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 benefit 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 manually for the case of standardized X's.

The derivation for the standardized case 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 $r = corr(X_1, X_2)$.

First, compute the eigenvalues λ_1, λ_2, which are the solutions to the determinantal 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 λ: $\lambda_1 = 1 + r$ 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.]

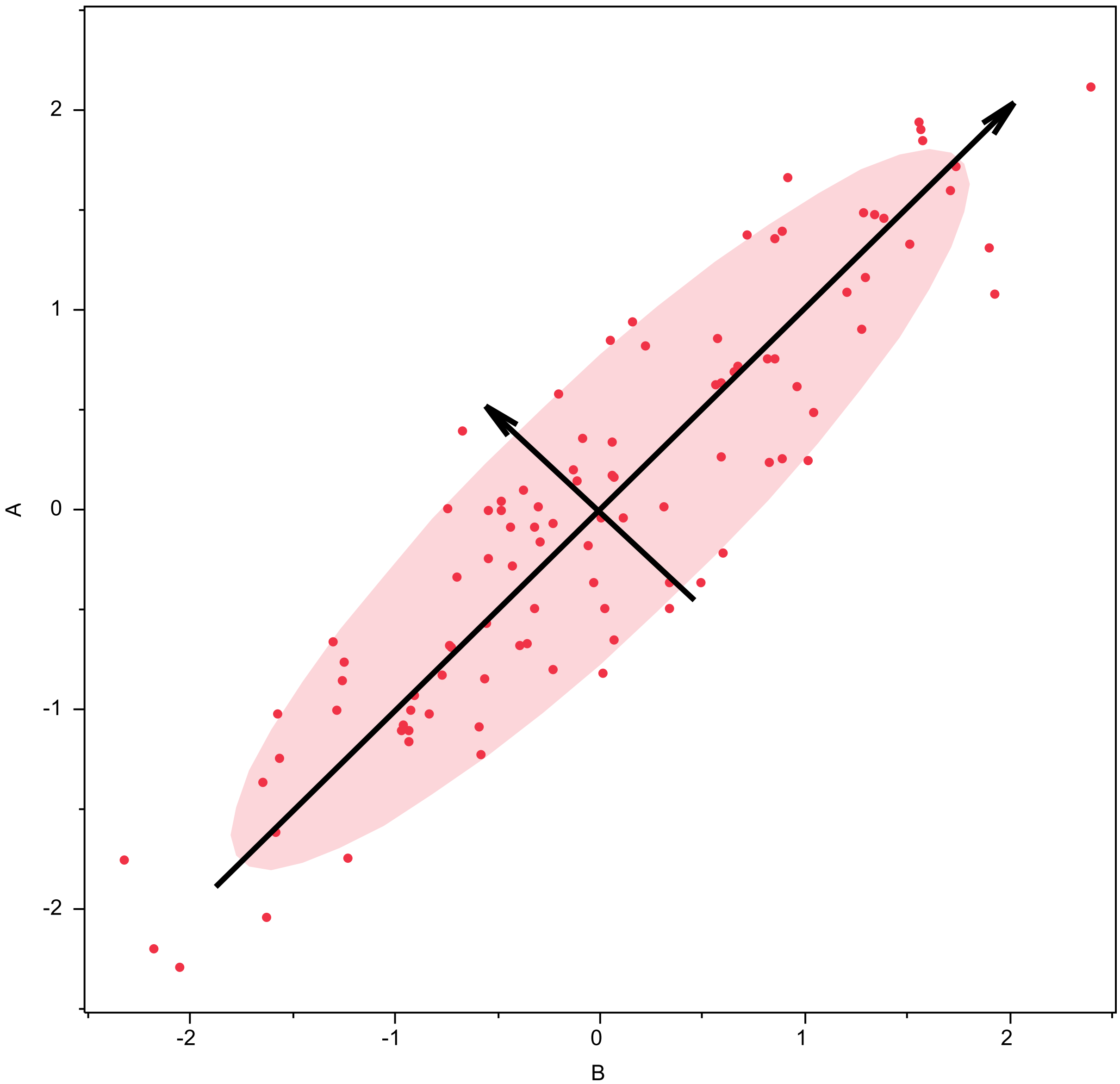
Second, for each eigenvalue, compute the eigenvectors (v_1, v_2). These will be the principal component coefficients. But by definition, the eigenvectors are solutions to the set of equations $[\mathbf{R} - \lambda_i \mathbf{I}]\mathbf{v} = \mathbf{0}$ or $\left[\begin{bmatrix} 1 & r \\ r & 1 \end{bmatrix} - \lambda_i \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right] \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. (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 $\begin{bmatrix} -rv_1 + rv_2 \\ rv_1 - rv_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. So any vector is a solution if $v_1 = v_2$. For $\lambda_i = \lambda_2 = 1 - r$, it becomes $\begin{bmatrix} rv_1 + rv_2 \\ rv_1 + rv_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. 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 form (ξ_1, ξ_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 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 $(a,-b)$. So 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. $a^2 - b^2 = 0$. 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

---

[1] This is the solution if $r \geq 0$. If $r \leq 0$, then $\lambda_1 = 1 - r$ and $\lambda_2 = 1 + r$ are the two solutions.

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

We see that the first PC $\xi_1 = \frac{1}{\sqrt{2}} x_1 + \frac{1}{\sqrt{2}} x_2$ is essentially the 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. 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 illustrates the situation. The two PCs are the two perpendicular arrows. PC1 has slope +1 and PC2 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 PC1 becomes the arrow with slope of -1, and PC2 becomes the arrow 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 A on B has slope *r,* and the regression of B on A has slope 1/*r*.