Penalized Regression

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STAT 7200–Multivariate Statistics

Objectives

- Introduce ridge regression and discuss the bias-variance trade-off
- Introduce Lasso regression and discuss variable selection
- Discuss cross-validation for parameter tuning

Recall: Least Squares Estimation i

- Let $\mathbf{Y}_1 \dots, \mathbf{Y}_n$ be a random sample of size n, and let $\mathbf{X}_1, \dots, \mathbf{X}_n$ be the corresponding sample of covariates.
    - $\mathbf{Y}_i$ and $\mathbf{X}_i$ are of dimension p and q, respectively.
- We will write $\mathbb{Y}$ and $\mathbb{X}$ for the matrices whose i-th row is $\mathbf{Y}_i$ and $\mathbf{X}_i$, respectively.
- From the linear model assumption, we can then write $E(\mathbb{Y} \mid \mathbb{X}) = \mathbb{X}B$.
- The least-squares criterion is given by

$$LS(B) = \mathrm{tr}\left[(\mathbb{Y} - \mathbb{X}B)^T(\mathbb{Y} - \mathbb{X}B)\right].$$

Recall: Least Squares Estimation ii

- The minimum is attained at at

$$\hat{B} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}.$$

- The least-squares estimator is *unbiased*:

$$E(\hat{B} \mid \mathbb{X}) = B.$$

- If we let $\hat{\beta}_i$ be the i-th column of $\hat{B}$, we have

$$\mathrm{Cov}(\hat{\beta}_i, \hat{\beta}_j) = \sigma_{ij}(\mathbb{X}^T\mathbb{X})^{-1},$$

  where σ_{ij} is the (i, j)-th entry of $\Sigma = \mathrm{Cov}\left(\mathbf{Y}_i \mid \mathbf{X}_i\right)$.

Multicollinearity

- As we can see, the variance of the regression coefficients depend on the inverse of $\mathbb{X}^T\mathbb{X}$.
- **Multicollinearity** is when the columns of $\mathbb{X}$ are *almost* linearly dependent.
    - Note: This can happen when a covariate is almost constant.
- As a consequence, $\mathbb{X}^T\mathbb{X}$ is nearly singular, and therefore the variance of the regression coefficients can blow up.

- **Solution**: Add a small positive quantity along the diagonal of $\mathbb{X}^T\mathbb{X}$.
    - $\mathbb{X}^T\mathbb{X} \to \mathbb{X}^T\mathbb{X} + \lambda I$
- The **Ridge estimator** of B is given by

$$\hat{B}_R = (\mathbb{X}^T\mathbb{X} + \lambda I_q)^{-1}\mathbb{X}^T\mathbb{Y}.$$

Example i

```r
library(tidyverse)
url <- "https://maxturgeon.ca/w20-stat7200/prostate.csv"
prostate <- read_csv(url)

# Separate into training and testing sets
data_train <- filter(prostate, train == TRUE) %>%
  dplyr::select(-train)
data_test <- filter(prostate, train == FALSE) %>%
  dplyr::select(-train)
```

Example ii

```
# OLS
model1 <- lm(lpsa ~ .,
             data = data_train)
pred1 <- predict(model1, data_test)

mean((data_test$lpsa - pred1)^2)
```

```
## [1] 0.521274
```

Example iii

```r
# Ridge regression
X_train <- model.matrix(lpsa ~ .,
                        data = data_train)
Y_train <- data_train$lpsa

B_ridge <- solve(crossprod(X_train) + diag(0.7, 9),
                 t(X_train)) %*% Y_train
```

Example iv

```r
X_test <- model.matrix(lpsa ~ .,
                       data = data_test)

pred2 <- X_test %*% B_ridge

mean((data_test$lpsa - pred2)^2)
```

```
## [1] 0.5180924
```

```r
# Compare both estimates
head(cbind(coef(model1), B_ridge))
```

Example v

```
##                         [,1]       [,2]
## (Intercept)  0.42917013  0.1323063
## lcavol       0.57654319  0.5709660
## lweight      0.61402000  0.6160020
## age         -0.01900102 -0.0173843
## lbph         0.14484808  0.1395858
## svi          0.73720864  0.6683160
```

Bias-Variance tradeoff i

- The ridge estimator is **biased**:

$$\begin{aligned}
E(\hat{B}_R \mid \mathbb{X}) &= (\mathbb{X}^T\mathbb{X} + \lambda I_q)^{-1}\mathbb{X}E(\mathbb{Y} \mid \mathbb{X}) \\
&= (\mathbb{X}^T\mathbb{X} + \lambda I_q)^{-1}\mathbb{X}^T\mathbb{X}B \\
&\neq B.
\end{aligned}$$

- But the variance is potentially smaller:

$$\mathrm{Cov}(\hat{\beta}_i, \hat{\beta}_j) = \sigma_{ij}(\mathbb{X}^T\mathbb{X} + \lambda I_q)^{-1}\mathbb{X}^T\mathbb{X}(\mathbb{X}^T\mathbb{X} + \lambda I_q)^{-1}.$$

- This is an example of the classical **bias-variance tradeoff**:
    - We increase bias and decrease variance.

Bias-Variance tradeoff ii

- Ideally, this is done in such a way to reduce the **mean squared error**:
$$MSE = \frac{1}{n}\mathrm{tr}\left[(\mathbb{Y} - \hat{\mathbb{Y}})^T(\mathbb{Y} - \hat{\mathbb{Y}})\right].$$
- *Should we compute the MSE with the training of the test data?*

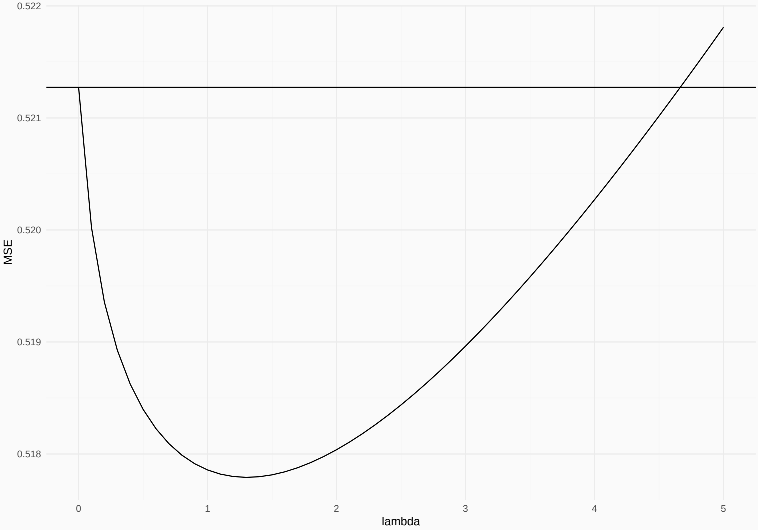
Example (cont'd) i

```
mse_df <- purrr::map_df(seq(0, 5, by = 0.1),
                        function(lambda) {
  B_ridge <- solve(crossprod(X_train) + diag(lambda, 9),
                  t(X_train)) %*% Y_train
  pred2 <- X_test %*% B_ridge

  mse <- mean((data_test$lpsa - pred2)^2)
  return(data.frame(MSE = mse,
                    lambda = lambda))
  })
```

Example (cont'd) ii

```r
ols_mse <- mean((data_test$lpsa - pred1)^2)

ggplot(mse_df, aes(lambda, MSE)) +
  geom_line() + theme_minimal() +
  geom_hline(yintercept = ols_mse)
```

Example (cont’d) iii



Regularized regression

- The ridge estimator can also be defined as a solution to a **regularized least squares problem**:

$$LS_R(B;\lambda) = \mathrm{tr}\left[(\mathbb{Y} - \mathbb{X}B)^T(\mathbb{Y} - \mathbb{X}B)\right] + \lambda \mathrm{tr}\left(B^T B\right).$$

- Yet another way to define the ridge estimator is as a solution to a **constrained least squares problem**:

$$\min_B \mathrm{tr}\left[(\mathbb{Y} - \mathbb{X}B)^T(\mathbb{Y} - \mathbb{X}B)\right], \qquad \mathrm{tr}\left(B^T B\right) \leq c.$$

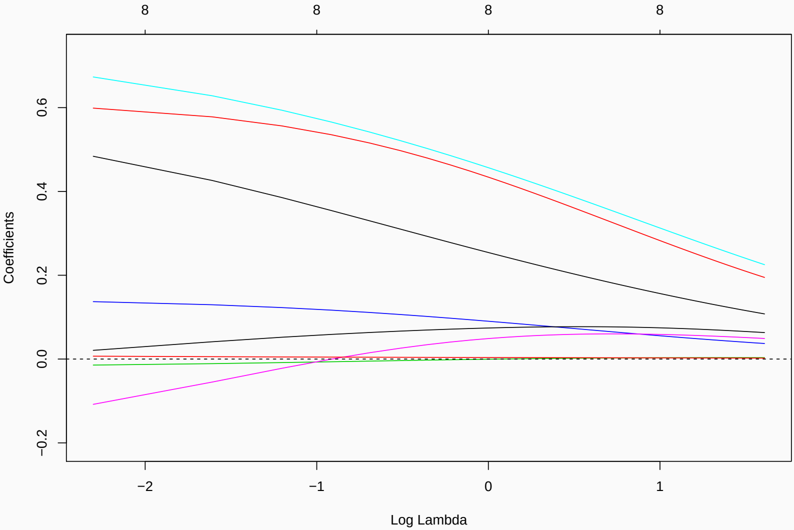
Solution path i

```r
library(glmnet)

# Fit for multiple values of lambda
X_train <- model.matrix(lpsa ~ . - 1,
                        data = data_train)
ridge_fit <- glmnet(X_train, data_train$lpsa,
                    alpha = 0,
                    lambda = seq(0, 5, by = 0.1))
```

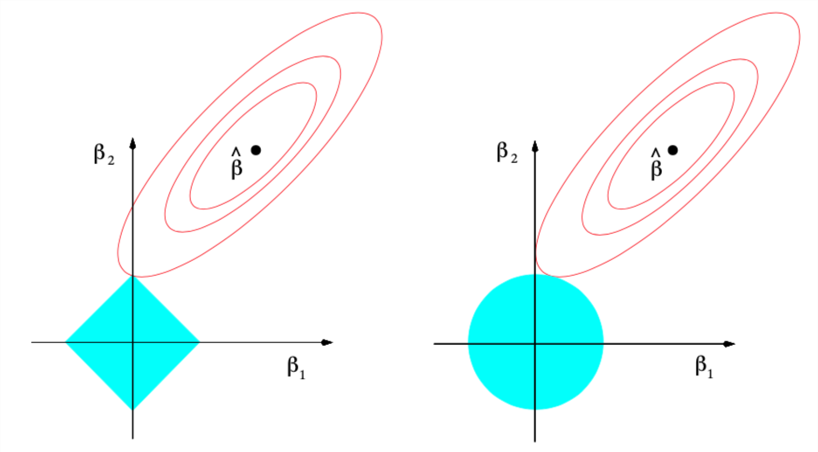
Solution path ii

```r
# Plot the value of the coefficients
# as a function of lambda
plot(ridge_fit, xvar = "lambda")
abline(h = 0, lty = 2)
```

Solution path iii



Constrained regression



Lasso regression

- **Lasso regression** puts a different constraint on the size of the regression coefficients B:
  - Ridge regression: $\mathrm{tr}\left(B^T B\right) = \sum_{ij} B_{ij}^2 \leq c$
  - Lasso regression: $\|B\|_1 = \sum_{ij} |B_{ij}| \leq c$
- Just as with ridge regression, this is also equivalent to a regularized least squares problem:

$$LS_L(B;\lambda) = \mathrm{tr}\left[(\mathbb{Y} - \mathbb{X}B)^T(\mathbb{Y} - \mathbb{X}B)\right] + \lambda\|B\|_1.$$

- **Major difference**: Lasso regression performs *variable selection*.

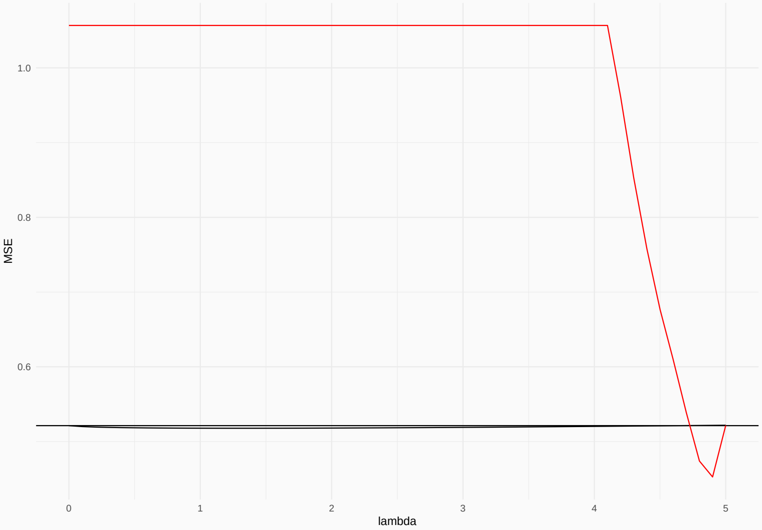
Example (cont'd) i

```
# Fit lasso regression along the same lambda sequence
lasso_fit <- glmnet(X_train, data_train$lpsa,
                    alpha = 1, # For lasso regression
                    lambda = seq(0, 5, by = 0.1))
```

```
X_test <- model.matrix(lpsa ~ . - 1,
                       data = data_test)
lasso_pred <- predict(lasso_fit, newx = X_test)
lasso_mse <- apply(lasso_pred, 2, function(col) {
  mean((data_test$lpsa - col)^2)
})
```

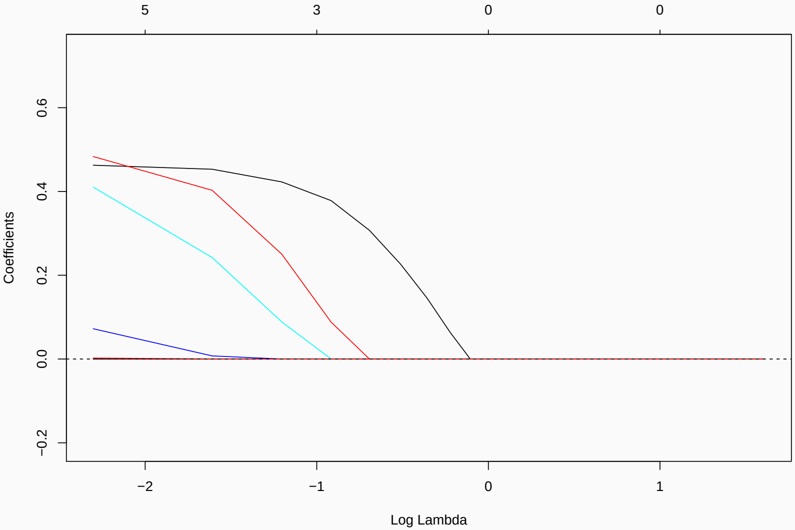
```r
lasso_mse_df <- data.frame(MSE = lasso_mse,
                           lambda = seq(0, 5, by = 0.1))
ggplot(mse_df, aes(lambda, MSE)) +
  geom_line() + theme_minimal() +
  geom_hline(yintercept = ols_mse) +
  geom_line(data = lasso_mse_df, colour = 'red')
```

Example (cont'd) iii



```r
# Plot the value of the coefficients
# as a function of lambda
plot(lasso_fit, xvar = "lambda")
abline(h = 0, lty = 2)
```

Example (cont'd) v



Example (cont'd) vi

```r
# Where is the min MSE?
filter(lasso_mse_df, MSE == min(MSE))
```

```
##           MSE lambda
## 1 0.4526232    4.9
```

```r
# What are the estimates?
coef(lasso_fit, s = 4.9)
```

Example (cont'd) vii

```
## 9 x 1 sparse Matrix of class "dgCMatrix"
##                    1
## (Intercept) 2.452345
## lcavol      .
## lweight     .
## age         .
## lbph        .
## svi         .
## lcp         .
## gleason     .
## pgg45       .
```

Comments

- There are other forms of penalized regression:
    - Elastic net, SCAD, adaptive lasso, group lasso, etc.
- They each have different *asymptotic* and *finite sample* properties.
    - E.g. Lasso is asymptotically biased; Elastic net and SCAD are asymptotically unbiased.
- In general, how do we select λ when we don't have a test set?
    - **Answer**: Cross-validation.

K-fold cross-validation

- Goal: Find the value of λ that minimises the MSE on test data.
- K-fold cross-validation (CV) is a resampling technique that estimates the test error from the training data.
- It is also an efficient way to use all your data, as opposed to separating your data into a training and a testing subset.

Algorithm

Let $K > 1$ be a positive integer.

1. Separate your data into K subsets of (approximately) equal size.
2. For $k = 1, \ldots, K$, put aside the k-th subset and use the remaining $K - 1$ subsets to train your algorithm.
3. Using the trained algorithm, predict the values for the held out data.
4. Calculate MSE_k as the Mean Squared Error for these predictions.
5. The overall MSE estimate is given by

$$MSE = \frac{1}{K} \sum_{k=1}^{K} MSE_k.$$

Example i

```r
# Take all the data
dataset <- dplyr::select(prostate, -train)
dim(dataset)
```

```
## [1] 97  9
```

```r
set.seed(7200)
library(caret)
```

```
## Loading required package: lattice
```

Example ii

```
##
## Attaching package: 'lattice'

## The following object is masked from 'package:openintro
##
##     lsegments

##
## Attaching package: 'caret'

## The following object is masked from 'package:openintro
##
##     dotPlot
```

Example iii

```
## The following object is masked from 'package:purrr':
##
##     lift
```

```r
# 5-fold CV
trainIndex <- createFolds(dataset$lpsa, k = 5)
str(trainIndex)
```

Example iv

```
## List of 5
##  $ Fold1: int [1:20] 6 8 22 23 25 27 28 32 41 46 ...
##  $ Fold2: int [1:19] 5 7 15 18 20 26 29 42 44 45 ...
##  $ Fold3: int [1:19] 1 11 19 21 24 30 33 48 49 50 ...
##  $ Fold4: int [1:19] 3 4 10 12 16 31 34 35 39 43 ...
##  $ Fold5: int [1:20] 2 9 13 14 17 36 37 38 40 47 ...
```

Example v

```r
# Define function to compute MSE
compute_mse <- function(prediction, actual) {
  # Recall: the prediction comes in an array
  apply(prediction, 2, function(col) {
    mean((actual - col)^2)
    })
}
```

Example vi

```
MSEs <- sapply(trainIndex, function(indices){
  X_train <- model.matrix(lpsa ~ . - 1,
                          data = dataset[-indices,])
  Y_train <- dataset$lpsa[-indices]
  X_test <- model.matrix(lpsa ~ . - 1,
                          data = dataset[indices,])
  lasso_fit <- glmnet(X_train, Y_train, alpha = 1,
                      lambda = seq(0, 5, by = 0.1))
  lasso_pred <- predict(lasso_fit, newx = X_test)
  compute_mse(lasso_pred, dataset$lpsa[indices])
  })
```

Example vii

```r
# Each column is for a different fold
dim(MSEs)
```

```
## [1] 51  5
```

```r
CV_MSE <- colMeans(MSEs)

seq(0, 5, by = 0.1)[which.min(CV_MSE)]
```

```
## [1] 0.4
```

Example viii

```r
# What are the estimates?
coef(lasso_fit, s = 0.4)
```

```
## 9 x 1 sparse Matrix of class "dgCMatrix"
##                      1
## (Intercept) 1.63646053
## lcavol      0.37816202
## lweight     0.08802054
## age         .
## lbph        .
## svi         .
```

Example ix

```
## lcp         .
## gleason     .
## pgg45       .
```

```
# Conveniently, glmnet has a function for CV
# It also chooses the lambda sequence for you
X <- model.matrix(lpsa ~ . -1, data = dataset)
lasso_cv_fit <- cv.glmnet(X, dataset$lpsa, alpha = 1,
                          nfolds = 5)
```

```
c("lambda.min" = lasso_cv_fit$lambda.min,
  "lambda.1se" = lasso_cv_fit$lambda.1se)
```

Example x

```
## lambda.min lambda.1se
## 0.03250172 0.14400281
```

```r
# What are the estimates?
coef(lasso_cv_fit, s = 'lambda.min')
```

```
## 9 x 1 sparse Matrix of class "dgCMatrix"
##                        1
## (Intercept)  0.161190494
## lcavol       0.508157223
## lweight      0.552486889
## age         -0.009374709
```

Example xi

```
## lbph              0.064736544
## svi               0.594693519
## lcp               .
## gleason           0.004797184
## pgg45             0.002351087
```

```r
# 1 SE rule
coef(lasso_cv_fit, s = 'lambda.1se')
```

Example xii

```
## 9 x 1 sparse Matrix of class "dgCMatrix"
##                     1
## (Intercept) 0.2975535
## lcavol      0.4725492
## lweight     0.3989087
## age         .
## lbph        .
## svi         0.4400593
## lcp         .
## gleason     .
## pgg45       .
```

Summary

- Regularized regression can help reduce the mean-squared error, especially in the presence of multicollinearity
  - **Ridge regression**: Penalizes the $L2$ norm of the coefficients
  - **Lasso regression**: Penalizes the $L1$ norm of the coefficients
- Unlike ridge regression, lasso regression also performs variable selection.
  - But this comes at a cost: **post-selection inference**.
- K-fold cross-validation can be used to find the best value of λ.