PCA - Step by Step.

Consider following dataset consisting of 3 rows & 3-dimensions to carry out PCA on it.

$$D = \begin{array}{c} \begin{array}{ccc} d_1 & d_2 & d_3 \end{array} \\ \begin{bmatrix} 9 & 6 & 6 \\ 9 & 9 & 9 \\ 6 & 6 & 6 \end{bmatrix} \end{array} \qquad n = 3, \quad d = 3$$

Step 1 - Compute covariance matrix for dataset D.

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

mean $(d_1) = [8]$ mean $(d_2) = 7$ mean $(d_3) = 7$.

$cov(d_1,d_1) = \frac{1}{3-1} \Sigma [(9-8)(9-8) + (9-8)(9-8) + (6-8)(6-8)] = \frac{1}{2}[1+1+4] = 3$

$cov(d_1,d_2) = \frac{1}{2}[(9-8)(6-7) + (9-8)(9-7) + (6-8)(6-7)] = \frac{1}{2}[-1+2+2] = \frac{3}{2} = 1.5$

$cov(d_1,d_3) = \frac{1}{2}[(9-8)(6-7) + (9-8)(9-7) + (6-8)(6-7)] = \frac{1}{2}[-1+2+2] = \frac{3}{2} = 1.5$

$cov(d_2,d_2) = \frac{1}{2}[(6-7)(6-7) + (9-7)(9-7) + (6-7)(6-7)] = \frac{1}{2}[1+4+1] = 3.$

$cov(d_2,d_3) = \frac{1}{2}[(6-7)(6-7) + (9-7)(9-7) + (6-7)(6-7)] = 3.$

$$A = CV(D) = \begin{array}{c|ccc} & d_1 & d_2 & d_3 \\ \hline d_1 & 3 & 1.5 & 1.5 \\ d_2 & 1.5 & 3 & 3 \\ d_3 & 1.5 & 3 & 3 \end{array}$$

$cov(d_3,d_3) = \frac{1}{2}[(6-7)(6-7) + (9-7)(9-7) + (6-7)(6-7)] = 3$

Step 2 - Compute eigenvalues for covariance matrix.

Eigenvalues of matrix A are roots of characteristic eq^n.

$\det(A - \lambda I) = 0$ where I is identity matrix.

$$(A - \lambda I) = \begin{bmatrix} 3 & 1.5 & 1.5 \\ 1.5 & 3 & 3 \\ 1.5 & 3 & 3 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 3-\lambda & 1.5 & 1.5 \\ 1.5 & 3-\lambda & 3 \\ 1.5 & 3 & 3-\lambda \end{bmatrix}$$

Lets solve $\det(A - \lambda I) = 0$

$$\det \left(\begin{vmatrix} 3-\lambda & 1.5 & 1.5 \\ 1.5 & 3-\lambda & 3 \\ 1.5 & 3 & 3-\lambda \end{vmatrix} \right) = 0.$$

$$(3-\lambda) \begin{vmatrix} 3-\lambda & 3 \\ 3 & 3-\lambda \end{vmatrix} - 1.5 \begin{vmatrix} 1.5 & 3 \\ 1.5 & 3-\lambda \end{vmatrix} + 1.5 \begin{vmatrix} 1.5 & 3-\lambda \\ 1.5 & 3 \end{vmatrix} = 0.$$

$(3-\lambda)[(3-\lambda)(3-\lambda) - 3 \times 3] - 1.5[1.5(3-\lambda) - 3 \times 1.5] + 1.5[1.5 \times 3 - (3-\lambda)1.5] = 0$

$(3-\lambda)[\cancel{9} - 3\lambda - 3\lambda + \lambda^2 - \cancel{9}] - 1.5[\cancel{4.5} - 1.5\lambda - \cancel{4.5}] + 1.5[\cancel{4.5} - \cancel{4.5} + 1.5\lambda] = 0$

$(3-\lambda)[\lambda^2 - 6\lambda] + 2.25\lambda + 2.25\lambda = 0.$

$3\lambda^2 - 18\lambda - \lambda^3 + 6\lambda^2 + 4.5\lambda = 0$

$-\lambda^3 + 9\lambda^2 - 13.5\lambda = 0$

$\lambda^3 - 9\lambda^2 + 13.5\lambda = 0 \implies \lambda(\lambda^2 - 9\lambda + 13.5) = 0$

$\lambda = 0$ is one of root

Lets solve $\lambda(\lambda^2 - 9\lambda + 13.5) = 0$ to get 3 eigenvalues

$\lambda = 0$ is one of root.

Lets solve quadratic eqⁿ $(\lambda^2 - 9\lambda + 13.5)$ to get other 2 roots.

$a = 1, \; b = -9, \; c = 13.5 \qquad \lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

$$\lambda = \frac{9 \pm \sqrt{(-9)^2 - 4(1)(13.5)}}{2 \times 1} = \frac{9 \pm \sqrt{81 - 54}}{2} = \frac{9 \pm \sqrt{27}}{2} = \frac{9 \pm 5.196}{2}.$$

$\lambda = 7.09$ or $\lambda = 1.902$

So eigenvalues are $\lambda = 0$, $\lambda = 7.09$ & $\lambda = 1.902$

Step3 – Lets compute eigenvectors now.

Need to solve $(A - \lambda I)\cancel{X} = 0$ where $\cancel{X}$ is eigenvector with eigen value λ.

i.e.
$$\left(\begin{bmatrix} 3-\lambda & 1.5 & 1.5 \\ 1.5 & 3-\lambda & 3 \\ 1.5 & 3 & 3-\lambda \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right) \begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0.$$

Assume $x = 1$. we get.

$\lambda = 0$.

$$\left(\begin{bmatrix} 3-0 & 1.5 & 1.5 \\ 1.5 & 3-0 & 3 \\ 1.5 & 3 & 3-0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right) \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0$$

$$\begin{bmatrix} 3-0 & 1.5 & 1.5 \\ 1.5 & 3 & 3 \\ 1.5 & 3 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0$$

$\therefore \quad 3 + 1.5y + 1.5z = 0 \Rightarrow 1.5y + 1.5z = -3 \Rightarrow y + z = -0.5$

$1.5 + 3y + 3z = 0 \Rightarrow 3y + 3z = -1.5 \Rightarrow y + z = -0.5$

$1.5 + 3y + 3z = 0 \qquad y + z = -0.5.$

put $y = 1$. then $z = -0.5 - y = -0.5 - 1 = -1.5$

$\therefore$ eigenvector is $[1 \quad 1 \quad -1.5]$ for $\lambda = 0$

for $\lambda = 7.09$

$x = 1$
$$\left(\begin{bmatrix} 3-7.09 & 1.5 & 1.5 \\ 1.5 & 3-7.09 & 3 \\ 1.5 & 3 & 3-7.09 \end{bmatrix} - \begin{bmatrix} 7.09 & 0 & 0 \\ 0 & 7.09 & 0 \\ 0 & 0 & 7.09 \end{bmatrix} \right) \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$$\left(\begin{bmatrix} -4.09 & 1.5 & 1.5 \\ 1.5 & -4.09 & 3 \\ 1.5 & 3 & -4.09 \end{bmatrix} - \begin{bmatrix} 7.09 & 0 & 0 \\ 0 & 7.09 & 0 \\ 0 & 0 & 7.09 \end{bmatrix} \right) \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0$$

$$\begin{bmatrix} -11.18 & 1.5 & 1.5 \\ 1.5 & -11.18 & 3 \\ 1.5 & 3 & 11.18 \end{bmatrix} \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$-11.18 + 1.5y + 1.5z = 0 \Rightarrow 1.5(y+z) = 11.18 \Rightarrow (y+z) = 7.45$

$1.5 - 11.18y + 3z = 0 \Rightarrow -11.18y + 3z = -1.5 \Rightarrow 11.18y - 3z = 1.5.$

$\Rightarrow \cancel{3.72y}$

$\Rightarrow 3(3.72y - z) = 1.5$

$\Rightarrow 3.72y - z = 0.5$

$y + z = 7.45$

$3.72y - z = 0.5$ Add y. $y + 3.72y = 7.45 + 0.5$

$4.72y = 7.95$

$y = 1.68.$

$y = 1.68$ in $y + z = 7.45 \Rightarrow z = 7.45 - y = 7.45 - 1.68 = 5.77.$

eigenvector for $\lambda = 7.09$ is $[1 \quad 1.68 \quad 5.77]$.

for $\lambda = 1.902$

$x = 1$

$$\left(\begin{bmatrix} 3-1.902 & 0 & 0 \\ 0 & 3-1.90 & 0 \\ 0 & 0 & 3-1.9 \end{bmatrix} - \begin{bmatrix} 1.9 & 0 & 0 \\ 0 & 1.9 & 0 \\ 0 & 0 & 1.9 \end{bmatrix}\right) \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$$\left(\begin{bmatrix} 1.1 & 0 & 0 \\ 0 & 1.1 & 0 \\ 0 & 0 & 1.1 \end{bmatrix} - \begin{bmatrix} 1.9 & 0 & 0 \\ 0 & 1.9 & 0 \\ 0 & 0 & 1.9 \end{bmatrix}\right) \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$$\begin{bmatrix} -0.8 & 0 & 0 \\ 0 & -0.8 & 0 \\ 0 & 0 & -0.8 \end{bmatrix} \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$-0.8 \cancel{+ 0y + 0z} =$

$$\left(\begin{bmatrix} 3-1.90 & 1.5 & 1.5 \\ 1.5 & 3-1.9 & 3 \\ 1.5 & 3 & 3-1.9 \end{bmatrix} - \begin{bmatrix} 1.9 & 0 & 0 \\ 0 & 1.9 & 0 \\ 0 & 0 & 1.9 \end{bmatrix}\right) \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$$\left(\begin{bmatrix} 1.1 & 1.5 & 1.5 \\ 1.5 & 1.1 & 3 \\ 1.5 & 3 & 1.1 \end{bmatrix} - \begin{bmatrix} 1.9 & 0 & 0 \\ 0 & 1.9 & 0 \\ 0 & 0 & 1.9 \end{bmatrix}\right) \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$$\begin{bmatrix} -0.8 & 1.5 & 1.5 \\ 1.5 & -0.8 & 3 \\ 1.5 & 3 & -0.8 \end{bmatrix} \begin{bmatrix} 1 \\ y \\ z \end{bmatrix} = 0.$$

$-0.8 + 1.5y + 1.5z = 0 \Rightarrow 1.5(y+z) = 0.8 \Rightarrow y+z = 0.53$
$1.5 - 0.8y + 3z = 0 \Rightarrow 0.8y - 3z = 1.5 \Rightarrow 0.8(y - 1.66z) = 1.5$
$1.5 + 3y - 0.8z = 0 \qquad \Rightarrow y - 1.66z = 1.70$

$y+z = 0.53 \Rightarrow 1.66y + 1.66z = 0.88$
$y - 1.66z = 1.7 \qquad + \; 1.66y - 1.66z = 1.7$

$$3.32y = 2.58$$
$$y = 0.77$$

$y+z = 0.53 \Rightarrow z = 0.53 - y = 0.53 - 0.77 = -0.24$

eigenvector is $[1 \quad 0.77 \quad -0.24]$

Step 4 ⇒ Sort eigenvectors as per decreasing order of eigenvalues.

$\lambda = 7.09 \qquad [1 \quad 1.68 \quad 5.77]$
$\lambda = 1.902 \qquad [1 \quad 0.77 \quad -0.24]$
$\lambda = 0 \qquad [1 \quad 1 \quad -1.5]$

W = d×k dimensional matrix where every column is vector
k=2

$$W = \begin{bmatrix} 1 & 1 \\ 1.68 & 0.77 \\ 5.77 & -0.24 \end{bmatrix}$$

Step 5 ⇒ Use W to transform samples into new subspace

$y = W^T \times x$ where x is d×1 dimensional vector showing one sample of dataset D.
y is transformed k×1 dimensional sample in new subspace.

$[9 \quad 6 \quad 6]$ first row ⟶ $\begin{bmatrix} 9 \\ 6 \\ 6 \end{bmatrix}$

$$W^T = \begin{bmatrix} 1 & 1.68 & 5.77 \\ 1 & 0.77 & -0.24 \end{bmatrix}$$

$$y = W^T x = \begin{bmatrix} 1 & 1.168 & 5.77 \\ 1 & 0.77 & -0.24 \end{bmatrix} \begin{bmatrix} 9 \\ 6 \\ 6 \end{bmatrix}$$

$$= \begin{bmatrix} 1\times9 + 6\times1.168 + 6\times5.77 \\ 1\times9 + 0.77\times6 - 0.24\times6 \end{bmatrix}$$

$$= \begin{bmatrix} 50.628 \\ 12.18 \end{bmatrix}$$

second row $\begin{bmatrix} 9 & 9 & 9 \end{bmatrix} \Longrightarrow \begin{bmatrix} 9 \\ 9 \\ 9 \end{bmatrix}$

$$y = w^T x = \begin{bmatrix} 1 & 1.68 & 5.77 \\ 1 & 0.77 & -0.24 \end{bmatrix} \begin{bmatrix} 9 \\ 9 \\ 9 \end{bmatrix} = \begin{bmatrix} 76.05 \\ 7.61 \end{bmatrix}$$

Third row $\begin{bmatrix} 6 & 6 & 6 \end{bmatrix} \Longrightarrow \begin{bmatrix} 6 \\ 6 \\ 6 \end{bmatrix}$

$$y = w^T x = \begin{bmatrix} 1 & 1.68 & 5.77 \\ 1 & 0.77 & -0.24 \end{bmatrix} \begin{bmatrix} 6 \\ 6 \\ 6 \end{bmatrix} = \begin{bmatrix} 50.7 \\ 9.18 \end{bmatrix}$$

transformed space: $\begin{bmatrix} 50.628 & 12.18 \\ 76.05 & 7.61 \\ 50.7 & 9.18 \end{bmatrix}$