

# Homework 2

## Stat 215A, Fall 2021

**Due:** push a `homework2.pdf` file to your `stat-215-a` GitHub repo by Thursday, October 07 at 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  $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_n] \in \mathbb{R}^{n \times n}$ ,  $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_p] \in \mathbb{R}^{p \times p}$ , and  $\mathbf{D} = \text{diag}(d_1, \dots, d_{\min\{n,p\}}) \in \mathbb{R}^{n \times p}$ . 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  $j$ ). Moreover,  $d_1 \geq \dots \geq d_{\min\{n,p\}} \geq 0$ .

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  $\lambda$  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  $\mathbf{X}$  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  $j = 1, \dots, p$

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

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

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

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:

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

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

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

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

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

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

4. Conclude that for each  $j = 1, \dots, p$ , the  $j^{\text{th}}$  PC direction,  $\hat{\mathbf{v}}_j$ , is equal to the  $j^{\text{th}}$  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

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

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.