Q1: A three-stimulus brain in a two-stimulus world

Consider a toy functional imaging experiment, in which the brain has 3 pixels, and there are two stimuli. Say that stimulus 1 causes an activation of +2 units in pixel 1, and -1 unit in pixels 2 and 3; say that stimulus 2 causes an activation of +2 units in pixel 2, and -1 unit in pixels 1 and 3. So we have a 3×2 data matrix Y.

A. Compute its principal components, \( Y = XB \), with the columns of \( X \) orthonormal, and the rows of \( B \) orthogonal (but not necessarily orthonormal).

\[
Y = \begin{pmatrix} 2 & -1 \\ -1 & 2 \\ -1 & -1 \end{pmatrix}, \text{ so } YY^* = \begin{pmatrix} 2 & -1 \\ -1 & 2 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} 2 & -1 \\ -1 & 2 \\ -1 & -1 \end{pmatrix} = \begin{pmatrix} 5 & -4 & -1 \\ -4 & 5 & -1 \\ -1 & -1 & 2 \end{pmatrix}.
\]

But it’s easier to determine the eigenvalues of \( YY^* \):

\[
\text{We use the approach described under “Symmetry—an important practical issue”: seek } Z \text{ as the first } p \text{ (row) eigenvectors of the } k \times k \text{ matrix } YY^*, \text{ and then find } X = YZ^* \Lambda^{-1/2} \text{ and } B = \Lambda^{1/2} Z, \text{ where } \Lambda \text{ is the matrix with the eigenvalues of } YY^* \text{ on the diagonal.}
\]

We could find the eigenvalues of \( YY^* \) by solving its characteristic equation, \( \det(\lambda I - YY^*) = 0 \). This is

\[
\text{det} \left( \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 6 & -3 \\ -3 & 6 \end{pmatrix} \right) = \text{det} \begin{pmatrix} \lambda - 6 & 3 \\ 3 & \lambda - 6 \end{pmatrix} = (\lambda - 6)^2 - 9 = \lambda^2 - 12\lambda + 27 = (\lambda - 9)(\lambda - 3), \text{ which has roots } \\
\lambda = 9 \text{ and } \lambda = 3.
\]

Or we could note that \( YY^* \) is symmetric under interchange of coordinates, so its eigenvectors must lie in subspaces that are preserved under interchange of coordinates, and therefore, must be proportional to \( v_+ = (1,1) \) and \( v_- = (1,-1) \)— and determine the eigenvectors by computing \( v_+ YY^* = 3v_+ \), and \( v_- YY^* = 9v_- \). Noting that \( v_+ = (1,1) \) and \( v_- = (1,-1) \) have squared-lengths of 2, we find the matrix of orthonormalized row eigenvectors, \( Z = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \), and \( \Lambda = \begin{pmatrix} 9 & 0 \\ 0 & 3 \end{pmatrix} \).

So \( B = \Lambda^{1/2} Z = \begin{pmatrix} 3 & 0 \\ 0 & \sqrt{3} \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 3 & -3 \\ \sqrt{3} & \sqrt{3} \end{pmatrix}. \)

\[
X = YZ^* \Lambda^{-1/2} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 9 & 0 \\ 0 & 3 \end{pmatrix}^{-1/2} = \frac{1}{\sqrt{2}} \begin{pmatrix} 2 & -1 \\ -1 & 2 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} 1/3 & 0 \\ 0 & 1/\sqrt{3} \end{pmatrix}.
\]

And

\[
= \frac{1}{\sqrt{2}} \begin{pmatrix} 3 & 1 \\ -3 & 1 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} 1/3 & 0 \\ 0 & 1/\sqrt{3} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1/\sqrt{3} \\ -1 & 1/\sqrt{3} \\ 0 & -2/\sqrt{3} \end{pmatrix}.
\]

Verify that \( Y = XB \), where the columns of \( X \) orthonormal, and the rows of \( B \) orthogonal.

\[ Y = XB \]
Note that the first principal component (i.e., the first column of \( X \)) is a mixture of the two responses – and is in some sense more complicated than either of them.

**Q2. Rotation of principal components.** Same setup as Q1. Let’s see if we can find a simple way to unmix these components. Let \( \tilde{u}_1 = \tilde{x}_1 \cos \theta + \tilde{x}_2 \sin \theta \), \( \tilde{u}_2 = -\tilde{x}_1 \sin \theta + \tilde{x}_2 \cos \theta \). Since the \( \tilde{u}_i \) are a non-singular linear combination of the \( \tilde{x}_i \), they necessarily also account for the data matrix \( Y \). We might consider a transformation to the \( \tilde{u}_i \) to be simpler if the coefficients in the \( \tilde{u}_i \) are smaller. The \( \tilde{u}_i \), like the \( \tilde{x}_i \), constitute the columns of a \( 3 \times 2 \) matrix, \( U(\theta) \). Is there a rotation \( \theta \) that minimizes the sum of the squares of these 6 quantities? If so, find it; if not, explain why and suggest alternative strategies.

The sum of the squares of the entries in \( U(\theta) \) is independent of \( \theta \), and identical to that of \( X \). The reason is that \( U = XR_\theta \), where \( R_\theta = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \), a rotation matrix. Since \( R_\theta R_\theta^* = I \),

\[
tr(UU^*) = tr\left(XR_\theta(XR_\theta)^*\right) = tr\left(XR_\theta R_\theta^* X^*\right) = tr(XX^*) .
\]

An alternative is to extremize the sum of the fourth powers of the entries of \( U(\theta) \). This will seek components whose entries have either very large values, or very small values (i.e., a “sparse” representation). This is effectively the “varimax” procedure.