**Principal Components Analysis for Two Variables**

There is software that computes principal components (PCs) very efficiently. No one wants to compute PCs by hand. But you may gain insight by seeing how it works in the simple case of two X's. So suppose you have data $(x_{11}, x_{12}, x_{13}, ..., x_{1n})$ and $(x_{21}, x_{22}, x_{23}, ..., x_{2n})$ on two variables $X_1$ and $X_2$. I will derive the two PCs and their eigenvalues manually for the case of standardized X's.

For the case of standardized X's, the PCs are the eigenvectors of the correlation matrix. So the derivation begins with the correlation matrix $R = \begin{bmatrix} corr(X_1, X_1) & corr(X_1, X_2) \\ corr(X_1, X_2) & corr(X_1, X_2) \end{bmatrix} = \begin{bmatrix} 1 & r \\ r & 1 \end{bmatrix}$, where $r = corr(X_1, X_2)$.

<u>First</u>, compute the eigenvalues $\lambda_1, \lambda_2$. By definition, they are the solutions to the determinant equation $|\mathbf{R} - \lambda \mathbf{I}| = 0$, i.e., $\left\| \begin{bmatrix} 1 & r \\ r & 1 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\| = 0$, or $\left\| \begin{bmatrix} 1-\lambda & r \\ r & 1-\lambda \end{bmatrix} \right\| = 0$. Expand the determinant to get $(1-\lambda)^2 - r^2 = 0$ and solve for $\lambda$: $\lambda_1 = 1 + r$ and $\lambda_2 = 1 - r$ are the two solutions.[1] [Note: The sum of the eigenvalues is $\lambda_1 + \lambda_2 = (1+r) + (1-r) = 2$, as it should be.]

<u>Second</u>, for each eigenvalue, compute the eigenvectors $(v_1, v_2)$. These will be the principal component coefficients. By definition, the eigenvectors are solutions to the set of equations $[\mathbf{R} - \lambda_i \mathbf{I}]\mathbf{v} = \mathbf{0}$ or $\left[ \begin{bmatrix} 1 & r \\ r & 1 \end{bmatrix} - \lambda_i \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right] \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. (There is one eigenvector for each eigenvalue, so you must solve this pair of equations for $\lambda_i = \lambda_1 = 1 + r$ and then again for $\lambda_i = \lambda_2 = 1 - r$.) The equations are $\begin{bmatrix} 1-\lambda_i & r \\ r & 1-\lambda_i \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. Hence $\begin{bmatrix} (1-\lambda_i)v_1 + rv_2 \\ rv_1 + (1-\lambda_i)v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. For $\lambda_i = \lambda_1 = 1 + r$, this becomes $\begin{bmatrix} -rv_1 + rv_2 \\ rv_1 - rv_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. The equations are linearly dependent, so there are infinitely many solutions. Any vector is a solution if $v_1 = v_2$. For $\lambda_i = \lambda_2 = 1 - r$, the equations become $\begin{bmatrix} rv_1 + rv_2 \\ rv_1 + rv_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. So any vector is a solution if $v_1 = -v_2$. Let $(a, a)$ denote a generic solution when $\lambda_i = \lambda_1 = 1 + r$. Let $(b, -b)$ denote a generic solution when $\lambda_i = \lambda_2 = 1 - r$. Then the equations that transform $(x_1, x_2)$ into their principal components $(\xi_1, \xi_2)$ have the form $\begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} a & a \\ b & -b \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. In order for this rotation matrix to qualify as the PC rotation, it must be

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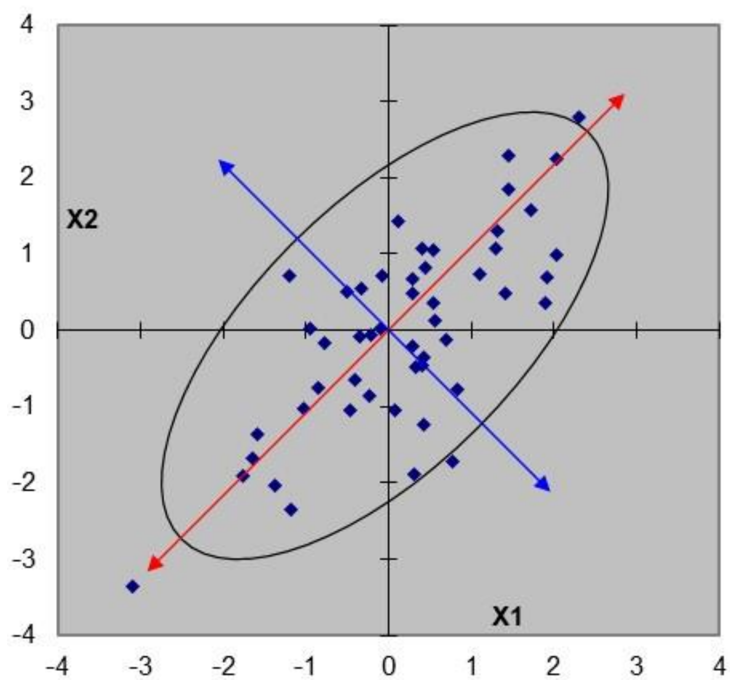
[1] By convention, $\lambda_1$ is the larger and $\lambda_2$ is the smaller. So if $r \geq 0$, then $\lambda_1 = 1 + r$ and $\lambda_2 = 1 - r$ are the two solutions; if $r \leq 0$, then $\lambda_1 = 1 - r$ and $\lambda_2 = 1 + r$.

orthonormal. Let us check that out. Now, $(x_1, x_2)$ = (1,0) is transformed into ($a$,$b$); and $(x_1, x_2)$ = (0,1) is transformed into ($a$,-$b$). For orthonormality, we must have the transformed lengths = 1; i.e., $\sqrt{a^2 + b^2} = 1$. And the angle between them must have cosine = 0; i.e. ($a$,$b$)•($a$,-$b$) = $a^2 - b^2 = 0$. Substituting the latter into the length constraint, we have $\sqrt{a^2 + a^2} = 1$. Hence $a = 1/\sqrt{2} = b$. Thus, the PC transformation is

$$\begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} x_1 + \frac{1}{\sqrt{2}} x_2 \\ \frac{1}{\sqrt{2}} x_1 - \frac{1}{\sqrt{2}} x_2 \end{bmatrix}$$

We see that the first PC $\xi_1 = \frac{1}{\sqrt{2}} x_1 + \frac{1}{\sqrt{2}} x_2$ is essentially the sum or the mean of the two X's, the second PC $\xi_2 = \frac{1}{\sqrt{2}} x_1 - \frac{1}{\sqrt{2}} x_2$ is essentially their difference. Curiously, the solution does not depend upon the value of the correlation between the two X's. These are the PCs for any two $X$'s! However, the variances of the two PCs do depend upon the correlation. The variances are $Var(\xi_1) = \lambda_1 = 1 + r$ and $Var(\xi_2) = \lambda_2 = 1 - r$.




The figure above illustrates the situation. The two PCs are the two perpendicular arrows. PC1 (red) has slope +1 and PC2 (blue) has slope -1. They cross at the origin. The larger the correlation, the more the data stretch out in the direction of PC1, the larger the variance of PC1, and the more elliptical the data plot appears. The closer the correlation is to 0, the less the data spread out, the smaller the variance of PC1, and the more circular the data plot appears. If the correlation is negative, then the orientation of the ellipse will rotate to upper left to lower right; PC1 will remain the long axis, but it will have slope of -1; and PC2 will remain the short axis, but with slope of +1, as footnote 1 suggests. In the original coordinates, the standardized $X_1$ and $X_2$ are correlated – indicated by the angled orientation of the data ellipse to the $X_1$ and $X_2$ axes. The principal components transformation replaces the original coordinate axes by the major and minor axes of the ellipse (the arrowed lines). In that new coordinate system, the data ellipse is flat – the data orientation is no longer angled; the correlation is zero.

It is worth noting that neither PC is the regression line for either variable. The regression of $X_2$ on $X_1$ has slope *r*, and the regression of $X_1$ on $X_2$ has slope 1/*r*. The regression lines rotate toward the original axes – illustrating the phenomenon of regression to the mean. The regression line for $X_2$ on $X_1$ minimizes the total squared *vertical up-and-down* distance from the points to the regression line; PC1 minimizes the total squared *perpendicular* distance from the points to the PC1 line.