Principal Components Analysis (PCA)

Step 1: Get the data. In this small example we will have $n = 6$ data points and $p = 2$ features. In reality we would have many more of each, and sometimes $p >> n$. The data matrix with n rows and p columns is called X_{orig}:

$$X_{\text{orig}} = \begin{bmatrix} 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \end{bmatrix} \qquad X = \begin{bmatrix} \quad & \quad \\ & \\ & \\ & \\ & \\ & \end{bmatrix}$$

Step 2: Subtract off the column-wise mean from each column (feature) to obtain X (fill in above). The mean of column f is:

$$\overline{f} = \frac{1}{n}\sum_{i=1}^{n} f_i$$

Step 3: Compute the covariance of each pair of features in X to obtain the $p \times p$ covariance matrix A. The covariance of feature f with feature g is:

$$\text{cov}(f, g) = \frac{1}{n-1}\sum_{i=1}^{n}(f_i - \overline{f})(g_i - \overline{g})$$

Note that in our case, we have set all the means to be 0. Also note that variance is a special case when $f = g$:

$$\text{cov}(f, f) = \text{var}(f) = \frac{1}{n-1}\sum_{i=1}^{n}(f_i - \overline{f})^2$$

Fill in A below:

$$A = \begin{bmatrix} \quad & \quad \\ & \end{bmatrix}$$

Step 4: Compute the eigenvalues (λ_1, λ_2 for $p = 2$) and eigenvectors ($\vec{v}_1$, $\vec{v}_2$) of A. The eigenvectors (sorted by eigenvalue) will become the directions of our principal components (i.e. new coordinate system). We want our eigenvectors and eigenvalues to satisfy:

$$A\vec{v} = \lambda\vec{v} \quad \Rightarrow \quad \det(A - \lambda I) = 0$$

If you've had linear algebra, verify that the eigenvalues are $\lambda_1 = \frac{3}{5}$ and $\lambda_2 = 0$, and the eigenvectors are $\vec{v}_1 = [1, -1]^T$ and $\vec{v}_2 = [1, 1]^T$. Otherwise use these directly in Step 5.

Step 5: Transform the data X using the eigenvector matrix W (one eigenvector on each *column*, sorted by eigenvalue). The number of eigenvectors we use corresponds to the number of dimensions we retain. Say we want to retain r dimensions, then we would obtain the transformed data $T_r = XW_r$. T_r will be an $n \times r$ matrix. In our case, use $r = 2$ and compute T_r.

$$T_2 = XW_2 = \begin{bmatrix} \quad & \quad \\ & \\ & \\ & \end{bmatrix} \begin{bmatrix} \quad & \quad \\ & \end{bmatrix} = \begin{bmatrix} \quad & \quad \\ & \\ & \\ & \end{bmatrix}$$

Step 6: Finally, plot the transformed data T_r with principal component 1 (PC1) on the x-axis and PC2 on the y-axis. We could plot further PCs on different coordinate systems when $p > 2$.