BIOS 635: Shrinkage Methods and Penalized Regression

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3/4/2021

Review

- Homework 5 due on 3/5 at 11PM through GitHub Classroom
- Last lecture: model selection

Model selection

- **Goal**: Choose/build model parameters and structure to create *optimal* model
- General methods:

  1. Subset Selection
  2. **Shrinkage**
  3. Dimension Reduction

Shrinkage

- **With regression**: estimate regression parameters by *minimizing squared residual error*
- **With subset selection**: fit multiple models by least squares, select *best*
- **With shrinkage**: fit model with all p predictors *once* with method that *shrinks* low magnitude coefficients to 0

Penalized regression

- With traditional regression:

$$
\begin{aligned}
&Y = \beta_0+\beta_1X_1+\ldots+\beta_pX_p+\epsilon \\
&\hat{\beta} = \min_{\beta} \sum_{i=1}^{n} [Y_i-(\beta_0+\beta_1X_1+\ldots+\beta_pX_p)]^2
\end{aligned}
$$

- With traditional regression:

```
\begin{align}
&Y = \beta_0+\beta_1X_1+\ldots+\beta_pX_p+\epsilon \\
&\hat{\beta} = \min_{\beta} \sum_{i=1}^{n} [Y_i-(\beta_0+\beta_1X_1+\ldots+\beta_pX_p)]^2+\lambda\sum_{j=1}^{p}||\beta_j||
\text{where } \lambda >0
\end{align}
```

- Penalized regression $\rightarrow$ need to minimize RSS **and** penalty from $\beta > 0$
  - *Will force low magnitude* $\beta \rightarrow 0$
  - *Need to choose how to compute magnitude of* β*, denoted norm*=$||.||_q$

Ridge regression

- **Recall**: Residual sum of squares (RSS)

$$RSS(\beta) = \sum_{i=1}^{n} [Y_i - (\beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p)]^2$$

- Use **square norm**:

$$\hat{\beta} = \min_{\beta} RSS(\beta) + \lambda \sum_{j=1}^{p} (\beta_j)^2$$

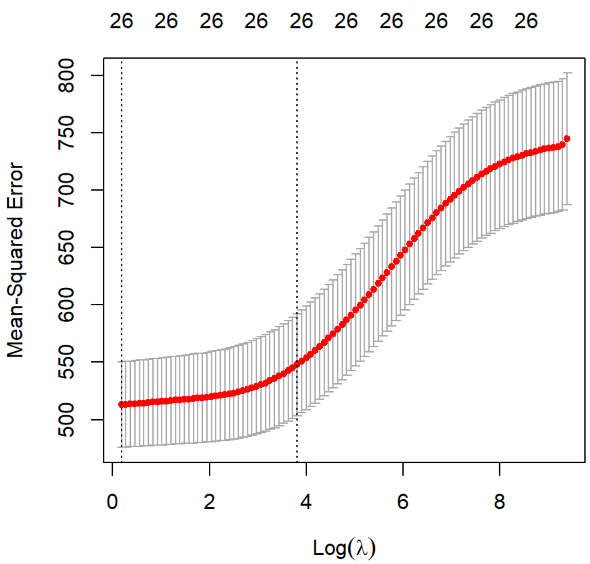
- $\lambda > 0$ is a *tuning parameter*, must be chosen and fixed
    - *Can use cross validation (CV), holdout, metrics like AIC, BIC, etc.*
    - *Generally **CV is best***

Ridge regression example

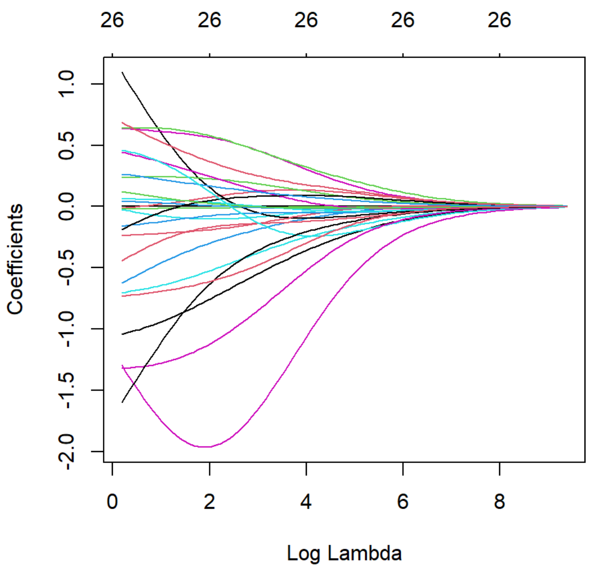
- Ex. cancer mortality at county level

```
cancer_data <- read_csv("../data/cancer_reg.csv") %>%
  select(-avgAnnCount, -avgDeathsPerYear, -incidenceRate, -binnedInc, -Geography) %>%
  select(TARGET_deathRate, medIncome, povertyPercent, MedianAge:BirthRate) %>%
  drop_na()

lm_ridge <- cv.glmnet(x=as.matrix(cancer_data[,-1]), y=unlist(cancer_data[,1]), alpha = 0)
plot(lm_ridge)
```




```
lm_ridge <- glmnet(x=as.matrix(cancer_data[,-1]), y=unlist(cancer_data[,1]),
                   alpha = 0)
plot(lm_ridge, xvar = "lambda")
```


26
26
26
26
26
Coefficients
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
0
2
4
6
8
Log Lambda

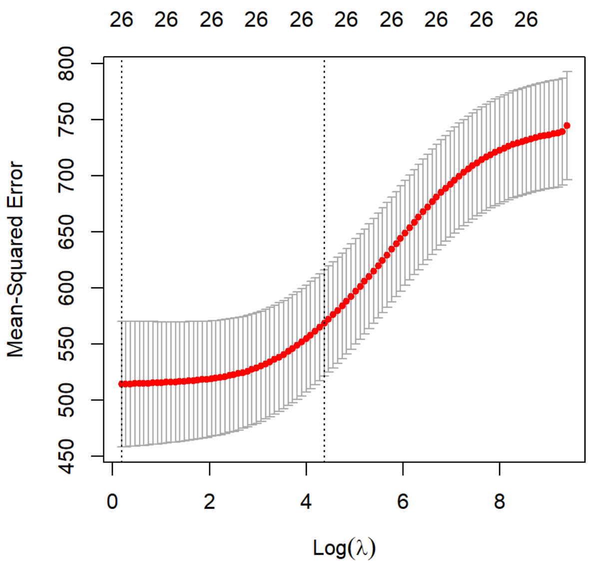
Ridge regression and scaling

- **Recall**: Standard least squares estimates are *scale equivalent*
  - *Multiplying predictor X_j by constant c simply re-scales $\hat{\beta}_j$ by $1/c*
  - $\rightarrow X_j\hat{\beta}_j$ *always the same*
- **Not the case** with penalized regression
  - *Scale of β_j determines if it is shrunk towards 0*
  - *Use of **squared norm** makes scaling even more impactful*
- Thus, best to apply after **standardizing the predictors**:

$$\tilde{x_{ij}} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x_j})^2}}$$

Scaling example in data

```
lm_ridge <-
  cv.glmnet(x=scale(as.matrix(cancer_data[,-1])),
            y=unlist(cancer_data[,1]),
            alpha = 0)
plot(lm_ridge)
```

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lm_ridge <- glmnet(x=scale(as.matrix(cancer_data[,-1])), y=unlist(cancer_data[,1]),
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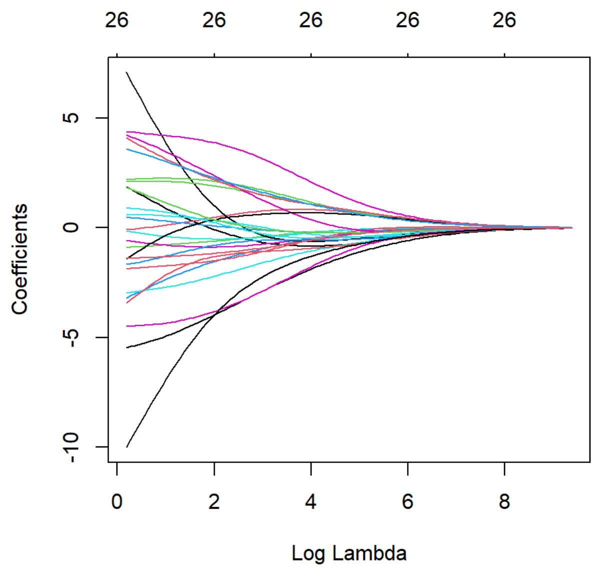
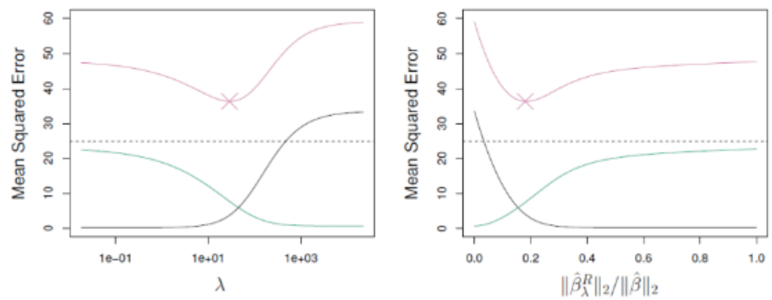

26
26
26
26
26
Coefficients
5
0
-5
-10
0
2
4
6
8
Log Lambda

How does ridge regression improve over least squares?

The Bias-Variance tradeoff



Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficients. Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of λ and $\|\hat{\beta}^R_\lambda\|_2/\|\hat{\beta}\|_2$. The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.

LASSO

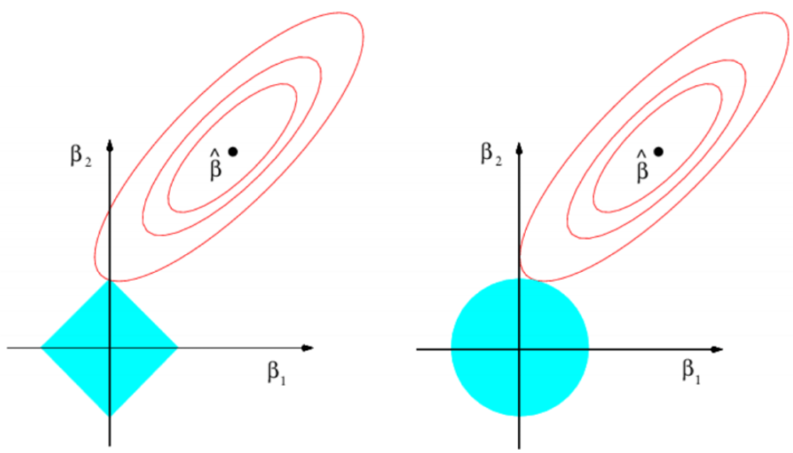
- Ridge regression **disadvantage**:
  - *Will **shrink unimportant coefficients to 0** but will **not** remove predictors near 0*
  - *Thus does not perform model selection, all p predictors still kept in model*
- **Solution**: *Lasso*
  - *Method:*

$$\hat{\beta} = \min_{\beta} RSS(\beta) + \lambda \sum_{j=1}^{p} |\beta_j|$$

- Uses L_1 norm, defined as $||\beta||_1 = \sum_j |\beta_j|$

LASSO vs ridge

- LASSO also shrinks coefficient estimates to 0
- **However**, will set low magnitude coefficients **to exactly 0**, thus removing them
  - *$\rightarrow$ can be used for model selection*
  - *Amount set to 0 depends on λ choice*
  - *$\rightarrow$ lasso yields sparse models*

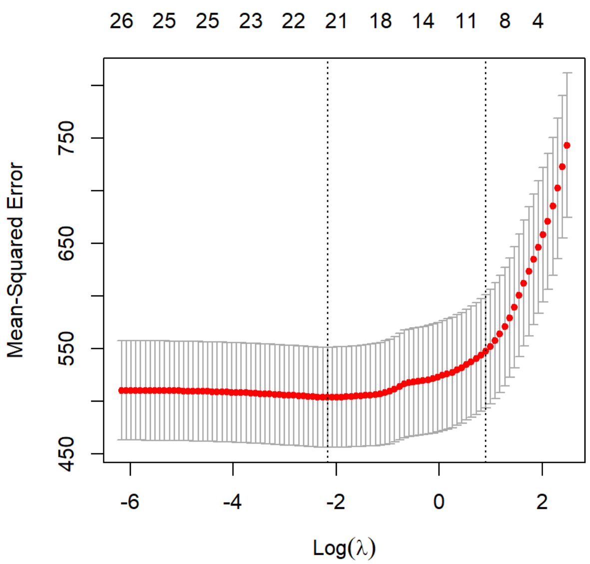


LASSO example

- Ex. cancer mortality at county level

```
cancer_data <- read_csv("../data/cancer_reg.csv") %>%
  select(-avgAnnCount, -avgDeathsPerYear, -incidenceRate, -binnedInc, -Geography) %>%
  select(TARGET_deathRate, medIncome, povertyPercent, MedianAge:BirthRate) %>%
  drop_na()

lm_ridge <- cv.glmnet(x=as.matrix(cancer_data[,-1]), y=unlist(cancer_data[,1]), alpha = 1)
plot(lm_ridge)
```

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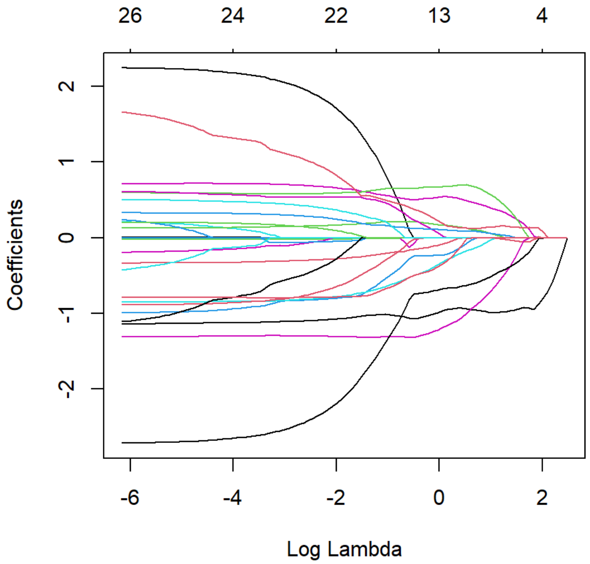
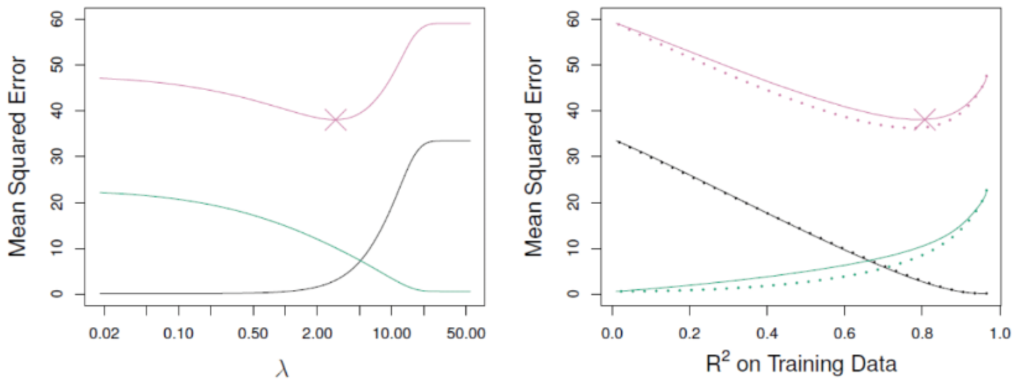
lm_ridge <- glmnet(x=as.matrix(cancer_data[,-1]), y=unlist(cancer_data[,1]),
                   alpha = 1)
plot(lm_ridge, xvar = "lambda")
```

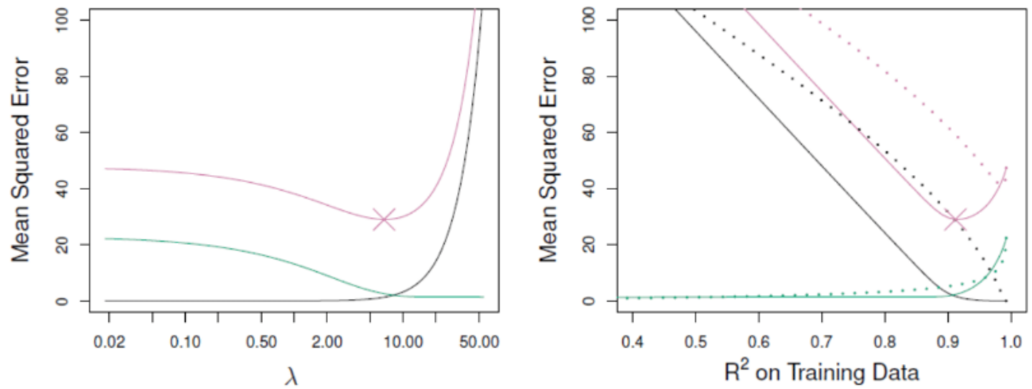

26
24
22
13
4
2
1
0
-1
-2
Coefficients
-6
-4
-2
0
2
Log Lambda

LASSO vs Ridge: Simulations



Simulated data with 45 features, all with non-zero coefficients.

LASSO vs Ridge: Simulations



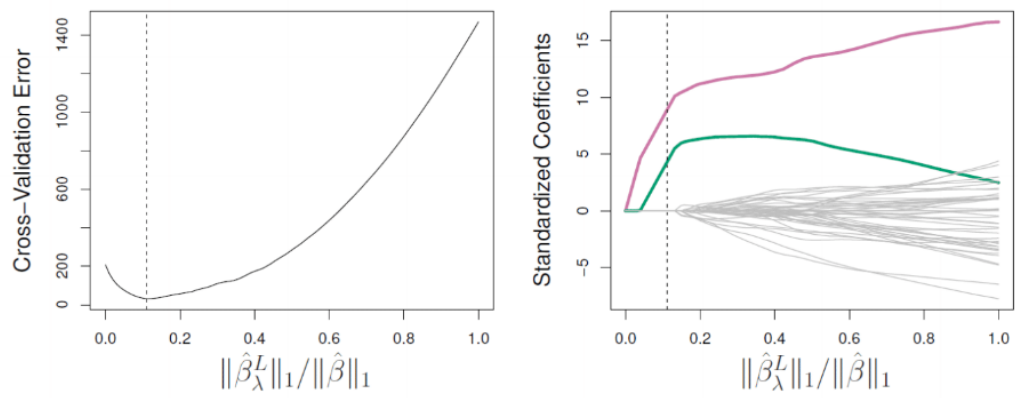
Simulated data with only two predictors that are related to response.

Tuning parameter selection

- Need to specify $\lambda > 0$ when using penalized regression
- Don't know which predictors are important before analysis, need some metric to guide selection
- **Cross validation** common way of doing this process
  - *First, setup grid of λ values to try*
  - *For each value, compute CV error*
  - *Choosen lambda which minimizes CV error*
  - *Refit penalized regression with chosen λ*

Tuning parameter selection: simulated data

Simulated data example



Simulated data with only two predictors that are related to response.

Other penalized regression methods

1. Smoothing splines

$$\text{minimize} \quad \underbrace{\sum_{i=1}^{n}(y_i - g(x_i))^2}_{\text{RSS}} + \underbrace{\lambda \int g''(t)^2 dt}_{\text{Roughness penalty}}$$

2. Group Lasso

3. Fused Lasso

- For data with temporal or spatial structure

4. Elastic Net

$$\hat{\beta} = \min_{\beta} RSS(\beta) + \lambda_1 \sum_{j=1}^{p} |\beta_j| + \lambda_2 \sum_{j=1}^{p} (\beta_j)^2$$

Song of the session

Africa Brasil by Jorge Ben Jor

O Plebeu by Jorge Ben Jor

Taj Mahal by Jorge Ben Jor