PCA: Numerical Example

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- Consider two attributes X and Y
- Each is sampled three times

$$X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}; \qquad Y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$$

- Combine these two into a matrix S

$$S = \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \\ -1 & 0 \end{bmatrix}$$

- Compute the (un-normalized) covariance matrix, C

$$C = S^T S = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 0 & 1 \\ -1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{bmatrix}$$

- Compute the eigenvalues and eigenvectors of C by solving $Cu = \lambda u \; or \; (C - \lambda I)u = 0$
- If all the attribute vectors are independent, then we have M=2 eigenvalues and M = 2 eigenvectors
- Because the Correlation matrix is real and symmetric all the eigenvalues are real and positive

- Plugging in the numbers, we get

$$\begin{bmatrix} 2-\lambda & -1 \\ -1 & 2-\lambda \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

- To solve for the eigenvalues, we use the determinant of the matrix to get a quadratic equation

$$(2-\lambda)^2 - 1 = \lambda^2 - 4\lambda + 3 = 0 \Rightarrow \lambda_1 = 3, \lambda_2 = 1$$

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- Note that the lambda's are listed in descending order of magnitude
- To solve for the eigenvectors, we simply substitute the two eigenvalues into the matrix equation.
- It is also general practice to find the simplest eigenvector in each case by normalizing it so that the sum of the squares of its components equals 1. Thus, we get:

Eigenvectors

- For $\lambda = 1$

$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

which gives $u_1 = u_2$

- For $\lambda = 3$

$$\begin{pmatrix} -1 & -1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

which gives $u_1 = -u_2$

Normalized Eigenvectors

- It is customary to normalize the eigenvectors
- The normalized eigenvectors are

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}; \qquad \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

- Note that u is the eigenvector associated with larger eigenvalue

Principal Components

- Now we are in a position to compute the principal components of S.

- The principal components are created by multiplying the components of each eigenvector by the attribute vectors and summing the result.

- That is, for the two principal components, P_1 and P_2, we can write

$P_1 = u_1 X + u_2 Y$, and $P_2 = v_1 X + v_2 Y$.

In Matrix Notation

- In matrix form, the principal component matrix is the product of the attribute matrix S and the eigenvector matrix U:

$$P = SU = \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{bmatrix} \begin{bmatrix} u_1 & v_1 \\ u_2 & v_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$$

- Therefore

$$P_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 2 \\ -1 \\ -1 \end{bmatrix}; \quad P_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}$$

- Note also that the principal component matrix has the property that when it is multiplied by its transpose we recover the eigenvalues in diagonal matrix form:

$$P^T P = \frac{1}{2} \begin{bmatrix} 2 & -1 & -1 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ -1 & 1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}$$

- Because the inverse and transpose of the eigenvector matrix are identical, we can write

$$PU^T = SUU^T = SUU^{-1} = S \Rightarrow$$

$$S = \frac{1}{2}\begin{bmatrix} 2 & 0 \\ -1 & 1 \\ -1 & -1 \end{bmatrix}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \\ -1 & 0 \end{bmatrix}$$

- These columns are the values of X & Y recovered!