Elements of Statistical Learning

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Contents

CHAPTER 2

Overview of Supervised Learning

Exercise 2.1. *Suppose that each of K-classes has an associated target t_k, which is a vector of all zeroes, except a one in the k-th position. Show that classifying the largest element of $\hat{y}$ amounts to choosing the closest target, $\min_k \|t_k - \hat{y}\|$ if the elements of $\hat{y}$ sum to one.*

Proof. The assertion is equivalent to showing that

$$\arg\max_i \hat{y}_i = \arg\min_k \|t_k - \hat{y}\| = \arg\min_k \|\hat{y} - t_k\|^2$$

by monotonicity of $x \mapsto x^2$ and symmetry of the norm.

WLOG, let $\|\cdot\|$ be the Euclidean norm $\|\cdot\|_2$. Let $k = \arg\max_i \hat{y}_i$, with $\hat{y}_k = \max y_i$. Note that then $\hat{y}_k \geq \frac{1}{K}$, since $\sum \hat{y}_i = 1$.

Then for any $k' \neq k$ (note that $y_{k'} \leq y_k$), we have

$$\begin{aligned}\|y - t_{k'}\|_2^2 - \|y - t_k\|_2^2 &= y_k^2 + (y_{k'} - 1)^2 - \left(y_{k'}^2 + (y_k - 1)^2\right) \\ &= 2\,(y_k - y_{k'}) \\ &\geq 0\end{aligned}$$

since $y_{k'} \leq y_k$ by assumption.

Thus we must have

$$\arg\min_k \|t_k - \hat{y}\| = \arg\max_i \hat{y}_i$$

as required. □

Exercise 2.2. *Show how to compute the Bayes decision boundary for the simulation example in Figure 2.5.*

Proof. The Bayes classifier is

$$\hat{G}(X) = \arg\max_{g \in \mathcal{G}} P(g|X = x).$$

In our two-class example ORANGE and BLUE, the decision boundary is the set where

$$P(g = \text{BLUE}|X = x) = P(g = \text{ORANGE}|X = x) = \frac{1}{2}.$$

By the Bayes rule, this is equivalent to the set of points where

$$P(X = x|g = \text{BLUE})P(g = \text{BLUE}) = P(X = x|g = \text{ORANGE})P(g = \text{ORANGE})$$

And since we know $P(g)$ and $P(X = x|g)$, the decision boundary can be calculated. □

Exercise 2.3. *Derive equation (2.24)*

Proof. TODO □

Exercise 2.4. *Consider N data points uniformly distributed in a p-dimensional unit ball centered at the origin. Show the the median distance from the origin to the closest data point is given by*

$$d(p, N) = \left(1 - \left(\frac{1}{2}\right)^{1/N}\right)^{1/p}$$

Proof. Let r be the median distance from the origin to the closest data point. Then

$$P(\text{All } N \text{ points are further than } r \text{ from the origin}) = \frac{1}{2}$$

by definition of the median.

Since the points x_i are independently distributed, this implies that

$$\frac{1}{2} = \prod_{i=1}^{N} P(\|x_i\| > r)$$

and as the points x_i are uniformly distributed in the unit ball, we have that

$$\begin{aligned} P(\|x_i\| > r) &= 1 - P(\|x_i\| \leq r) \\ &= 1 - \frac{Kr^p}{K} \\ &= 1 - r^p \end{aligned}$$

Putting these together, we obtain that

$$\frac{1}{2} = (1 - r^p)^N$$

and solving for r, we have

$$r = \left(1 - \left(\frac{1}{2}\right)^{1/N}\right)^{1/p}$$

□

Exercise 2.5. *Consider inputs drawn from a spherical multivariate-normal distribution $X \sim N(0, \mathbf{1}_p)$. The squared distance from any sample point to the origin has a χ^2_p distribution with mean p. Consider a prediction point x_0 drawn from this distribution, and let $a = \frac{x_0}{\|x_0\|}$ be an associated unit vector. Let $z_i = a^T x_i$ be the projection of each of the training points on this direction.*

Show that the z_i are distributed $N(0,1)$ with expected squared distance from the origin 1, while the target point has expected squared distance p from the origin. Hence for $p = 10$, a randomly drawn test point is about 3.1 standard deviations from the origin, while all the training points are on average one standard deviation along direction a. So most prediction points see themselves as lying on the edge of the training set.

PROOF. Let $z_i = a^T x_i = \frac{x_0^T}{\|x_0\|} x_i$. Then z_i is a linear combination of $N(0,1)$ random variables, and hence normal, with expectation zero and variance

$$\mathrm{Var}(z_i) = \|a^T\|^2 \mathrm{Var}(x_i) = \mathrm{Var}(x_i) = 1$$

as the vector a has unit length and $x_i \sim N(0,1)$.

For each target point x_i, the squared distance from the origin is a χ_p^2 distribution with mean p, as required. □

Exercise 2.6. *(a) Derive equation (2.27) in the notes.*
(b) Derive equation (2.28) in the notes.

PROOF. (i) We have

$$\begin{aligned} EPE(x_0) &= E_{y_0|x_0} E_{\mathcal{T}} (y_0 - \hat{y}_0)^2 \\ &= \mathrm{Var}(y_0|x_0) + E_{\mathcal{T}}[\hat{y}_0 - E_{\mathcal{T}}\hat{y}_0]^2 + [E_{\mathcal{T}} - x_0^T\beta]^2 \\ &= \mathrm{Var}(y_0|x_0) + \mathrm{Var}_{\mathcal{T}}(\hat{y}_0) + \mathrm{Bias}^2(\hat{y}_0). \end{aligned}$$

We now treat each term individually. Since the estimator is unbiased, we have that the third term is zero. Since $y_0 = x_0^T\beta + \epsilon$ with ϵ an $N(0,\sigma^2)$ random variable, we must have $\mathrm{Var}(y_0|x_0) = \sigma^2$.

The middle term is more difficult. First, note that we have

$$\begin{aligned} \mathrm{Var}_{\mathcal{T}}(\hat{y}_0) &= \mathrm{Var}_{\mathcal{T}}(x_0^T\hat{\beta}) \\ &= x_0^T \mathrm{Var}_{\mathcal{T}}(\hat{\beta}) x_0 \\ &= E_{\mathcal{T}} x_0^T \sigma^2 (\mathbf{X}^T\mathbf{X})^{-1} x_0 \end{aligned}$$

by conditioning (3.8) on $\mathcal{T}$.

(ii) TODO

□

Exercise 2.7. *Consider a regression problem with inputs x_i and outputs y_i, and a parameterized model $f_\theta(x)$ to be fit with least squares. Show that if there are observations with* tied *or* identical *values of x, then the fit can be obtained from a reduced weighted least squares problem.*

Proof. This is relatively simple. WLOG, assume that $x_1 = x_2$, and all other observations are unique. Then our RSS function in the general least-squares estimation is

$$RSS(\theta) = \sum_{i=1}^{N} \left(y_i - f_\theta(x_i)\right)^2 = \sum_{i=2}^{N} w_i \left(y_i - f_\theta(x_i)\right)^2$$

where

$$w_i = \begin{cases} 2 & i = 2 \\ 1 & \text{otherwise} \end{cases}$$

Thus we have converted our least squares estimation into a reduced weighted least squares estimation. This minimal example can be easily generalised. □

Exercise 2.8. *Suppose that we have a sample of N pairs x_i, y_i, drawn IID from the distribution such that*

$$\begin{aligned} x_i &\sim h(x), \\ y_i &= f(x_i) + \epsilon_i, \\ E(\epsilon_i) &= 0, \\ Var(\epsilon_i) &= \sigma^2. \end{aligned}$$

We construct an estimator for f linear in the y_i,

$$\hat{f}(x_0) = \sum_{i=1}^{N} \ell_i(x_0; \mathcal{X}) y_i$$

where the weights $\ell_i(x_0; X)$ do not depend on the y_i, but do depend on the training sequence x_i denoted by $\mathcal{X}$.

(a) *Show that the linear regression and k-nearest-neighbour regression are members of this class of estimators. Describe explicitly the weights $\ell_i(x_0; \mathcal{X})$ in each of these cases.*

(b) *Decompose the conditional mean-squared error*

$$E_{\mathcal{Y}|\mathcal{X}} \left(f(x_0) - \hat{f}(x_0)\right)^2$$

into a conditional squared bias and a conditional variance component. $\mathcal{Y}$ represents the entire training sequence of y_i.

(c) *Decompose the (unconditional) MSE*

$$E_{\mathcal{Y},\mathcal{X}} \left(f(x_0) - \hat{f}(x_0)\right)^2$$

into a squared bias and a variance component.

(d) *Establish a relationship between the square biases and variances in the above two cases.*

Proof. (a) Recall that the estimator for f in the linear regression case is given by

$$\hat{f}(x_0) = x_0^T \beta$$

where $\beta = (X^T X)^{-1} X^T y$. Then we can simply write

$$\hat{f}(x_0) = \sum_{i=1}^{N} \left(x_0^T (X^T X)^{-1} X^T \right)_i y_i .$$

Hence

$$\ell_i(x_0; \mathcal{X}) = \left(x_0^T (X^T X)^{-1} X^T \right)_i .$$

In the k-nearest-neighbour representation, we have

$$\hat{f}(x_0) = \sum_{i=1}^{N} \frac{y_i}{k} \mathbf{1}_{x_i \in N_k(x_0)}$$

where $N_k(x_0)$ represents the set of k-nearest-neighbours of x_0. Clearly,

$$\ell_i(x_0; \mathcal{X}) = \frac{1}{k} \mathbf{1}_{x_i \in N_k(x_0)}$$

(b) TODO
(c) TODO
(d) TODO

□

Exercise 2.9. *Compare the classification performance of linear regression and k-nearest neighbour classification on the* `zipcode` *data. In particular, consider on the 2's and 3's, and $k = 1, 3, 5, 7, 15$. Show both the training and test error for each choice.*

Proof. TODO - Plot error rates, etc.

```
# Load training data
zip.train <- as.data.frame(read.table(file="zip.train", header=FALSE))
colnames(zip.train) <- c("Y",paste("X.",1:256,sep=""))
zip.train.filtered <- subset(zip.train, Y == 2 | Y == 3)
# Create linear regression
mod <- lm(Y ˜ ., data = zip.train.filtered)

# Load testing data
zip.test <- as.data.frame(read.table(file="zip.test", header=FALSE))
colnames(zip.test) <- c("Y",paste("X.",1:256,sep=""))
zip.test.filtered <- subset(zip.test, Y == 2 | Y == 3)
# Predict categories
zip.test.filtered$Ypred <- predict(mod, zip.test.filtered)

category_f <- function(x) {
if (x > 2.5) 3 else 2
}
# Round predictions
zip.test.filtered$Yround <- sapply(zip.test.filtered$Ypred, category_f)
```

```
##### KNN
knn.test.data <- subset(zip.test, Y == 2 | Y == 3)
knn.train.data <- subset(zip.train, Y == 2 | Y == 3)
knn.train.data$Y <- as.factor(knn.train.data$Y)

knn.results <- sapply(1:15, function(k) { knn(train=knn.train.data, test=knn.test.data, knn.↩
    train.data$Y, k = k) })
install.packages("mclust")
errors <- sapply(knn.results, function(classification) { classError(knn.test.data$Y, ↩
    classification)$errorRate})
```

□

Exercise 2.10. *Consider a linear regression model with p parameters, fitted by OLS to a set of trainig data $(x_i, y_i)_{1\leq i\leq N}$ drawn at random from a population. Let $\hat\beta$ be the least squares estimate. Suppose we have some test data $(\tilde{x}_i, \tilde{y}_i)_{1\leq i\leq M}$ drawn at random from the same population as the training data.*

If $R_{tr}(\beta) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i\beta^T x_i\right)^2$ and $R_{te}(\beta) = \frac{1}{M}\sum_{i=1}^{M}\left(\tilde{y}_i - \beta^T\tilde{x}_i\right)^2$, prove that

$$E(R_{tr}(\hat\beta)) \leq E(R_{te}(\hat\beta))$$

where the expectation is over all that is random in each expression.

CHAPTER 3

Linear Methods for Regression

Exercise 3.1. *Show that the F statistic for dropping a single coefficient from a model is equal to the square of the corresponding z-score.*

Proof. Recall that the F statistic is defined by the following expression

$$\frac{(RSS_0 - RSS_1)/(p_1 - p_0)}{RSS_1/(N - p_1 - 1)}.$$

where RSS_0, RSS_1 and $p_0 + 1, p_1 + 1$ refer to the residual sum of squares and the number of free parameters in the smaller and bigger models, respectively. Recall also that the F statistic has a $F_{p_1 - p_0, N - p_1 - 1}$ distribution under the null hypothesis that the smaller model is correct.

Next, recall that the z-score of a coefficient is

$$z_j = \frac{\hat{\beta}_j}{\hat{\sigma}\sqrt{v_j}}$$

and under the null hypothesis that β_j is zero, z_j is distributed according to a t-distribution with $N - p - 1$ degrees of freedom.

Hence, by dropping a single coefficient from a model, our F statistic has a $F_{1,N-p-1}$ where $p + 1$ are the number of parameters in the original model. Similarly, the corresponding z-score is distributed according to a t_{N-p-1} distribution, and thus the square of the z-score is distributed according to an $F_{1,N-p-1}$ distribution, as required.

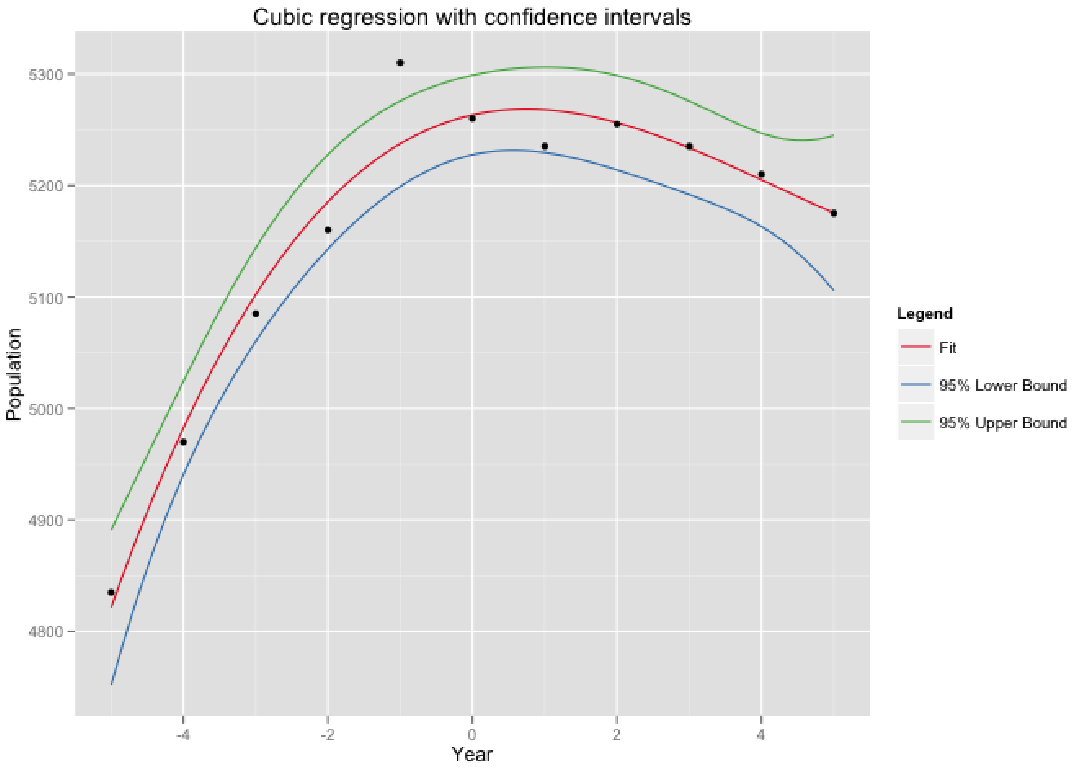
Thus both the z-score and the F statistic test identical hypotheses under identical distributions. Thus they must have the same value in this case. □

Exercise 3.2. *Given data on two variables X and Y, consider fitting a cubic polynomial regression model $f(X) = \sum_{j=0}^{3} \beta_j X^j$. In addition to plotting the fitted curve, you would like a 95% confidence band about the curve. Consider the following two approaches:*

(1) At each point x_0, form a 95% confidence interval for the linear function $a^T\beta = \sum_{j=0}^{3} \beta_j x_0^j$.

(2) Form a 95% confidence set for β as in (3.15), which in tun generates confidence intervals for $f(x_0)$.

How do these approaches differ? Which band is likely to be wider? Conduct a small simulation experiment to compare the two methods.



Proof. The key distinction is that in the first case, we form the set of points such that we are 95% confident that $\hat{f}(x_0)$ is within this set, whereas in the second method, we are 95% confident that an arbitrary point is within our confidence interval. This is the distinction between a *pointwise* approach and a *global* confidence estimate.

In the pointwise approach, we seek to estimate the variance of an individual prediction - that is, to calculate $\mathrm{Var}(\hat{f}(x_0)|x_0)$. Here, we have

$$\begin{aligned}\sigma_0^2 = \mathrm{Var}(\hat{f}(x_0)|x_0) &= \mathrm{Var}(x_0^T\hat{\beta}|x_0)\\ &= x_0^T\mathrm{Var}(\hat{\beta})x_0\\ &= \hat{\sigma}^2 x_0^T(X^TX)^{-1}x_0.\end{aligned}$$

where $\hat{\sigma}^2$ is the estimated variance of the innovations ϵ_i.

We can implement this algorithm in R as follows:

```
library("ggplot2")
library("reshape2")

# Raw data
```

```
simulation.xs <- c(1959, 1960, 1961, 1962, 1963, 1964, 1965, 1966, 1967, 1968, 1969)
simulation.ys <- c(4835, 4970, 5085, 5160, 5310, 5260, 5235, 5255, 5235, 5210, 5175)
simulation.df <- data.frame(pop = simulation.ys, year = simulation.xs)

# Rescale years
simulation.df$year <- simulation.df$year - 1964

# Generate regression, construct confidence intervals
fit <- lm(pop ~ year + I(year^2) + I(year^3), data=simulation.df)
xs <- seq(-5, 5, 0.1)
fit.confidence <- predict(fit, data.frame(year=xs), interval="confidence", level=0.95)


# Create data frame containing variables of interest
df <- as.data.frame(fit.confidence)
df$year <- xs
df <- melt(df, id.vars="year")

p <- ggplot()
p <- p + geom_line(aes(x=year, y=value, colour=variable),
                   df)
P <- p + geom_point(aes(x=year, y=pop),
                    simulation.df)
p <- p + scale_x_continuous('Year')
p <- p + scale_y_continuous('Population')
p <- p + opts(title="Cubic regression with confidence intervals")
p <- p + scale_color_brewer(name="Legend",
        labels=c("Fit",
                 "95% Lower Bound",
                 "95% Upper Bound"),
        palette="Set1")
```

TODO: Part 2. □

Exercise 3.3 (The Gauss-Markov Theorem). *(1) Prove the Gauss-Markov theorem: the least squares estimate of a parameter $a^T\beta$ has a variance no bigger than that of any other linear unbiased estimate of $a^T\beta$.*

(2) Secondly, show that if $\hat{V}$ is the variance-covariance matrix of the least squares estimate of β and $\tilde{V}$ is the variance covariance matrix of any other linear unbiased estimate, then $\hat{V} \leq \tilde{V}$, where $B \leq A$ if $A - B$ is positive semidefinite.

Proof. Let $\hat{\theta} = a^T\hat{\beta} = a^T(X^TX)^{-1}X^Ty$ be the least squares estimate of $a^T\beta$. Let $\tilde{\theta} = c^Ty$ be any other unbiased linear estimator of $a^T\beta$. Now, let $d^T = c^T - a^T(X^{-1}X)^{-1}X^T$. Then as c^Ty is unbiased, we must have

$$\begin{aligned} E(c^Ty) &= E\left(a^T(X^TX)^{-1}X^T + d^T\right)y \\ &= a^T\beta + d^TX\beta \\ &= a^T\beta \end{aligned}$$

as $c^T y$ is unbiased, which implies that $d^T X = 0$.

Now we calculate the variance of our estimator. We have

$$\begin{aligned}
\mathrm{Var}(c^T y) &= c^T \mathrm{Var}(y) c \\
&= \sigma^2 c^T c \\
&= \sigma^2 \left(a^T (X^T X)^{-1} X^T + d^T \right) \left(a^T (X^T X)^{-1} X^T + d^T \right)^T \\
&= \sigma^2 \left(a^T (X^T X)^{-1} X^T + d^T \right) \left(X (X^T X)^{-1} a + d \right) \\
&= \sigma^2 \left(a^T (X^T X)^{-1} X^T X (X^T X)^{-1} a + a^T (X^T X)^{-1} \underbrace{X^T d}_{=0} + \underbrace{d^T X}_{=0} (X^T X)^{-1} a + d^T d \right) \\
&= \sigma^2 \left(\underbrace{a^T (X^T X)^{-1} a}_{\mathrm{Var}(\hat{\theta})} + \underbrace{d^t d}_{\geq 0} \right)
\end{aligned}$$

Thus $\mathrm{Var}(\hat{\theta}) \leq \mathrm{Var}(\tilde{\theta})$ for all other unbiased linear estimators $\tilde{\theta}$.

The proof of the matrix version is almost identical, except we replace our vector d with a matrix D. It is then possible to show that $\tilde{V} = \hat{V} + D^T D$, and as $D^T D$ is a positive semidefinite matrix for any D, we have $\hat{V} \leq \tilde{V}$. □

Exercise 3.4. *Show how the vector of least square coefficients can be obtained from a single pass of the Gram-Schmidt procedure. Represent your solution in terms of the QR decomposition of X.*

Proof. Recall that by a single pass of the Gram-Schmidt procedure, we can write our matrix X as

$$X = Z\Gamma,$$

where Z contains the orthogonal columns z_j, and Γ is an upper-diagonal matrix with ones on the diagonal, and $\gamma_{ij} = \frac{\langle z_i, x_j \rangle}{\|z_i\|^2}$. This is a reflection of the fact that by definition,

$$x_j = z_j + \sum_{k=0}^{j-1} \gamma_{kj} z_k.$$

Now, by the QR decomposition, we can write $X = QR$, where Q is an orthogonal matrix and R is an upper triangular matrix. We have $Q = ZD^{-1}$ and $R = D\Gamma$, where D is a diagonal matrix with $D_{jj} = \|z_j\|$.

Now, by definition of $\hat{\beta}$, we have

$$(X^T X)\hat{\beta} = X^T y.$$

Now, using the QR decomposition, we have

$$\begin{aligned}(R^TQ^T)(QR)\hat{\beta} &= R^TQ^Ty \\ R\hat{\beta} &= Q^Ty\end{aligned}$$

As R is upper triangular, we can write

$$\begin{aligned}R_{pp}\hat{\beta}_p &= \langle q_p, y\rangle \\ \|z_p\|\hat{\beta}_p &= \|z_p\|^{-1}\langle z_p, y\rangle \\ \hat{\beta}_p &= \frac{\langle z_p, y\rangle}{\|z_p\|^2}\end{aligned}$$

in accordance with our previous results. Now, by back substitution, we can obtain the sequence of regression coefficients $\hat{\beta}_j$. As an example, to calculate $\hat{\beta}_{p-1}$, we have

$$\begin{aligned}R_{p-1,p-1}\hat{\beta}_{p-1} + R_{p-1,p}\hat{\beta}_p &= \langle q_{p-1}, y\rangle \\ \|z_{p-1}\|\hat{\beta}_{p-1} + \|z_{p-1}\|\gamma_{p-1,p}\hat{\beta}_p &= \|z_{p-1}\|^{-1}\langle z_{p-1}, y\rangle\end{aligned}$$

and then solving for $\hat{\beta}_{p-1}$. This process can be repeated for all β_j, thus obtaining the regression coefficients in one pass of the Gram-Schmidt procedure. □

Exercise 3.5. *Consider the ridge regression problem (3.41). Show that this problem is equivalent to the problem*

$$\hat{\beta}^c = \arg\min_{\beta^c}\left(\sum_{i=1}^{N}\left(y_i - \beta_0^c - \sum_{j=1}^{p}(x_{ij} - \hat{x}_j)\beta_j^c\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^{c2}\right)^2.$$

Proof. Consider rewriting our objective function above as

$$L(\beta^c) = \sum_{i=1}^{N}\left(y_i - \left(\beta_0^c - \sum_{j=1}^{p}\bar{x}_j\beta_j^c\right) - \sum_{j=1}^{p}x_{ij}\beta_j^c\right)^2 + \lambda\sum_{j=1}^{p}{\beta_j^2}^2$$

Note that making the substitutions

$$\begin{aligned}\beta_0 &\mapsto \beta_0^c - \sum_{j=1}^{p}\hat{x}_j\beta_j \\ \beta_j &\mapsto \beta_j^c, j = 1, 2, \ldots, p\end{aligned}$$

that $\hat{\beta}$ is a minimiser of the original ridge regression equation if $\hat{\beta}^c$ is a minimiser of our modified ridge regression.

The modified solution merely has a shifted intercept term, and all other coefficients remain the same. □

Exercise 3.6. *Show that the ridge regression estimate is the mean (and mode) of the posterior distribution, under a Gaussian prior $\beta \sim N(0, \tau\mathbf{I})$, and Gaussian sampling model $y \sim N(X\beta, \sigma^2\mathbf{I})$. Find the relationship between the regularization parameter λ in the ridge formula, and the variances τ and σ^2.*

Exercise 3.7. *Assume*

$$y_i \sim N(\beta_0 + x_i^T\beta, \sigma^2), i = 1, 2, \dots, N$$

and the parameters β_j are are each distributed as $N(0, \tau^2)$, independently of one another. Assume σ^2 and τ^2 are known, show that the minus log-posterior density of β is proportional to

$$\sum_{i=1}^{N}\left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2$$

where $\lambda = \frac{\sigma^2}{\tau^2}$.

Exercise 3.8. *Consider the QR decomposition of the uncentred $N \times (p+1)$ matrix X, whose first column is all ones, and the SVD of the $N \times p$ centred matrix $\tilde{X}$. Show that Q_2 and U share the same subspace, where Q_2 is the submatrix of Q with the first column removed. Under what circumstances will they be the same, up to sign flips?*

Proof. Denote the columns of X by $x_0, \dots, x_p$, the columns of Q by $z_0, \dots, z_p$, the columns of $\tilde{X}$ by $\tilde{x}_1, \dots, x_n$, and the columns of U by $u_1, \dots, u_p$. Without loss of generality, we can assume that for all i, $\|x_i\| = 1$ and that X is non-singular (this cleans up the proof somewhat).

First, note that by the QR decomposition, we have that $\text{span}(x_0, \dots, x_j) = \text{span}(z_0, \dots, z_j)$ for any $0 \le j \le p$.

By our assumption, we have that $\tilde{x}_i = x_i - \bar{x}_i\mathbf{1}$ for $i = 1, \dots, p$. Thus we can write $\tilde{x}_i = \sum_{j \le i} \alpha_j z_j$, and as the z_j are orthogonal, we must be able to write $\tilde{x}_i$ in terms of z_j for $j = 1, 2, \dots, i$. Thus $\text{span}(\tilde{x}_1, \dots, \tilde{x}_i) = \text{span}(z_1, \dots, z_i)$.

Finally, we calculate $\text{span}(u_1, \dots, u_p)$. We have that U is a unitary $N \times p$ matrix, and thus the columns of U span the column space of $\tilde{X}$, and thus the span of Q_2 is equal to the span of U.

TODO: When is Q_2 equal to U up to parity? Is it where columns of □

Exercise 3.9 (Forward stepwise regression)**.** *Suppose that we have the QR decomposition for the $N \times q$ matrix X_1 in a multiple regression problem with response y, and we have an additional $p - q$ predictors in matrix X_2. Denote the current residual by r. We wish to establish which one of these additional variables will reduce the residual-sum-of-squares the most when included with those in X_1. Describe an efficient procedure for doing this.*

PROOF. Select the vector $x_{j'}$ where

$$x_{j'} = \operatorname*{arg\,min}_{j=q+1,\ldots,p} \left| \left\langle \frac{x_q}{\|x_q\|}, r \right\rangle \right|$$

This selects the vector that explains the maximal amount of variance in r given X_1, and thus reduces the residual sum of squares the most. It is then possible to repeat this procedure by updating X_2 as in Algorithm 3.1. □

Exercise 3.10 (Backward stepwise regression)**.** *Suppose that we have the multiple regression fit of y on X, along with standard errors and z-scores. We wish to establish which variable, when dropped, will increase the RSS the least. How would you do this?*

PROOF. By Exercise 3.1, we can show that the F-statistic for dropping a single coefficient from a model is equal to the square of the corresponding z-score. Thus, we drop the variable that has the lowest squared z-score from the model. □

Exercise 3.11. *Show that the solution to the multivariate linear regression problem (3.40) is given by (3.39). What happens if the covariance matrices Σ_i are different for each observation?*

Exercise 3.12. *Show that the ridge regression estimates can be obtained by OLS on an augmented data set. We augment the centred matrix X with p additional rows $\sqrt{\lambda}\mathbf{I}$, and augment y with p zeroes.*

PROOF. For our augmented matrix X_1, equal to appending $\sqrt{\lambda I}$ to the original observation matrix X, we have that the RSS expression for OLS regression becomes

$$\begin{aligned} RSS &= \sum_{i=1}^{N+p} \left(y_i - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 \\ &= \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \sum_{i=N+1}^{N+p} \left(\sum_{j=1}^{p} x_{ij}\beta_j \right)^2 \\ &= \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \sum_{j=1}^{p} \lambda\beta_j^2 \end{aligned}$$

which is the objective function for the ridge regression estimate. □

CHAPTER 4

Linear Methods for Classification

Exercise 4.1. *Show how to solve the geenralised eigenvalue problem* $\max a^T Ba$ *subject to* $a^T W a = 1$ *by transforming it to a standard eigenvalue problem.*

Proof. By Lagrange multipliers, we have that the function $\mathcal{L}(a) = a^T Ba - \lambda(a^T Wa - 1)$ has a critical point where

$$\frac{d\mathcal{L}}{da} = 2a^T B^T - 2\lambda a^T W^T = 0,$$

that is, where $Ba = \lambda Wa$. If we let $W = D^T D$ (Cholesky decomposition), $C = D^{-1}BD^{-1}$, and $y = Da$, we obtain that our solution becomes

$$Cy = \lambda y,$$

and so we can convert our problem into an eigenvalue problem. It is clear that if y_m and λ_m are the maximal eigenvector and eigenvalue of the reduced problem, then $D^{-1}y_m$ and λ_m are the maximal eigenvector and eigenvalue of the generalized problem, as required. □

Exercise 4.2. *Suppose that we have features* $x \in \mathbb{R}^p$*, a two-class response, with class sizes* N_1, N_2*, and the target coded as* $-N/N_1, N/N_2$*.*

1. *Show that the LDA rule classifies to class 2 if*

$$x^T \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1) > \frac{1}{2}\hat{\mu}_2^T \hat{\Sigma}^{-1}\hat{\mu}_2 - \frac{1}{2}\hat{\mu}_1^T \hat{\Sigma}^{-1}\hat{\mu}_1 + \log\frac{N_1}{N} - \log\frac{N_2}{N}$$

2. *Consider minimization of the least squares criterion*

$$\sum_{i=1}^{N} \left(y_i - \beta_0 - \beta^T x_i\right)^2$$

   Show that the solution $\hat{\beta}$ *satisfies*

$$\left((N-2)\hat{\Sigma} + \frac{N_1 N_2}{N}\hat{\Sigma}_B\right)\beta = N(\hat{\mu}_2 - \hat{\mu}_1)$$

   where $\hat{\Sigma}_B = (\hat{\mu}_2 - \hat{\mu}_1)(\hat{\mu}_2 - \hat{\mu}_1)^T$*.*

3. *Hence show that* $\hat{\Sigma}_B\beta$ *is in the direction* $(\hat{\mu}_2 - \hat{\mu}_1)$*, and thus*

$$\hat{\beta} \propto \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1)$$

and therefore the least squares regression coefficient is identical to the LDA coefficient, up to a scalar multiple.

(4) *Show that this holds for any (distinct) coding of the two classes.*

(5) *Find the solution $\hat{\beta}_0$, and hence the predicted values $\hat{\beta}_0 + \hat{\beta}^T x$. Consider the following rule: classify to class 2 if $\hat{y}_i > 0$ and class 1 otherwise. Show that this is not the same as the LDA rule unless the classes have equal numbers of observations.*

Proof. We use the notation of Chapter 4.

(1) Since in the two class case, we classify to class 2 if $\delta_1(x) < \delta_2(x)$. Substituting this into our equation for the Linear discriminant functions, we have

$$\delta_1(x) < \delta_2(x)$$
$$x^T \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1) > \frac{1}{2}\hat{\mu}_2^T \hat{\Sigma}^{-1}\hat{\mu}_2 - \frac{1}{2}\hat{\mu}_1^T \hat{\Sigma}^{-1}\hat{\mu}_1 + \log\frac{N_1}{N} - \log\frac{N_2}{N}$$

as required.

(2) Let U_i be the n element vector with j-th element 1 if the j-th observation is class i, and zero otherwise. Then we can write our target vector Y as $t_1 U_1 + t_2 U_2$, where t_i are our target labels, and we have $\mathbf{1} = U_1 + U_2$. Note that we can write our estimates $\hat{\mu}_1, \hat{\mu}_2$ as $X^T U_i = N_i \hat{\mu}_i$, and that $X^T Y = t_1 N_1 \hat{\mu}_1 + t_2 N_2 \hat{\mu}_2$.

By the least squares criterion, we can write

$$RSS = \sum_{i=1}^{N}(y_i - \beta_0 - \beta^T X)^2 = (Y - \beta_0\mathbf{1} - X\beta)^T(Y - \beta_0\mathbf{1} - X\beta)$$

Minimizing this with respect to β and β_0, we obtain

$$2X^T X\beta - 2X^T Y + 2\beta_0 X^T\mathbf{1} = 0$$
$$2N\beta_0 - 2\mathbf{1}^T(Y - X\beta) = 0.$$

These equations can be solved for β_0 and β by substitution as

$$\hat{\beta}_0 = \frac{1}{N}\mathbf{1}^T(Y - X\beta)$$
$$\left(X^T X - \frac{1}{N}X^T\mathbf{1}\mathbf{1}^T X\right)\hat{\beta} = X^T Y - \frac{1}{N}X^T\mathbf{1}\mathbf{1}^T Y$$

The RHS can be written as

$$X^T Y - \frac{1}{N}X^T\mathbf{1}\mathbf{1}^T Y = t_1 N_1\hat{\mu}_1 + t_2 N_2\hat{\mu}_2 - \frac{1}{N}(N_1\hat{\mu}_1 + N_2\hat{\mu}_2)(t_1 N_1 + t_2 N_2)$$
$$= \frac{N_1 N_2}{N}(t_1 - t_2)(\hat{\mu}_1 - \hat{\mu}_2)$$

where we use our relations for $X^T U_i$ and the fact that $\mathbf{1} = U_1 + U_2$.

Similarly, the bracketed term on the LHS of our expression for β can be rewritten as

$$X^T X = (N-2)\hat{\Sigma} + N_1 \hat{\mu}_1 \hat{\mu}_1^T + N_2 \hat{\mu}_2 \hat{\mu}_2^T,$$

and by substituting in the above and the definition of $\hat{\Sigma}_B$, we can write

$$X^T X - \frac{1}{N} X^T \mathbf{1}\mathbf{1}^T X = (N-2)\hat{\Sigma} + \frac{N_1 N_2}{N} \hat{\Sigma}_B$$

as required.

Putting this together, we obtain our required result,

$$\left((N-2)\hat{\Sigma} + \frac{N_1 N_2}{N} \hat{\Sigma}_B \right) \hat{\beta} = \frac{N_1 N_2}{N} (t_1 - t_2)(\hat{\mu}_1 - \hat{\mu}_2),$$

and then substituting $t_1 = -N/N_1, t_2 = N/N_2$, we obtain our required result,

$$\left((N-2)\hat{\Sigma} + \frac{N_1 N_2}{N} \hat{\Sigma}_B \right) \hat{\beta} = N(\hat{\mu}_2 - \hat{\mu}_1)$$

(3) All that is required is to show that $\hat{\Sigma}_B \beta$ is in the direction of $(\hat{\mu}_2 - \hat{\mu}_1)$. This is clear from the fact that

$$\hat{\Sigma}_B \hat{\beta} = (\hat{\mu}_2 - \hat{\mu}_1)(\hat{\mu}_2 - \hat{\mu}_1)^T \hat{\beta} = \lambda(\hat{\mu}_2 - \hat{\mu}_1)$$

for some $\lambda \in \mathbb{R}$. Since $\hat{\Sigma}\hat{\beta}$ is a linear combination of terms in the direction of $(\hat{\mu}_2 - \hat{\mu}_1)$, we can write

$$\hat{\beta} \propto \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1)$$

as required.

(4) Since our t_1, t_2 were arbitrary and distinct, the result follows.

(5) From above, we can write

$$\begin{aligned} \hat{\beta}_0 &= \frac{1}{N} \mathbf{1}^T (Y - X\hat{\beta}) \\ &= \frac{1}{N}(t_1 N_1 + t_2 N_2) - \frac{1}{N} \mathbf{1}^T X \hat{\beta} \\ &= -\frac{1}{N}(N_1 \hat{\mu}_1^T + N_2 \hat{\mu}_2^T)\hat{\beta}. \end{aligned}$$

We can then write our predicted value $\hat{f}(x) = \hat{\beta}_0 + \hat{\beta}^T x$ as

$$\begin{aligned} \hat{f}(x) &= \frac{1}{N} \left(N x^T - N_1 \hat{\mu}_1^T - N_2 \hat{\mu}_2^T \right) \hat{\beta} \\ &= \frac{1}{N} \left(N x^T - N_1 \hat{\mu}_1^T - N_2 \hat{\mu}_2^T \right) \lambda \hat{\Sigma}^{-1} (\hat{\mu}_2 - \hat{\mu}_1) \end{aligned}$$

for some $\lambda \in \mathbb{R}$, and so our classification rule is $\hat{f}(x) > 0$, or equivalently,

$$\begin{aligned} N x^T \lambda \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1) &> (N_1 \hat{\mu}_1^T + N_2 \hat{\mu}_2^T)\lambda \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1) \\ x^T \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1) &> \frac{1}{N}\left(N_1 \hat{\mu}_1^T + N_2 \hat{\mu}_2^T\right) \hat{\Sigma}^{-1}(\hat{\mu}_2 - \hat{\mu}_1) \end{aligned}$$

which is different to the LDA decision rule unless $N_1 = N_2$.

□

Exercise 4.3. *Suppose that we transform the original predictors X to $\hat{Y}$ by taking the predicted values under linear regression. Show that LDA using $\hat{Y}$ is identical to using LDA in the original space.*

Exercise 4.4. *Consier the multilogit model with K classes. Let β be the $(p+1)(K-1)$-vector consisting of all the coefficients. Define a suitable enlarged version of the input vector x to accommodate this vectorized coefficient matrix. Derive the Newton-Raphson algorithm for maximizing the multinomial log-likelihood, and describe how you would implement the algorithm.*

Exercise 4.5. *Consider a two-class regression problem with $x \in \mathbb{R}$. Characterise the MLE of the slope and intercept parameter if the sample x_i for the two classes are separated by a point $x_0 \in \mathbb{R}$. Generalise this result to $x \in \mathbb{R}^p$ and more than two classes.*

Exercise 4.6. *Suppose that we have N points $x_i \in \mathbb{R}^p$ in general position, with class labels $y_i \in \{-1, 1\}$. Prove that the perceptron learning algorithm converges to a separating hyperplane in a finite number of steps.*

(1) *Denote a hyperplane by $f(x) = \beta^T x^\star = 0$. Let $z_i = \frac{x_i^\star}{\|x_i^\star\|}$. Show that separability implies the existence of a β_{sep} such that $y_i \beta_{sep}^T z_i \geq 1$ for all i.*

(2) *Given a current β_{old}, the perceptron algorithm identifies a pint z_i that is misclassified, and produces the update $\beta_{new} \leftarrow \beta_{old} + y_i z_i$. Show that*

$$\|\beta_{new} - \beta_{sep}\|^2 \leq \|\beta_{old} - \beta_{sep}\|^2 - 1$$

and hence that the algorithm converges to a separating hyperplane in no more than $\|\beta_{start} - \beta_{sep}\|^2$ steps.

Proof. Recall that the definition of separability implies the existence of a separating hyperplane - that is, a vector β_{sep} such that $\operatorname{sgn}\left(\beta_{\text{sep}}^T x_i^\star\right) = y_i$.

(1) By assumption, there exists $\epsilon > 0$ and β_{sep} such that

$$y_i \beta_{\text{sep}}^T z_i^\star \geq \epsilon$$

for all i. Then the hyperplane $\frac{1}{\epsilon}\beta_{\text{sep}}$ is a separating hyperplane that by linearity satisfies the constraint

$$y_i \beta_{\text{sep}}^T z_i^\star \geq 1.$$

(2) We have

$$\begin{aligned}
\|\beta_{\text{new}} - \beta_{\text{sep}}\|^2 &= \|\beta_{\text{new}}\|^2 + \|\beta_{\text{sep}}\|^2 - 2\beta_{\text{sep}}^T\beta_{\text{new}} \\
&= \|\beta_{\text{old}} + y_i z_i\|^2 + \|\beta_{\text{sep}}\|^2 - 2\beta_{\text{sep}}^T\left(\beta_{\text{old}} + y_i z_i\right) \\
&= \|\beta_{\text{old}}\|^2 + \|y_i z_i\|^2 + 2y_i\beta_{\text{old}}^T z_i + \|\beta_{\text{sep}}\|^2 - 2\beta_{\text{sep}}^T\beta_0 - 2y_i\beta_{\text{sep}}^T z_i \\
&\leq \|\beta_{\text{old}}\|^2 + \|\beta_{\text{sep}}\|^2 - 2\beta_{\text{sep}}^T\beta_{\text{old}} + 1 - 2 \\
&= \|\beta_{\text{old}} - \beta_{\text{sep}}\|^2 - 1.
\end{aligned}$$

Let $\beta_k, k = 0, 1, 2, \ldots$ be the sequence of iterates formed by this procedure, with $\beta_0 = \beta_{\text{start}}$. Let $k^\star = \left\lceil \|\beta_{\text{start}} - \beta_{\text{sep}}\|^2 \right\rceil$. Then by the above result, we must have $\|\beta_{k^\star} - \beta_{\text{sep}}\|^2 = 0$, and by properties of the norm we have that $\beta_{k^\star} = \beta_{\text{sep}}$, and so we have reached a separating hyperplane in no more than $k^\star$ steps.

□