PCA Manual Example

Given dataset matrix $X = \begin{bmatrix} 126 & 78 \\ 128 & 80 \\ 128 & 82 \\ 130 & 82 \\ 130 & 84 \\ 132 & 86 \end{bmatrix}$, assume both features use same measurements

Find the principle components.

Step 1: Standardize the data

- Since both features use the same measurements, we only need to center the dataset:

$$X := \begin{bmatrix} 126-129 & 78-82 \\ 128-129 & 80-82 \\ 128-129 & 82-82 \\ 130-129 & 82-82 \\ 130-129 & 84-82 \\ 132-129 & 86-82 \end{bmatrix} = \begin{bmatrix} -3 & -4 \\ -1 & -2 \\ -1 & 0 \\ 1 & 0 \\ 1 & 2 \\ 3 & 4 \end{bmatrix}$$

Step 2: Form covariance matrix C

$$C = \frac{1}{m-1} X^T X = \begin{bmatrix} 4.4 & 5.6 \\ 5.6 & 8 \end{bmatrix}$$

Step 3: Calculate eigenvalues and eigenvectors

Calculate eigenvalues:

$$\det|C - \lambda I| = 0$$

$$\Leftrightarrow \det\left|\begin{bmatrix} 4.4-\lambda & 5.6 \\ 5.6 & 8-\lambda \end{bmatrix}\right| = 0$$

$$\Leftrightarrow (4.4-\lambda)(8-\lambda) - 5.6^2 = 0$$

$$\Leftrightarrow 3.84 - 12.4\lambda + \lambda^2 = 0$$

$$\Rightarrow \left[\begin{array}{l} \lambda_1 = 0.32 \\ \lambda_2 = 12.08 \end{array}\right.$$

Calculate eigenvector:

- Case $\lambda_2 = 12.08$:

$$C v_2 = \lambda_2 v_2$$

$$\Leftrightarrow \begin{bmatrix} 4.4 & 5.6 \\ 5.6 & 8.0 \end{bmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = 12.08 \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\Rightarrow \begin{cases} x = 1 \\ y = 1.37 \end{cases}$$

$$\Rightarrow v_2 = \begin{bmatrix} 1 \\ 1.37 \end{bmatrix}$$

Normalize v_2: $v_2 := \dfrac{v_2}{\|v_2\|} = \begin{bmatrix} 0.59 \\ 0.81 \end{bmatrix}$

Do the same for λ_1, then $v_1 = \begin{bmatrix} -0.81 \\ 0.59 \end{bmatrix}$

Sort the eigenvectors based on eigenvalues, form orthonormal matrix V:

$$V = (v_2 \mid v_1)$$

$$= \begin{bmatrix} 0.59 & -0.81 \\ 0.81 & 0.59 \end{bmatrix}$$

Step 4: Calculate principle components

$$X \cdot V = \begin{bmatrix} -3 & -4 \\ -1 & -2 \\ -1 & 0 \\ 1 & 0 \\ 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 0.59 & -0.81 \\ 0.81 & 0.59 \end{bmatrix} = \begin{array}{cc} PC1 & PC2 \\ \left[\begin{array}{c} -5.0 \\ -2.2 \\ -0.6 \\ 0.6 \\ 2.2 \\ 5.0 \end{array}\right. & \left.\begin{array}{c} 0.1 \\ -0.4 \\ 0.8 \\ -0.8 \\ 0.4 \\ -0.1 \end{array}\right] \\ \lambda_1 = 12.08 & \lambda_2 = 0.32 \end{array}$$

Step 5: Intepret the PCA

- We can see that:

$$\%\ var = \frac{\lambda_1}{\lambda_1 + \lambda_2} = \frac{12.08}{12.08 + 0.32} = 97.4\%$$

$\Rightarrow$ PC1 captures 97.4% of the total variance

So we can reduce the dimensions to just PC1, so:

$$X \cdot v_1 = \begin{bmatrix} \vdots & \vdots \\ \end{bmatrix} \begin{bmatrix} 0.59 \\ 0.81 \end{bmatrix} = \underbrace{\begin{bmatrix} \vdots \\ \end{bmatrix}}_{PC1}$$