

Principal Component Analysis

Step 1: Compute Covariance Matrix

In R^2 space

Example 1

$$\vec{d}_i = \begin{bmatrix} x_i \\ y_i \end{bmatrix}$$

$$\bar{x} = \sum_{i=1}^n \frac{x_i}{n}$$

$$\text{cov}(X, Y) = (\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})) / (n - 1)$$

Tries to capture the correlation / covariance between two variables

$$\text{cov}(X, X) = \text{Var}(X) = (\sum_{i=1}^n (x_i - \bar{x})^2) / (n - 1)$$

$$\text{cov}(Y, Y) = \text{Var}(Y) = (\sum_{i=1}^n (y_i - \bar{y})^2) / (n - 1)$$

$$P(x \in [a, b]) = \int_a^b f(x) dx$$

Where:

- $f(x) \geq 0$ for all x
- Area under $f(x)$ from $-\infty$ to $+\infty = 1$

$f(x)$ = normal distribution bell like curve

Example 2

When the points are uniformly distributed across the plane:

$$\text{cov}(X, Y) = 0$$

Create Covariance Matrix for R^2

$$\text{COV} = \begin{bmatrix} \text{cov}(X, X) & \text{cov}(X, Y) \\ \text{cov}(Y, X) & \text{cov}(Y, Y) \end{bmatrix}$$

Example in R^3

$$\text{Stars} = \{s_1, s_2, \dots, s_n\}$$

$$s_i = \begin{bmatrix} x_i \\ y_i \\ z_i \end{bmatrix}$$

$$COV = \begin{bmatrix} \text{cov}(X, X) & \text{cov}(X, Y) & \text{cov}(X, Z) \\ \text{cov}(Y, X) & \text{cov}(Y, Y) & \text{cov}(Y, Z) \\ \text{cov}(Z, X) & \text{cov}(Z, Y) & \text{cov}(Z, Z) \end{bmatrix}$$

COV matrix is always symmetric

Step 2: Eigen Decomposition:

$$\det(C - \lambda I) = 0$$

$$\text{Roots of } \text{spectrum}(C) = \{\lambda_1, \lambda_2, \lambda_3\}$$

Without loss of generality:

$$\lambda_1 \geq \lambda_2 \geq \lambda_3$$

Principal Components: $E_{\lambda_1}, E_{\lambda_2}, E_{\lambda_3}$

Take the **first 2 eigenspaces** to bring down to R^2

Step 3: Orthogonal Projection

$$U = \text{span}\{E_{\lambda_1}, E_{\lambda_2}\}$$

$$B = [E_{\lambda_1}, E_{\lambda_2}]$$

Use OP to bring data down from R^3 to R^2 :

- Maximising data retention
- Minimising data loss
 - By picking the **first 2 eigenspaces**

Example 3

In R^2

$$\text{Stars} = \{s_1, s_2, s_3\} = \left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 3 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 3 \end{bmatrix} \right\}$$

Step 1: Compute Covariance Matrix:

$$C = \begin{bmatrix} \text{cov}(X, X) & \text{cov}(X, Y) \\ \text{cov}(Y, X) & \text{cov}(Y, Y) \end{bmatrix} = \begin{bmatrix} 3 & -3/2 \\ -3/2 & 3 \end{bmatrix}$$

Step 2: Eigen Decomposition

$$\text{Characteristic Polynomial} = \lambda^2 - 6\lambda + 27/4$$

$$\text{Spectrum}(C) = \{9/2, 3/2\}$$

Pick highest value = 9/2

$$E_{9/2} = \text{1st Principal Component} = \text{span}\left\{\begin{bmatrix} -1 \\ 1 \end{bmatrix}\right\}$$

Step 3: Orthogonal Projection:

$$U = \text{span}\{E_{9/2}\}$$

$$B = [E_{9/2}] = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$\text{Projection Matrix} = B(B^T B)^{-1} B^T = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \left(\begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \right)^{-1} \begin{bmatrix} -1 & 1 \end{bmatrix} = 1/2 \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} = P$$

$$Ps_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$Ps_2 = \begin{bmatrix} 3/2 \\ -3/2 \end{bmatrix}$$

$$Ps_3 = \begin{bmatrix} -3/2 \\ 3/2 \end{bmatrix}$$

Step 2: Eigen Decomposition

Step 3: Orthogonal Projection

Covariance Theorem

$$\text{cov}(X, Y)^2 \leq \text{Var}(X)\text{Var}(Y)$$