1\cdot 8}}{2\cdot 1} = \frac{7 \pm \sqrt{17}}{2}$$
$$e_1 = \frac{7+\sqrt{17}}{2} \qquad e_2 = \frac{7-\sqrt{17}}{2}$$

③ Solve for eigenvalues

$$(A - \lambda I)\vec{v} = 0$$

$$\lambda_1 = \frac{7+\sqrt{17}}{2} = 5'56$$

$$\begin{bmatrix} 4-5'56 & 2 \\ 2 & 3-5'56 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \end{bmatrix} = 0$$

$$\Rightarrow \begin{bmatrix} -1.56 & 2 \\ 2 & -2.56 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \end{bmatrix} = 0$$

$$\Rightarrow \left.\begin{matrix} -1.56x + 2y = 0 \\ 2x - 2.56y = 0 \end{matrix}\right\}$$

$$x = \frac{2'56y}{2} \Rightarrow \boxed{x = 1'28y}$$

$$\vec{v}_1 = \begin{bmatrix} 1'28y \\ y \end{bmatrix} = \begin{bmatrix} 1'28 \\ 1 \end{bmatrix} = \begin{bmatrix} 1'28/1'5 \\ 1/1'5 \end{bmatrix} = \begin{bmatrix} 0'85 \\ 0'66 \end{bmatrix}$$

$$\|\vec{v}_1\| = \sqrt{1'28^2 + 1^2} = 1'5$$

We normalize the eigenvector have length 1

$$\lambda_2 = \frac{7-\sqrt{17}}{2} = 1'438$$

$$\begin{bmatrix} 4-1'438 & 2 \\ 2 & 3-1'438 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \end{bmatrix} = 0$$

$$\begin{bmatrix} 2'562 & 2 \\ 2 & 1'562 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \end{bmatrix} = 0$$

$$\left.\begin{matrix} 2'562x + 2y = 0 \\ 2x + 1'562y = 0 \end{matrix}\right\}$$

$$y = \frac{2'562x}{2} = 1'281x$$

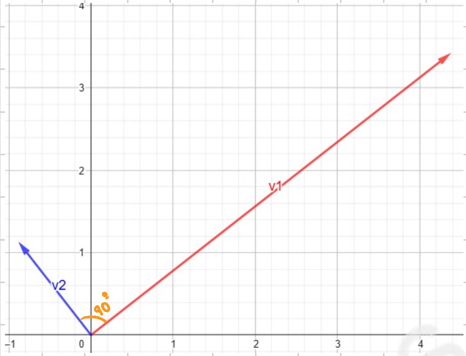
$$\vec{v}_2 = \begin{bmatrix} x \\ 1'281x \end{bmatrix} = \begin{bmatrix} 1 \\ 1'281 \end{bmatrix} = \begin{bmatrix} 1/1'625 \\ 1'281/1'625 \end{bmatrix} = \begin{bmatrix} 0'615 \\ 0'788 \end{bmatrix}$$

$$\|v_2\| = \sqrt{1^2 + 1'281^2} = 1'625$$

Therefore:

Eigenvalues: 5'56 and 1'438

Eigenvectors: $\begin{bmatrix} 0'85 \\ 0'66 \end{bmatrix}$ and $\begin{bmatrix} 0'615 \\ 0'788 \end{bmatrix}$



- If you observe the plotting of both vector, you will realize that both vector are orthogonal
- Two orthogonal vectors form 90-degree angle and their dot product is zero $\boxed{(v1 \cdot v2 = 0)}$

This means they don't share component in the same direction, they are completely independent

- Finally, if each Principal Component is orthogonal they captures a unique type of variance.
- PC2 is orthogonal to PC1
- PC3 is orthogonal to both PC1 and PC2

Steps to calculate PCA

Mean of X

1. Standardize the data $(X - \bar{X})$
2. Compute the covariance matrix $A = \frac{1}{N} X^T X$
3. Compute eigenvalues and eigenvectors $A\vec{v} = \lambda\vec{v}$
4. Sort eigenvectors by eigenvalues in descending order (top k eigenvector = top k principal components)
5. Project the data (reduce the dimension while keeping the variance)

$$X_{new} = X_{old} \cdot W_k$$

Matrix with top k eigenvectors

My current data

Data with K dimension

Dimension of each element

(n_samples, k_eigenvalues) = (n_samples, n_features) @ (n_features, K_eigenvalues)