Notes

STA314H1 - Fall 2020

Ziyue Yang

November 26, 2020

Contents

1 Week 5

1.1 Norms

1.1.1 Induced Norm of a Matrix

Question 1.1. If we have a vector x and a matrix A, how big is Ax compared to x?

Suppose that we find a constant $C_{A,q}$ such that

$$\|Ax\|_q \leq C_{A,q}\|x\|_q, \tag{1.1}$$

then the **smallest such constant** would be a good indication of how much multiplying by A changes the length of a vector.

▌ This lets us define the **induced norm** of a matrix

Definition 1.1 (The Induced Norm of a Matrix)**.** The induced norm of a matrix A is defined as

$$\|A\|_q = \sup_x \frac{\|Ax\|_q}{\|x\|_q}. \tag{1.2}$$

▌ NB: This works when A is rectangular.

1.1.2 jj2-Norm of a Matrix

We hold a special place for 2-norms, as well as the induced 2-norm of a matrix.

Definition 1.2 (The Induced 2-Norm of a Matrix)**.**

$$\|A\|_2^2 = \sup_x \frac{\|Ax\|_2^2}{\|x\|_2^2} = \sup_x \frac{x^T A^T Ax}{x^T x}. \tag{1.3}$$

Note that this is the **largest eigenvalue of** $A^T A$. Hence the 2-norm of a matrix A is the square root of the largest eigenvalue of $A^T A$.

1.1.3 Orthogonal Invariance

It turns out that both the matrix and vector 2-norms are invariant to multiplication by an orthogonal matrix. Note that this is NOT true for other norms.

Example 1.1. Suppose U is a $p \times p$ orthogonal matrix, then

$$\|Ux\|_2^2 = x^T Y^T Y x = x^T x = \|x\|_2^2. \tag{1.4}$$

Suppose A is an $n \times p$ matrix, V is an $n \times n$ orthogonal matrix. Then

$$\|U^T AVx\|_2^2 = \|U^T A\tilde{x}\|_2^2 = \tilde{x}^T A^T U U^T A\tilde{x} = \tilde{x}^T A^T A\tilde{x}, \tag{1.5}$$

where $\tilde{x} = Vx$, $\|\tilde{x}\|_2^2 = \|x\|_2$ and so

$$\|U^T AV\|_2 = \|A\|_2. \tag{1.6}$$

1.2 The Singular Value Decomposition (of Non-Symmetic and Rectangular Matrices)

Remark 1.1. We know that $\|X\|_2$ is the square root of the largest eigenvalue of $X^T X$, hence at some point , whenever we see one of the inner product matrices, we should recall the **PCA**.

The SVD is a good way to understand exactly how PCA is working in terms of the feature matrix X.

Theorem 1.1 (The Singular Value Decomposition)**.** Assume that $p < n$.

Let X be an $n \times p$ matrix. Then there exists an orthogonal $p \times p$ matrix V (i.e. $V^T V = VV^T = I$) and an orthogonal $n \times n$ matrix U such that

$$U^T X V = D, \tag{1.7}$$

where $D = \text{diag}(\sigma_1, \ldots, \sigma_p)$, and $\sigma_1 \geq \cdots \geq \sigma_p \geq 0$.

Proof. Omitted for now. □

1.2.1 The SVD and Principal Components

Remark 1.2. So what good is an SVD?

The SVD is like the *eigendecomposition* of a symmetic matrix, except it is defined for **all** matrices.

We can express the SVD of an $n \times p$ matrix X in several equivalent ways:

1. As a singular tuple (σ, u, v) that satisfies $Xv = \sigma u$ and $X^T u = \sigma v$.
2. As a matrix decomposition $X = UDV^T$, where V is a $p \times p$ orthogonal matrix, and U is a $n \times n$ orthogonal matrix.
3. As a way of representing the matrix as a sum

$$X = \sum_{j=1}^{p} \sigma_j u_j v_j^T. \tag{1.8}$$

Remark 1.3 (The SVD and Principal Components)**.** Recall that the factor loadings are the eigenvectors of $X^T X$.

If $X = UDV^T$, then $X^T X = V^T D U^T U D V^T = V D^2 V^T$.

- The V in the SVD is exactly the matrix of factor loadings.
- The eigenvalues of $X^T X$ are the squares of the singular values.

Note that the score vectors were defined as $t_j = X v_j$, and We can use one of the representations of singular vectors to see that

$$t_j = X v_j = \sigma_j u_j. \tag{1.9}$$

1.2.2 SVD and Principlal Component Regression

Remark 1.4. The SVD makes it easy to solve the normal equations.

Recall that

$$\begin{aligned}\hat{\beta} &= (X^T X)^{-1} X^T y && (1.10)\\ &= V D^{-2} V^T V D U^T y && (1.11)\\ &= V D^{-1} U^T y && (1.12)\\ &= \sum_{j=1}^{p} \frac{u_j^T y}{\sigma_j} v_j. && (1.13)\end{aligned}$$

PCR just snipes off the small eigenvectors:

$$\hat{\beta}_{\text{pcr}} = V_k D_k^{-2} V_k^T V D U^T = \sum_{j=1}^{k} \frac{u_j^T y}{\sigma_j} v_j. \tag{1.14}$$

1.3 Ridge Regression

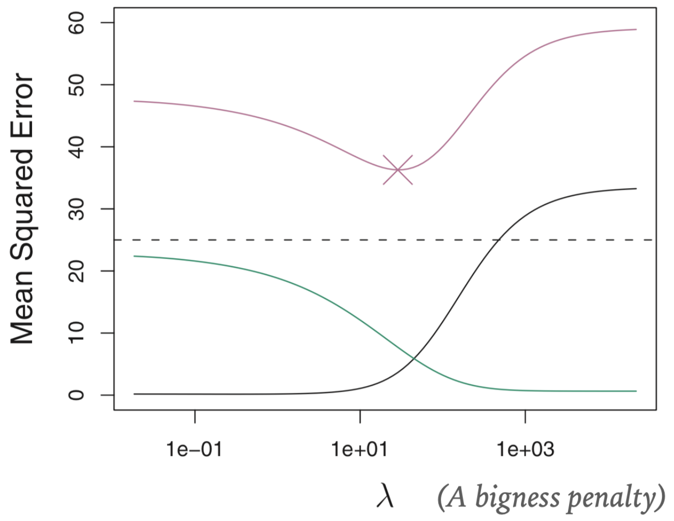
1.3.1 Overfitting Discussion

As we add more features to our regression, our training error will decrease, as our test error will go down for a while, then will increase again. A sign that something has gone wrong is that we have wildly varying regression coefficients, reasons include

- (Almost) co-linearity of features;
- Big feature weights are needed to fit data perfectly,

which can lead to out-of-sample *bias*.

What if we force the coefficients to be small?



The idea is: *Don't let things get to big.*

1.3.2 Ridge Regression Objective Function

Instead of solving our standard least-squares problem, we should use the **ridge regression** objective function.

Definition 1.3 (Ridge Regression Objective Function)**.**

$$\min_{\beta_0,\beta} \sum_{i=1}^{n} (y_i - \beta_0 - X\beta)^2 + \lambda \|\beta\|_2^2. \tag{1.15}$$

This means that we need to **balance** the goodness of fit with the requirements that the β_j aren'r too big. The parameter λ controls the balance.

If $\lambda = 0$, we recover LS;

If $\lambda \to \infty$, then all the coefficeints are zero.

Side note about the intercept...

If we want to include an intercept term, it's importatnt to make sure the features are **centred**, in which we can do quick maths to show that the first row of the normal equation is

$$1^T \begin{pmatrix} 1 & X \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta \end{pmatrix} = 1^T y. \tag{1.16}$$

If X is centred (such that $1^T X = 0$), then it follows that

$$\beta_0 = \frac{1}{n} \sum_{i=1}^{n} y_i \tag{1.17}$$

Points to y_i: don't shirnk.

What does the solution look like?

Assuming we cetre the predictors, we already know what the value of β_0 is. Now assume that the data has the mean of zero. Notice that the objective function (1.15) is *smooth* and quadratic, so we can minimize it as before.

The components of the gradient are

$$\begin{aligned} \frac{\partial}{\partial \beta_k} \left[\sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right] &= 2 \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} \beta_j x_{ij} \right) x_{ik} + 2\lambda \beta_k && (1.18) \\ &= 2X^T y - 2X^T X \beta - \lambda \beta && (1.19) \\ &= 0 \qquad \text{when } (X^T X + \lambda I)\beta = X^T y. && (1.20) \end{aligned}$$

1.3.3 Ridge Regression Estimates

By performing a **singular value decomposition** of X, we obtain

$$X = UDV^T, \tag{1.21}$$

here

U and V have orthonormal columns,

D is diagonal

This is related to the eigendecomposition by

$$X^TX = VDU^TUDV^T = VD^2V^T, \tag{1.22}$$

plugging which into the ridge regression equations (?ref here), we get

$$\begin{aligned}
(X^TX + \lambda I)\beta &= X^Ty && (1.23)\\
V(D^2 + \lambda I)V^T\beta &= VDU^Ty && (1.24)\\
V^T\beta &= (D^2 + \lambda I)^{-1}DU^Ty && (1.25)\\
\beta &= V(D^2 + \lambda I)^{-1}DU^Ty. && (1.26)
\end{aligned}$$

What does the fit look like?

Comparison of β_{ridge} and β_{LS}:

$$\begin{aligned}
\beta_{bridge} &= \sum_{j=1}^{p} \frac{\sigma_j}{\sigma_j^2 + \lambda} v_j u_j^T y && (1.27)\\
\beta_{LS} &= \sum_{j=1}^{p} \frac{1}{\sigma_j} v_j u_j^T y && (1.28)
\end{aligned}$$

Hence the ridge regression shrinks each coefficient by a factor of

$$\frac{\sigma_i^2}{\sigma_i^2 + \lambda}. \tag{1.29}$$

> Note that the shrinkage is NOT uniform.
>
> Refers to *Week 5, Part 3: Ridge Regression.*

2 Week 6 (Quiz 1)

3 Week 7

3.1 Introduction to Lasso

Remark 3.1. Ridge regression stabilizes the least-squares estimates by shrinking low-variance directions, which makes it like a *softer* version of **principal component regression**.

> Can we use penalized regression to make a softer version of variable selection? Yes. But we need to use a different penalty.

OMITTED TO SAVE TIME

4 Week 8/9

4.1 Logistic Regression

4.1.1 Classification Boundaries

From the Bayes' classifier we know that the best decision boundary is $Pr(y = 1 \mid x) = 0.5$.

Taking logs, we observe that

$$\log(Pr(y = 1 \mid x)) = -\log 2 \tag{4.1}$$

$$\log(1 - Pr(y = 1 \mid x)) = -\log 2 \tag{4.2}$$

implying that the decision boundary is

$$\implies \log\left(\frac{Pr(y = 1 \mid x)}{1 - Pr(y = 1 \mid x)}\right) = \beta_0 + x^T\beta = 0. \tag{4.3}$$

> This is a linear boundary.

4.1.2 Separation and Remedies

Separation *occasionally/almost* happens with real data, especially when there are a lot of predictors.

An option to prevent this is to add a penalty, which prevents us from being able to increase the value of β forever.

L1-penalized logistic regression/logistic lasso minimizes

$$-\frac{1}{n}\sum_{i=1}^{n}(y_i \log(p(\beta, x_i)) + (1 - y)\log(1 - p(\beta, x_i))) + \lambda\|\beta\|_1 \tag{4.4}$$

L2-penalized logistic regression minimizes

$$-\frac{1}{n}\sum_{i=1}^{n}(y_i \log(p(\beta, x_i)) + (1 - y)\log(1 - p(\beta, x_i))) + \lambda\|\beta\|_2^2 \tag{4.5}$$