Numerical on PCA

* Consider dataset,

Feature	Sample 1	Sample 2	Sample 3	Sample 4
a	4	8	13	7
b	11	4	5	14

- Step-1 : Getting the dataset

Feature	Sample 1	Sample 2	Sample 3	Sample 4
a	4	8	13	7
b	11	4	5	14

- step-2 : Representing data into a structure

	Feature	
~~Feature~~	a	b
Sample 1	4	11
Sample 2	8	4
Sample 3	13	5
Sample 4	7	14

Step - 3: Calculate Mean

No. of features, $n = 2$ (a,b)

No. of samples, $N = 4$ (Sample1, Sample 2, Sample 3, Sample4)

Calculating mean,

$$\bar{a} = \frac{4+8+13+7}{4} = 8$$

$$\bar{b} = \frac{11+4+5+14}{4} = 8.5$$

Step - 4: Calculation of the covariance matrix

Calculating covariance matrix between features, In the given dataset, ordered features are as,
(a,a), (a,b), (b,a), (b,b).

$$Cov(a,a) = \frac{1}{N-1} \sum_{k=1}^{N} (a_i - \bar{a})(a_i - \bar{a})$$

$$= \frac{1}{N-1} \sum_{k=1}^{N} (a_i - \bar{a})^2 \quad \text{[for same feature]}$$

$$= \frac{1}{4-1} \left[(4-8)^2 + (8-8)^2 + (13-8)^2 + (7-8)^2 \right]$$

$$= \frac{(-4)^2 + 0^2 + 5^2 + 1^2}{3}$$

$$= \frac{14}{}$$

$$Cov(a,b) = \frac{1}{N-1} \sum_{K=1}^{N} (a_i - \bar{a})(b_i - \bar{b})$$

$$= \frac{1}{4-1} \Big[(4-8)(11-8.5) + (8-8)(4-8.5) + (13-8)(5-8.5) + (7-8)(14-8.5) \Big]$$

$$= \frac{1}{3} \Big[(-4)(2.5) + 0 \cdot (-4.5) + (5) \cdot (-3.5) + (-1)(5.5) \Big]$$

$$= \frac{1}{3} \Big[-10 + 0 - 17.5 - 5.5 \Big]$$

$$= \frac{-33}{3}$$

$$= -11$$

$$Cov(b,a) = \frac{1}{N-1} \sum_{K=1}^{N} (b_i - \bar{b})(a_i - \bar{a})$$

$$= Cov(a,b)$$

$$= -11$$

$$Cov(b,b) = \frac{1}{N-1} \sum_{k=1}^{N} (b_i - \bar{b})(b_i - \bar{b})$$

$$= \frac{1}{N-1} \sum_{K=1}^{N} (b_i - \bar{b})^2$$

$$= \frac{1}{4-1} \Big[(11-8.5)^2 + (4-8.5)^2 + (5-8.5)^2 + (14-8.5)^2 \Big]$$

$$= \frac{1}{3} \Big[(2.5)^2 + (-4.5)^2 + (-3.5)^2 + (5.5)^2 \Big]$$

$$= \frac{1}{3}\left[6.25 + 20.25 + 12.25 + 30.25\right]$$

$$= \frac{69}{3}$$

$$= 23$$

Hence covariance matrix can be

$$S = \begin{bmatrix} Cov(a,a) & Cov(a,b) \\ Cov(b,a) & Cov(b,b) \end{bmatrix}$$

$$= \begin{bmatrix} 14 & -11 \\ -11 & 23 \end{bmatrix}$$

Step-5: Eigenvalues of the covariance matrix

Inorder to calculate Eigenvalue,

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

$$I = \text{Identity Matrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\lambda I = \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}$$

$$\det\left(\begin{bmatrix} 14 & -11 \\ -11 & 23 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}\right) = 0$$

$$\det\begin{pmatrix} 14-\lambda & -11 \\ -11 & 23-\lambda \end{pmatrix} = 0$$

$$\Rightarrow (14-\lambda)(23-\lambda)-(-11)(-11)=0$$

$$\Rightarrow 322-14\lambda-23\lambda+\lambda^2-121=0$$

$$\Rightarrow \lambda^2-37\lambda+201=0$$

'λ' can be calculated by quadratic equation,

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

$$=\frac{-(-37)\pm\sqrt{(37)^2-4(1)(201)}}{2\times 1}$$

$$=\frac{\cancel{-}37\pm\sqrt{1369-804}}{2}$$

$$=\frac{\cancel{-}37\pm\sqrt{565}}{2}$$

$$=\frac{\cancel{-}37\pm 23.76}{2}$$

$$=\frac{\cancel{-}37+23.76}{2},\ \frac{37-23.76}{2}$$

$$=30.38,\ 6.62$$

$\therefore$ Eigenvalues, $\lambda_1=30.38$, $\lambda_2=6.62$

So, while arranging in descending order,

$\lambda_1 > \lambda_2 > \ldots$

Hence, $\lambda_1 = 30.38$

$\lambda_2 = 6.62$

Step-6: Computation of the eigenvectors

First, we are going to find out Eigenvector for eigenvalue, $\lambda_1 = 30.38$

$$U = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = (S - \lambda_1 I) U$$

$$= \begin{bmatrix} 14-\lambda_1 & -11 \\ -11 & 23-\lambda_1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$= \begin{bmatrix} (14-\lambda_1) u_1 - 11 u_2 \\ -11 u_1 + (23-\lambda_1) u_2 \end{bmatrix}$$

$(14-\lambda_1) u_1 - 11 u_2 = 0 \quad \cdots\cdots \text{(i)}$

$-11 u_1 + (23-\lambda_1) u_2 = 0 \quad \cdots\cdots \text{(ii)}$

from (i)

$$\frac{U_1}{11} = \frac{U_2}{14-\lambda_1} = A \quad \text{(assigning)}$$

Assume, $A = 1$

$$\frac{U_1}{11} = \frac{U_2}{14-\lambda_1} = A = 1$$

Hence,

$$\frac{U_1}{11} = 1 \Rightarrow U_1 = 11$$

$$\frac{U_2}{14-\lambda_1} = 1 \Rightarrow U_2 = 14 - \lambda_1$$
$$= 14 - 30.38$$
$$= -16.38$$

Hence, Eigenvector for λ_1

$$\Rightarrow \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 11 \\ -16.38 \end{bmatrix}$$

To ~~a~~ find a unit eigenvector, we compute the length of U_1 which is given by,

$$\|U_1\| = \sqrt{11^2 + (-16.38)^2}$$

$= \sqrt{121 + 268.30}$

$\simeq 19.73$

$$e_1 = \begin{bmatrix} 11/\|U_1\| \\ -16.38/\|U_1\| \end{bmatrix}$$

$$= \begin{bmatrix} 0.5575 \\ -0.8302 \end{bmatrix}$$

Now, calculate eigen vector for $\lambda_2 = 6.62$

$$(S - \lambda_2 I) \cdot U_2 = 0$$

$$\begin{bmatrix} (14-\lambda_2) & -11 \\ -11 & (23-\lambda_2) \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$(14-\lambda_2)u_1 - 11u_2 = 0$ .... (iii)

$-11u_1 + (23-\lambda_2)u_2 = 0$ .... (iv)

from (iii)

$(14-\lambda_2)u_1 - 11u_2 = 0$

$\Rightarrow (14-\lambda_2)u_1 = 11u_2$

$\Rightarrow \frac{u_1}{11} = \frac{u_2}{14-\lambda_2} = B$ (assigning)

Assume, $\beta = 1$

$$\frac{u_1}{11} = \frac{u_2}{14-\lambda_2} = \beta = 1$$

Hence, $\frac{u_1}{11} = 1 \Rightarrow u_1 = 1$

$$\frac{u_2}{14-\lambda_2} = 1 \Rightarrow u_2 = 14 - \lambda_2$$

$$= 14 - 6.62$$

$$= 7.38$$

Hence, Eigenvector for $\lambda_2 = \begin{bmatrix} 11 \\ 7.38 \end{bmatrix}$

To find a unit eigenvector, we compute the length of U_2 which is given by

$$\|U_2\| = \sqrt{11^2 + (7.38)^2}$$

$$= 13.24$$

$$e_2 = \begin{bmatrix} 11/\|U_2\| \\ 7.38/\|U_2\| \end{bmatrix}$$

$$= \begin{bmatrix} 11/13.24 \\ 7.38/13.24 \end{bmatrix} = \begin{bmatrix} 0.8308 \\ \cancel{0.5891} \\ 0.5574 \end{bmatrix}$$

Step-7: Computation of first principle components

Feature	Sample1	Sample2	Sample3	Sample4
a	4	8	13	7
b	11	4	5	14

$$P_{11} = e_1^T \begin{bmatrix} 4-8 \\ 11-8.5 \end{bmatrix}$$

$$= \begin{bmatrix} 0.5575 & -0.8302 \end{bmatrix} \begin{bmatrix} -4 \\ 2.5 \end{bmatrix}$$

$$= (-2.23 - 2.0755)$$

$$= -4.3055$$

$$P_{12} = e_1^T \begin{bmatrix} 8-8 \\ 4-8.5 \end{bmatrix}$$

$$= \begin{bmatrix} 0.5575 & -0.8302 \end{bmatrix} \begin{bmatrix} 0 \\ -4.5 \end{bmatrix}$$

$$= 0 + 3.7359 = 3.7359$$

$$P_{13} = e_1^T \begin{bmatrix} 13-8 \\ 5-8.5 \end{bmatrix}$$

$$= \begin{bmatrix} 0.5575 & -0.8302 \end{bmatrix} \begin{bmatrix} 5 \\ -3.5 \end{bmatrix}$$

$P_{13} = 2.787 + 2.905$

$= 5.692$

$P_{14} = e_1^T \begin{bmatrix} 7-8 \\ 14-8.5 \end{bmatrix}$

$= \begin{bmatrix} 0.5575 & -0.8302 \end{bmatrix} \begin{bmatrix} -1 \\ 5.5 \end{bmatrix}$

$= -0.5575 - 4.5661$

$= -5.123$

Step-8: Geometrical meaning of first principal components