Stats 790

Assignment 2

1. a) Derivation of linear regression coefficients.

Naive Linear Algebra

Given $Y = X\beta + \epsilon$, we want to solve for β by minimizing the sum of squared residuals $\sum \epsilon_i^2 = \epsilon^T \epsilon$.

$$\epsilon^{T} \epsilon = (Y - X\beta)^{T} (Y - X\beta)$$

$$= (Y^{T} - \beta^{T} X^{T}) (Y - X\beta)$$

$$= Y^{T} Y - \beta^{T} X^{T} Y - Y^{T} X\beta + \beta^{T} X^{T} X\beta$$

We take the derivative of this equation with respect to β :

$$= -X^T Y - Y^T X + X^T X \beta$$
$$= -2X(Y - X\beta)$$

Setting this equal to 0 we get:

$$0 = -2X^{T}(Y - X\beta)$$
$$0 = X^{T}Y - X^{T}X\beta$$
$$X^{T}X\beta = X^{T}Y$$
$$(X^{T}X)^{-1}X^{T}X\beta = (X^{T}X)^{-1}X^{T}Y$$
$$\beta = (X^{T}X)^{-1}X^{T}Y$$

QR Decomposition

We want A = QR where Q is an orthogonal matrix $(Q^TQ = I)$, and R is upper triangular. Let X = QR.

Starting from the result from earlier:

$$X^{T}X\beta = X^{T}Y$$
$$(QR)^{T}(QR)\beta = (QR)^{T}Y$$
$$R^{T}Q^{T}QR\beta = R^{T}Q^{T}Y$$
$$R^{T}R\beta = R^{T}Q^{T}Y$$
$$R\beta = Q^{T}Y$$

Following which we backwards solve for β .

SVD

We will let $X = UDV^T$, where D is a diagonal matrix, V is orthogonal. We then know the following:

$$Y = X\beta$$

$$Y = UDV^{T}\beta$$

$$(UDV^{T})^{-1}Y = (UDV^{T})^{-1}UDV^{T}\beta$$

$$VD^{-1}U^{T}Y = VD^{-1}U^{T}(UDV^{T})\beta$$

$$VD^{-1}U^{T}Y = \beta$$

Which we can solve for in R.

Cholesky Decomposition

We want $A = LL^T$ where A is a symmetric and positive definite matrix and L is a lower triangular matrix.

$$X^{T}Y = X^{T}X\beta$$
$$X^{T}Y = LL^{T}\beta$$
$$X^{T}Y = L(L^{T}\beta)$$
$$X^{T}Y = L^{T}\beta$$

Following which you backwards solve the upper triangular matrix L^T .

b) Implementation in R.

First, we load packages needed.

```
library(dplyr)
library(magrittr)
library(readr)
library(ggplot2)
library(ISLR2)
library(leaps)
library(glmnet)
library(pls)
library(matlib)
library(microbenchmark)
set.seed(5)
```

Then, we can create functions for solving linear regression using naive linear algebra, Cholesky decomposition, and QR decomposition.

```
# naive linear algebra;
linalg <- function(X1,y1) {
   xtr <- t(X1)
   b_la <- (inv(xtr %*% X1) %*% xtr %*% y1)</pre>
```

```
yhat_la <- X1 %*% b_la</pre>
# Cholesky decomposition;
cholesky <- function(X1,y1){</pre>
  xtr <- t(X1)
  L <- chol(xtr %*% X1)
  cp <- crossprod(X1, y1)</pre>
  a <- xtr %*% X1 %*% cp
  b_cd <- backsolve(L, a, transpose = T)</pre>
  yhat_cd <- X1 %*% b_cd
# QR decomposition;
qrd <- function(X1,y1){</pre>
  qrdecomp <- qr(X1)</pre>
  qr_q <- qr.Q(qrdecomp)</pre>
  qr_r <- qr.R(qrdecomp)</pre>
  qr_qty <- crossprod(qr_q,y1)</pre>
  b_qrd <- backsolve(qr_r, qr_qty)</pre>
  yhat_qrd <- X1 %*% b_qrd</pre>
```

Next, we will write a function to run each of the above functions and time them.

```
# create function to run each function above for various n, p
solve_lr <- function(n, p){</pre>
  X <- matrix(rnorm(n*p),ncol=p) #matrix x, p*n x p
  y <- matrix(rnorm(n), nrow=n) #vector y, 1 x n
  list(X=X,y=y)
  qrd(X,y)
  cholesky(X,y)
  linalg(X,y)
  timing <- microbenchmark(qrd(X,y),</pre>
                             cholesky(X,y),
                             linalg(X,y))
  summ <- summary(timing)</pre>
  results <- c(summ$mean,n,p)
  df <<- rbind(df,results)</pre>
  #return(df)
}
```

Then, we can create a data frame of average times for each method of solving and use various values of n and p.

```
ns <- round(10^seq(2, 5, by = 0.25))
ps <- round(2^seq(2, 5, by = 0.25))
```

```
df <- data.frame()

for (i in seq_along(ns)) {
    solve_lr(ns[i], p=10)
}

for (i in seq_along(ps)) {
    solve_lr(n=100, ps[i])
}

names(df) = c("QRD","CD","LA","n","p")</pre>
```

We can create plots to show the log-linear relationship between n and time and p and time.

```
df %>% filter(p==10) %>%
 ggplot() +
  geom_point(aes(x = log(QRD), y = log(n)), color = "pink") +
 geom_point(aes(x = log(CD), y = log(n)), color = "blue") +
  geom_point(aes(x = log(LA), y = log(n)), color = "purple")+
 xlab("Time")+
 ylab("n")+
 theme_bw()
df %>% filter(n==100) %>%
  ggplot() +
  geom_point(aes(x = log(QRD), y = log(p)), color = "pink") +
  geom_point(aes(x = log(CD), y = log(p)), color = "blue") +
  geom_point(aes(x = log(LA), y = log(p)), color = "purple")+
 xlab("Time")+
 ylab("p")+
  theme_bw()
```

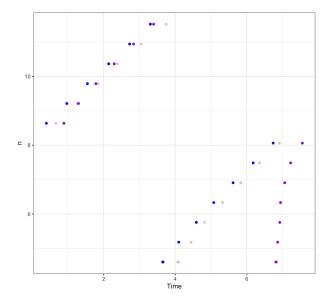


Figure 1: Plot of log(n) against log(time) for Cholesky decomposition(blue), QR decomposition (pink) and linear algebra solving (purple) for p=10.

Lastly, we will create log-log models of average time using the value of n.

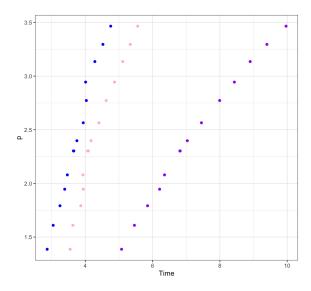


Figure 2: Plot of log(p) against log(time) for Cholesky decomposition(blue), QR decomposition (pink) and linear algebra solving (purple) for n=100.

```
#create log log model of average times to n
df2 <- df %>% filter(p==10)
lmqr <- lm(log(QRD) ~ log(n), data= df2)</pre>
summary(lmqr)
Call:
lm(formula = log(QRD) \sim log(n), data = df2)
Residuals:
   Min
            1Q Median
                             3Q
-2.9526 -1.0021 -0.1323 1.1035 3.0860
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept)
            6.7491
                     1.6985
                                3.974 0.00185 **
            -0.3631
                         0.2089 -1.738 0.10769
log(n)
\Signif. codes: 0 ***
                          0.001
                                        0.01
                                                    0.05
                                                               0.1
Residual standard error: 1.765 on 12 degrees of freedom
Multiple R-squared: 0.2012, Adjusted R-squared: 0.1346
F-statistic: 3.022 on 1 and 12 DF, p-value: 0.1077
lmcd <- lm(log(CD) ~ log(n), data= df2)</pre>
summary(lmcd)
Call:
lm(formula = log(CD) \sim log(n), data = df2)
Residuals:
   Min
            1Q Median
                             3Q
                                    Max
-2.9258 -1.1234 -0.1202 0.9922 3.2052
```

```
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept)
             6.4314
                        1.7370
                                 3.702 0.00302 **
log(n)
            -0.3599
                        0.2136 -1.685 0.11786
___
\Signif. codes: 0 ***
                         0.001
                                                  0.05 .
                                                              0.1
                                       0.01
                                                                        1
Residual standard error: 1.805 on 12 degrees of freedom
Multiple R-squared: 0.1913, Adjusted R-squared: 0.1239
F-statistic: 2.838 on 1 and 12 DF, p-value: 0.1179
lmla <- lm(log(LA) ~ log(n), data= df2)</pre>
summary(lmla)
lm(formula = log(LA) ~ log(n), data = df2)
Residuals:
   Min
            10 Median
                            3Q
                                   Max
-3.3274 -0.7810 0.0206 1.2441 2.8536
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 11.4564
                      1.7239
                                 6.646 2.38e-05 ***
log(n)
            -0.8385
                        0.2120 -3.955 0.00191 **
                        0.001
                                                  0.05
                                                             0.1
\Signif. codes: 0 ***
                                       0.01
Residual standard error: 1.791 on 12 degrees of freedom
Multiple R-squared: 0.5659, Adjusted R-squared: 0.5298
F-statistic: 15.65 on 1 and 12 DF, p-value: 0.001909
```

The linear algebra method is the only one that has the log(n) term significant in the model. All models have a coefficient value for log(n) between -1 and 0, so the models display a relatively linear relationship. R-squared is much higher for linear algebra than for the other models, indicating a stronger linear relationship.

2. First, we will import necessary packages.

```
library(dplyr)
library(magrittr)
library(readr)
library(ggplot2)
library(ISLR2)
library(leaps)
library(glmnet)
library(pls)
```

Next, the data is imported and scaled as described in the data information.

```
data <- read.table('prostatedata.txt')

train <- data %>% filter(train == TRUE)
test <- data %>% filter(train == FALSE)

Xmat <- model.matrix(lpsa ~ ., data)[, -10]
preds <- data[,1:8]
p <- ncol(Xmat)
y <- data$lpsa
xscaled <- scale(preds,TRUE,TRUE)</pre>
```

For data augmentation, we append $\sqrt{\lambda}I$ to X (where $\lambda = 0.01$ to get $X = \begin{pmatrix} X \\ \sqrt{\lambda}I \end{pmatrix}$, and p zeros to Y.

```
# append 0's to y vector and sqrt(lambda)*I to x
os <- matrix(0, (dim(xaug)[1]-length(y)), 1)
yaug <- rbind(y, os)
aug <- sqrt(0.01) * diag(8)
xaug <- rbind(xscaled, aug)
ridge_aug <- glmnet(xaug, yaug, alpha = 0)</pre>
```

For the native implementation of ridge regression, we use the scaled matrix of predictors and the response column.

```
#native implementation of ridge regression
ridge_nat <- glmnet(xscaled, y, family = gaussian, alpha = 0)</pre>
```

Next, we will examine the plots of both ridge models to compare. As we can see below, the plots look pretty much identical.

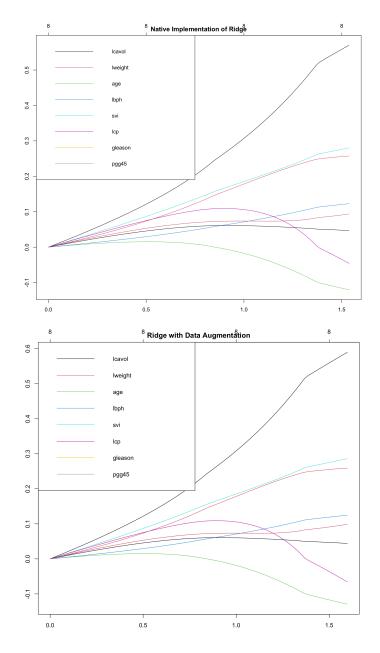
```
plot(ridge_aug, main = "Ridge with Data Augmentation")
legend("topleft", legend = rownames(coef(ridge_aug))[-1], lty = 1, col = 1:p)

plot(ridge_nat, main = "Native Implementation of Ridge")
legend("topleft", legend = rownames(coef(ridge_nat))[-1], lty = 1, col = 1:p)
```

Looking at timing for each method, the data augmentation method is much faster than native ridge implementation.

```
library(microbenchmark)

ridgetime <- microbenchmark(
  ridge_nat = glmnet(xscaled, y, family = gaussian, alpha = 0),</pre>
```



```
ridge_aug = glmnet(xaug, yaug, alpha = 0)
ridgetime
Unit: microseconds
          min
                        lq
                             mean
                                         median
ridge_nat 79390.596 81461.8340 86378.4503 83297.3220 91084.4315
           490.483
                   516.3745 587.1573 557.0055
                                                  653.6015
ridge_aug
      max neval
101190.542
            100
   823.649
            100
```

From Equation 3.41 and 3.43 in ESL, we have:

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

$$RSS(\lambda) = (Y - X\beta)^{T}(Y - X\beta) + \lambda \beta^{T}\beta$$

We can begin by taking the product of the Gaussian distributions:

$$\begin{split} P(\beta|D) &= N(X^T\beta, \sigma^2 I) * N(0, \tau I) \\ &= \frac{1}{\sigma\sqrt{2\pi}} exp\left(\frac{-(Y - X^T\beta)^2}{2\sigma^2}\right) * \frac{1}{\tau\sqrt{2\pi}} exp\left(\frac{-(Y - 0)^2}{2\tau}\right) \end{split}$$

We can take the log of the likelihood:

$$\begin{split} &= \log \left(\frac{1}{\sigma \sqrt{2\pi}} exp \left(\frac{-(Y - X^T \beta)^2}{2\sigma^2} \right) \right) + \log \left(\frac{1}{\tau \sqrt{2\pi}} exp \left(\frac{-(Y - 0)^2}{2\tau} \right) \right) \\ &= \frac{-(Y - X^T \beta)^2}{2\sigma^2} - \frac{Y^2}{2\tau} \\ &= \frac{-(Y - X^T \beta)^T (Y - X^T \beta)}{2\sigma^2} - \frac{\beta^T \beta}{2\tau} \end{split}$$

Then,

$$\begin{aligned} & argmin_{\beta} \left[\frac{-(Y - X^{T}\beta)^{T}(Y - X^{T}\beta)}{2\sigma^{2}} - \frac{\beta^{T}\beta}{2\tau} \right] \\ &= RSS + \lambda \beta^{T}\beta \\ &= RSS + \lambda \sum \beta_{j}^{2} \end{aligned}$$

Where $\lambda = 2\sigma^2/\tau$. Thus, this is the ridge estimate.

From Equation 3.44 in ESL we have:

$$\hat{\beta}^{ridge} = (X^T X + \lambda I)^{-1} X^T Y$$

Using SVD and setting $X = UDV^T$, this becomes,

$$= ((UDV^{T})^{T}(UDV^{T}) + \lambda I)^{-1}(UDV^{T})^{T}Y$$

$$= (VD^{T}U^{T} + \lambda I)^{-1}(VD^{T}U^{T})Y$$

$$= (VDU^{T}UDV^{T} + \lambda I)^{-1}(VDU^{T})Y$$

$$= D^{2} + \lambda I)^{-1}(VDU^{T})Y$$

$$||\hat{\beta}^{ridge}||^{2} = (D^{2} + \lambda I)^{-1} (VDU^{T}) Y)^{2}$$

$$= Y^{T} (VDU^{T})^{T} (D^{2} + \lambda I)^{-2} (VDU^{T}) Y$$

$$= Y^{T} (UD) (D^{2} + \lambda I)^{-2} (DU^{T}) Y$$

$$= \sum_{j=1}^{p} y u_{j} d_{j} \frac{1}{(dj + \lambda)^{2}} d_{j} u_{j} y$$

$$= \sum_{j=1}^{p} \frac{y u_{j} d_{j} d_{j} u_{j} y}{(dj + \lambda)^{2}}$$

Which increases as λ goes to 0.

Lasso

We can look at table 3.4 to see the estimators in the case of orthonormal columns of X. For lasso, this is $sign(\hat{\beta}_j)(|\hat{\beta}_j| - \lambda)_+$. AS λ goes to zero, $(|\hat{\beta}_j| - \lambda)$ will increase since λ is getting smaller, and so the entire estimator will increase.

This can be seen for the ridge estimator as well, $\hat{\beta}_j/1 + \lambda$, so as λ goes to 0 the estimator increases.

The lasso solution is given by Equation 3.52 in ESL:

$$\hat{\beta}^{lasso} = argmin_{\beta} \left[1/2 \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right]$$

Subject to $\sum_{j=1}^{p} |\beta_j| \le t$.

Let $X' = [X_j X_j^*]$ and $\beta^{*'} = [\beta_j \beta_j^*]$ so that $X\beta^* = X\beta_j + X\beta_J^*$.

Then we have

$$\hat{\beta}^{lasso} = argmin_{\beta} \left[\frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right]$$

$$= argmin_{\beta} \left[\frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - x \beta_j - x \beta_j^*)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right]$$

$$= argmin_{\beta} \left[\frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - x (\beta_j + \beta_j^*))^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right]$$

$$= argmin_{\beta} \left[\frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - x (\beta_j + \beta_j^*))^2 + \lambda (|\beta_j| + |\beta_j^*|) \right]$$

Subject to $\sum_{j=1}^p |\beta_j| \le t$ i.e., $(|\beta_j| + |\beta_j^*|) \le t$. and $(|\beta_j| + a) \le t$.

Let
$$X = \begin{pmatrix} X \\ \lambda I \end{pmatrix}$$
, and $Y = \begin{pmatrix} y \\ 0 \end{pmatrix}$.

We want to show how this can turn into the lasso problem.

$$min||y - X\beta||^2 + \lambda[\alpha||\beta||_2^2 + (1 - \alpha)||\beta||_1]$$

$$\begin{aligned} & \min ||y - X\beta||^2 \\ &= ||y - X\beta||_2^2 + ||0 - \lambda\beta||_2^2 \\ &= ||y - X\beta||_2^2 + ||\lambda\beta||_2^2 \\ &= ||y - X\beta||_2^2 + \lambda ||\beta||_2^2 \end{aligned}$$

Setting α to 1 we get:

$$\begin{split} &= ||y - X\beta||_2^2 + \lambda ||\beta||_2^2 + \lambda ||\beta||_2^2 \\ &= ||y - X\beta||_2^2 + \lambda ||\beta||_2^2 \end{split}$$

Which is equal to $\hat{\beta}^{lasso}$.