Homework 2
Stat 215A, Fall 2019

Due: provide a hard copy at the beginning of the lab on Friday October 11th or push a `homework2.pdf` file to your `stat-215-a` GitHub repo by Thursday October 10 11:59pm

0 Linear Algebra Review

Recall that the SVD of $\mathbf{X} \in \mathbb{R}^{n \times p}$ is a matrix decomposition such that $\mathbf{X} = \mathbf{U}\,\mathbf{D}\,\mathbf{V}^\top$, where $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_n] \in \mathbb{R}^{n \times n}$, $\mathbf{V} = [\mathbf{v}_1, \ldots, \mathbf{v}_p] \in \mathbb{R}^{p \times p}$, and $\mathbf{D} = \mathrm{diag}(d_1, \ldots, d_{\min\{n,p\}}) \in \mathbb{R}^{n \times p}$. In addition, $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices so that $\mathbf{U}^\top\,\mathbf{U} = \mathbf{U}\,\mathbf{U}^\top = \mathbf{I}$ and $\mathbf{V}^\top\,\mathbf{V} = \mathbf{V}\,\mathbf{V}^\top = \mathbf{I}$ (i.e., $\mathbf{u}_j^\top\,\mathbf{u}_i = \mathbf{v}_j^\top\,\mathbf{v}_i = 0$ for all $i \neq j$ and $\mathbf{u}_j^\top\,\mathbf{u}_j = \mathbf{v}_j^\top\,\mathbf{v}_j = 1$ for all i). Moreover, $d_1 \geq \cdots \geq d_{\min\{n,p\}} \geq 0$.

Now, while the SVD can be used for any rectangular matrix, square matrices have an additional special property and can be decomposed via an eigendecomposition. Given a square matrix $\mathbf{A} \in \mathbb{R}^{p \times p}$, we say that $\mathbf{v} \in \mathbb{R}^p$ is an *eigenvector* of $\mathbf{A}$ if $\mathbf{v} \neq \mathbf{0}$ and $\mathbf{A}\,\mathbf{v} = \lambda\,\mathbf{v}$ for some $\lambda \in \mathbb{R}$. We also call λ the *eigenvalue* of $\mathbf{A}$ corresponding to the eigenvector $\mathbf{v}$. For a more intuitive (geometric) interpretation of eigenvalues and eigenvectors, see this reference.

There is a close connection between the SVD and eigendecomposition. Namely, for any matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, $\mathbf{v} \in \mathbb{R}^p$ is a right singular vector of $\mathbf{X}$ with singular value d if and only if $\mathbf{v} \in \mathbb{R}^p$ is an eigenvector of $\mathbf{X}^\top\,\mathbf{X}$ corresponding to the eigenvalue d^2. You may use this fact without proof.

1 Principal Components Analysis and SVD

Let $\mathbf{X}$ be an $n \times p$ data matrix, where n is the number of observations and p is the number of features. For simplicity, we will assume that $\mathbf{X}$ has been mean-centered (i.e., each column of X has mean 0) and that $n \leq p$. In the lab section, we used projections in order to introduce the population version of PCA as solving for each $j = 1, \ldots, p$

$$\mathbf{v}_j^* = \underset{\mathbf{v} \in \mathbb{R}^p}{\mathrm{argmax}}\ \mathbf{v}^\top\,\mathrm{Var}(\mathbf{X})\,\mathbf{v} \qquad \text{subject to} \quad \|\mathbf{v}\|_2^2 = 1, \quad \mathbf{v}^\top\,\mathbf{v}_i^* = 0\ \forall\, i < j. \tag{1.1}$$

However, since $\mathrm{Var}(\mathbf{X})$ is almost always unknown in practice, we typically estimate $\mathrm{Var}(\mathbf{X})$ with the sample covariance $\frac{1}{n}\,\mathbf{X}^\top\,\mathbf{X}$. Thus, in practice, the principal component (PC) directions, $\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_p$, are the solution to the following system of optimization problems:

$$\hat{\mathbf{v}}_j = \underset{\mathbf{v} \in \mathbb{R}^p}{\mathrm{argmax}}\ \mathbf{v}^\top\,\mathbf{X}^\top\,\mathbf{X}\,\mathbf{v} \qquad \text{subject to} \quad \|\mathbf{v}\|_2^2 = 1, \quad \mathbf{v}^\top\,\hat{\mathbf{v}}_i = 0\ \ \forall\, i < j. \tag{1.2}$$

In this problem, we will take small steps through the proof to show that the PC directions are precisely the right singular vectors of $\mathbf{X}$.

1. To begin, prove that the first PC direction $\hat{\mathbf{v}}_1$ is equal to the first right singular vector $\mathbf{v}_1$. To show this, use Lagrange multipliers to solve the PC1 optimization problem:

$$\hat{\mathbf{v}}_1 = \underset{\mathbf{v} \in \mathbb{R}^p}{\mathrm{argmax}}\ \mathbf{v}^\top\,\mathbf{X}^\top\,\mathbf{X}\,\mathbf{v} \qquad \text{subject to} \quad \|\mathbf{v}\|_2^2 = 1. \tag{1.3}$$

If you are not familiar with matrix calculus, Wikipedia is a convenient resource for common derivative identities, which you may find useful here.

2. Next, let $j \in \{2, \dots, p\}$ be given. Use the SVD and matrix multiplication to show that for all $\mathbf{v} \in \mathbb{R}^p$ satisfying $\mathbf{v}^\top \mathbf{v}_i = 0$ for each $i < j$, we have

$$\mathbf{v}^\top \mathbf{X}^\top \mathbf{X}\,\mathbf{v} = \sum_{k=j}^{p} \mathbf{v}^\top \left(d_k^2\, \mathbf{v}_k\, \mathbf{v}_k^\top \right) \mathbf{v}, \tag{1.4}$$

where we define $d_k = 0$ for $k = n+1, \dots, p$.

3. Then, show that for each $j = 2, \dots, p$, the original (sample) PCA formulation in (1.2) is equivalent to

$$\hat{\mathbf{v}}_j = \underset{\mathbf{v} \in \mathbb{R}^p}{\operatorname{argmax}}\ \mathbf{v}^\top \left(\mathbf{X}_{(j)}^\top\, \mathbf{X}_{(j)} \right) \mathbf{v} \qquad \text{subject to} \quad \|\mathbf{v}\|_2^2 = 1, \tag{1.5}$$

where $\mathbf{X}_{(j)} = \widetilde{\mathbf{U}}\widetilde{\mathbf{D}}\widetilde{\mathbf{V}}^\top$, $\widetilde{\mathbf{U}} = [\mathbf{u}_j, \dots, \mathbf{u}_n, \mathbf{u}_1, \dots, \mathbf{u}_{j-1}] \in \mathbb{R}^{n \times n}$, $\widetilde{\mathbf{D}} = \operatorname{diag}(d_j, \dots, d_n, 0, \dots, 0) \in \mathbb{R}^{n \times p}$, and $\widetilde{\mathbf{V}} = [\mathbf{v}_j, \dots, \mathbf{v}_p, \mathbf{v}_1, \dots, \mathbf{v}_{j-1}] \in \mathbb{R}^{p \times p}$.

4. Conclude that for each $j = 1, \dots, p$, the j^{th} PC direction, $\hat{\mathbf{v}}_j$, is equal to the j^{th} right singular vector $\mathbf{v}_j$. (Hint: Problem 1 may be useful).

2 Ordinary Least Squares

Suppose that we observe our usual data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ and response vector $\mathbf{y} \in \mathbb{R}^n$, where n is the number of samples/observations and p is the number of features. Suppose also that $\mathbf{X}$ has rank $p < n$. Under this setting, the ordinary least squares (OLS) estimator is given by

$$\hat{\boldsymbol{\beta}}_{OLS} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}}\ \|\mathbf{y} - \mathbf{X}\,\boldsymbol{\beta}\|_2^2.$$

1. Provide an expression for $\hat{\boldsymbol{\beta}}_{OLS}$ in terms of $\mathbf{X}$ and $\mathbf{y}$ by solving the optimization problem above. Why do we require the assumption that $\operatorname{rank}(\mathbf{X}) = p < n$?

2. Show that the OLS predictions $\hat{\mathbf{y}} = \mathbf{X}\,\hat{\boldsymbol{\beta}}_{OLS}$ can be written as $\hat{\mathbf{y}} = \mathbf{H}\,\mathbf{y}$, where $\mathbf{H}^2 = \mathbf{H}$.

3. Prove that the residuals $\hat{\mathbf{r}} = \mathbf{y} - \hat{\mathbf{y}}$ are orthogonal to the OLS predictions $\hat{\mathbf{y}}$. Draw a picture to show what this means geometrically.