Exercise: PCA via successive deflation

Let $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k$ be the first k eigenvectors with largest eigenvalues of $\mathbf{C} = \frac{1}{n}\mathbf{X}^T\mathbf{X}$, i.e., the principal basis vectors. These satisfy

$$\mathbf{v}_j^T\mathbf{v}_k = \begin{cases} 0 & \text{if } j \neq k \\ 1 & \text{if } j = k \end{cases} \tag{1}$$

We will construct a method for finding the $\mathbf{v}_j$ sequentially.

As we showed in class, $\mathbf{v}_1$ is the first principal eigenvector of $\mathbf{C}$, and satisfies $\mathbf{C}\mathbf{v}_1 = \lambda_1\mathbf{v}_1$. Now define $\tilde{\mathbf{x}}_i$ as the orthogonal projection of $\mathbf{x}_i$ onto the space orthogonal to $\mathbf{v}_1$:

$$\tilde{\mathbf{x}}_i = \mathbf{P}_{\perp\mathbf{v}_1}\ \mathbf{x}_i = (\mathbf{I} - \mathbf{v}_1\mathbf{v}_1^T)\mathbf{x}_i \tag{2}$$

Define $\tilde{\mathbf{X}} = [\tilde{\mathbf{x}}_1; ...; \tilde{\mathbf{x}}_n]$ as the **deflated matrix** of rank $d-1$, which is obtained by removing from the d dimensional data the component that lies in the direction of the first principal direction:

$$\tilde{\mathbf{X}} = (\mathbf{I} - \mathbf{v}_1\mathbf{v}_1^T)^T\mathbf{X} = (\mathbf{I} - \mathbf{v}_1\mathbf{v}_1^T)\mathbf{X} \tag{3}$$

1. Using the facts that $\mathbf{X}^T\mathbf{X}\mathbf{v}_1 = n\lambda_1\mathbf{v}_1$ (and hence $\mathbf{v}_1^T\mathbf{X}^T\mathbf{X} = n\lambda_1\mathbf{v}_1^T$) and $\mathbf{v}_1^T\mathbf{v}_1 = 1$, show that the covariance of the deflated matrix is given by

$$\tilde{\mathbf{C}} \triangleq \frac{1}{n}\tilde{\mathbf{X}}^T\tilde{\mathbf{X}} = \frac{1}{n}\mathbf{X}^T\mathbf{X} - \lambda_1\mathbf{v}_1\mathbf{v}_1^T \tag{4}$$

2. Let $\mathbf{u}$ be the principal eigenvector of $\tilde{\mathbf{C}}$. Explain why $\mathbf{u} = \mathbf{v}_2$. (You may assume $\mathbf{u}$ is unit norm.)

3. Suppose we have a simple method for finding the leading eigenvector and eigenvalue of a pd matrix, denoted by $[\lambda, \mathbf{u}] = f(\mathbf{C})$. Write some pseudo code for finding the first K principal basis vectors of $\mathbf{X}$ that only uses the special f function and simple vector arithmetic, i.e., your code should not use SVD or the `eig` function. Hint: this should be a simple iterative routine that takes 2–3 lines to write. The input is $\mathbf{C}$, K and the function f, the output should be $\mathbf{v}_j$ and λ_j for $j = 1 : K$. Do not worry about being syntactically correct.