

Compute Co-variance

$$\text{Cov}(x_1, x_2) = \frac{1}{n-1} \sum_{i=1}^n (x_{1i} - \bar{x}_1)(x_{2i} - \bar{x}_2)$$



## How to compute Co-variance matrix

$x_1$	$x_2$	$y$
1	2	4
2	3	5
3	4	6
4	5	7
5	6	8

Step: 1

dataset

Calculate Covariance matrix??

→ To calculate the Covariance matrix, we need to compute the covariance between each pair of features  $x_1$  and  $x_2$ .

Let me calculate covariance matrix:

Step 2

Covariance matrix.

(a) Calculate mean's

$$\bar{x}_1 = \frac{1+2+3+4+5}{5} = 3$$

$$\bar{x}_2 = \frac{2+3+4+5+6}{5} = 4$$

(b) Centre the data  
Subtract the mean from each Value.

Centred  $x_1: [-2, -1, 0, 1, 2]$

Centred  $x_2: [-2, -1, 0, 1, 2]$

3. Compute 'Covariance':

Covariance between  $x_1$  and  $x_2$

$$\text{Var}(x_1) = \frac{1}{4} [(-2)^2 + (-1)^2 + (0)^2 + (1)^2 + (2)^2] = 2.5$$

Covariance between  $x_1$  and  $x_2$

$$\text{Cov}(x_1, x_2) = \frac{1}{4} [(-2)(-2) + (-1)(-1) + (0)(0) + (1)(1) + (2)(2)] = 2.5$$

Covariance matrix

$$\Sigma = \begin{pmatrix} 2.5 & 2.5 \\ 2.5 & 2.5 \end{pmatrix}$$

# Find Eigen values and Eigen vectors

## 1. Eigen value equation

Solve characteristic equation

$$\det(\mathbf{E} - \lambda \mathbf{I}) = 0$$

identity matrix.

Substituting the covariance

$$\begin{vmatrix} 2.5 - \lambda & 2.5 \\ 2.5 & 2.5 - \lambda \end{vmatrix} = 0$$

Solve determinant:  $\Rightarrow \lambda^2 - 5\lambda = 0$

$$\lambda_1 = 0, \lambda_2 = 5$$

Eigen vectors

$$(\mathbf{E} - \lambda \mathbf{I}) \mathbf{v} = 0$$

$$\lambda_1 = 0$$

$$(\mathbf{E} - 0 \mathbf{I}) \cdot \mathbf{v} = 0$$

$$\mathbf{E} \mathbf{v} = 0$$

$$\begin{pmatrix} 2.5 & 2.5 \\ 2.5 & 2.5 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 0$$



Solving  $v_1$  and  $v_2$

$$v_1 = -v_2$$

$$\boxed{\lambda_1 = 0} \quad v_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\boxed{\text{Eigen vector}} \quad \boxed{\lambda_2 = 5}$$

$$(E - 5I) \cdot v = 0$$

$$\begin{pmatrix} 2.5 - 5 & 2.5 \\ 2.5 & 2.5 - 5 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$-2.5v_1 + 2.5v_2 = 0$$

$$\boxed{v_1 = v_2}$$

$$v_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

• Eigen vector  $\lambda_1 = 0 \Rightarrow v_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$$\lambda_2 = 5 \Rightarrow v_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

PCA

① Feature reduction technique.

## Principal Components

Principal components are the directions of maximum variance in the data, which correspond to the eigen vectors of the covariance matrix. These components are ranked by the magnitude of their corresponding eigen values:

• Eigen values  $\lambda_1 = 0, \lambda_2 = 5$

Eigen vectors (Principal components)

For  $\lambda_1 = 0$ ,  $V_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$\lambda_2 = 5$ ,  $V_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Interpretation

## Interpretation

• First principal component corresponds to the eigen vector with the largest eigen value. In this case,

## Partial Least Squares

	$x_1$	$x_2$	$y$
1	2.0	3.0	5.0
2	1.5	2.5	4.5
3	3.0	4.0	6.0
4	2.5	3.5	5.5

Step 1:

Standardize predictors

① Calculate the mean and variance of each predictor.

For  $x_1$ :

$$\bar{x}_1 = \frac{2.0 + 1.5 + 3.0 + 2.5}{4} = 2.0$$

$$\text{Var}(x_1) = \frac{(2.0 - 2.0)^2 + (1.5 - 2.0)^2 + (3.0 - 2.0)^2 + (2.5 - 2.0)^2}{3} = 0.25$$

Standardize  $x_1$  and  $x_2$



$$z_1^{(0)} = \frac{x_1 - \bar{x}_1}{\sqrt{\text{Var}(x_1)}}$$

$$z_2^{(0)} = \frac{x_2 - \bar{x}_2}{\sqrt{\text{Var}(x_2)}}$$

After Standardization data look like:

	$z_1^{(0)}$	$z_2^{(0)}$	$y$
1	0.0	6.0	5.0
2	-0.5	-0.5	4.5
3	1.0	1.0	6.0
4	0.5	0.5	5.5

Step 2: Perform PLS Iteration.

Iteration 1:

(a) compute  $Z$ :

Compute  $\hat{\theta}_{ij}$

$$\hat{\theta}_{11} = (z_1^{(0)}, y) = 0.0 \cdot 5.0 + (-0.5) \cdot 4.5 + 1.0 \cdot 6.0 + 0.5 \cdot 5.5$$

4



$$\hat{\theta}_{12} = (x_2^{(0)}, y) = 0.0 + 5.0 + (-0.5) \cdot 4.5 + \frac{(1.0) \cdot 6.0 + 0.5 \cdot 5.5}{4} = 0.75$$

Compute  $z_1$ :

$$z_1 = \hat{\theta}_{11} \cdot x_1^{(0)} + \hat{\theta}_{12} \cdot x_2^{(0)}$$

$$z_1 = 0.75 \cdot x_1^{(0)} + 0.75 \cdot x_2^{(0)}$$

$$z_1 = 0.75 + (x_1^{(0)} + x_2^{(0)})$$

① Compute  $\hat{\theta}_1$ :  $\hat{\theta}_1 = \frac{(z_1, y)}{z_1 \cdot z_1}$

Compute  $(z_1, y)$

$$(z_1, y) = 0.75 \cdot (0.0 + 0.0) \cdot 5.5 + (-0.5 - 0.5) \cdot 4.5 + 0.75 \cdot (1.0 + 1.0) \cdot 6.0$$

Compute  $(z_1, z_1)$ :

$$(z_1, z_1) = 0.75 \cdot (0.0 + 0.0) \cdot (0.0 + 0.0) + 0.75 \cdot (-0.5 - 0.5) \cdot (-0.5 - 0.5) + 0.75$$

20.75

$$\text{Therefore } \hat{\theta}_1 = \frac{4.875}{2.25} = 2.167$$

② update fitted value  $\hat{y}^{(1)}$

$$\hat{y}^{(1)} = \hat{y}^{(0)} + \hat{\theta}_1 z_1$$

$$y^{(1)} = 5.0 + 2.167 z_1$$

③ orthogonalize the predictors:  
update  $x_1^{(1)}$  and  $x_2^{(1)}$ .

$$x_1^{(1)} = x_1^{(0)} - \frac{(z_1 \cdot x_1^{(0)})}{(z_1 \cdot z_1)} \cdot z_1$$

$$x_2^{(1)} = x_2^{(0)} - \frac{z_1 \cdot x_2^{(0)}}{(z_1 \cdot z_1)} \cdot z_1$$

if need repeat in iteration 2