Model Building & Scoring for Prediction

Institute for Advanced Analytics
MSA Class of 2022

Model Building

- Linear regression is a great initial approach to model building, but it isn't the only form of regression.
- Linear regression is the **best linear unbiased estimator (BLUE)**.

Best Linear Unbiased Estimator

- What does it mean to be **unbiased**?

$$\hat{\beta}_j \sim N\left(\beta_j, s_{\hat{\beta}_j}\right)$$

Best Linear Unbiased Estimator

- What does it mean to be **unbiased**?

$$\hat{\beta}_j \sim N\left(\beta_j, s_{\hat{\beta}_j}\right)$$

On average, coefficients from all samples are centered around the true coefficient.

Best Linear Unbiased Estimator

- What does it mean to be **unbiased**?

$$\hat{\beta}_j \sim N\left(\beta_j, s_{\widehat{\beta}_j}\right)$$

- What does it mean to be **best**?
  - *IF* assumptions hold, $s_{\widehat{\beta}_j}$ is the minimum variance of all the unbiased estimators.

Best Linear Unbiased Estimator

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What if assumptions don't hold?

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Best Linear Unbiased Estimator

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- What does it mean to be **best**?
  - ***IF* assumptions hold**, $s_{\hat{\beta}_j}$ is the **minimum variance of all the unbiased estimators**.

What if biased estimators had smaller variance?

Regularized Regression

Potential Problems

- As the number of variables increases, more problems tend to arise.
  - Assumptions start to fail.
  - Multicollinearity concerns.

- Multicollinearity problems → coefficients vary widely.
  - Variations lead to **overfitting** (only predicting the training data well, but not generalizing to the test dataset).
  - Higher variance than desired.

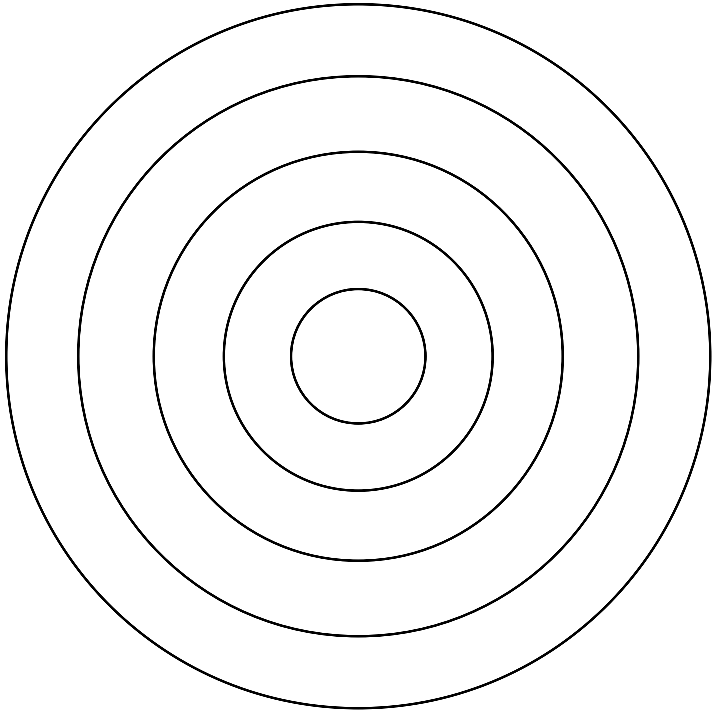
- More variables than observations (genetic modeling).

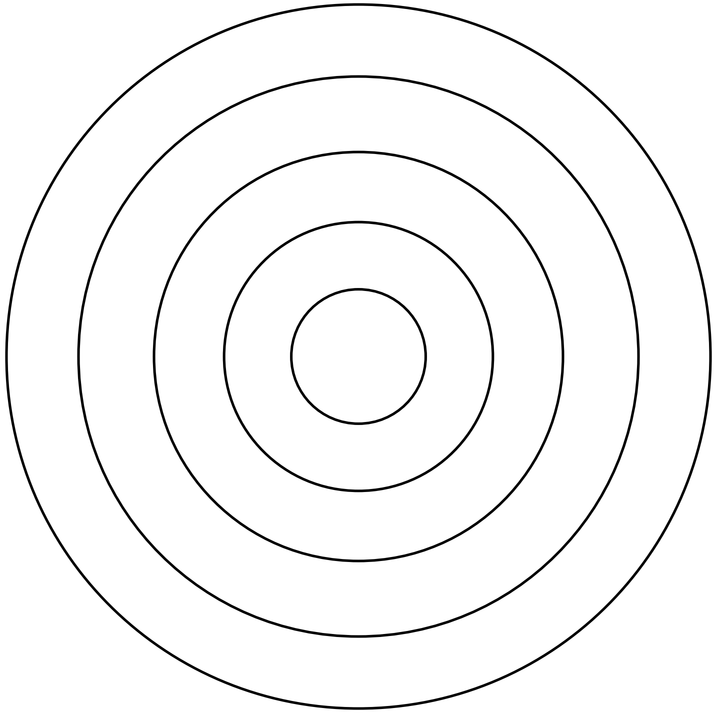
Regularized Regression

- **Regularized regression** (or penalized / shrinkage regression) puts constraints on the estimated coefficients in our model and *shrink* these estimates to 0.

- Coefficients become biased, but potentially improve variance of the model.

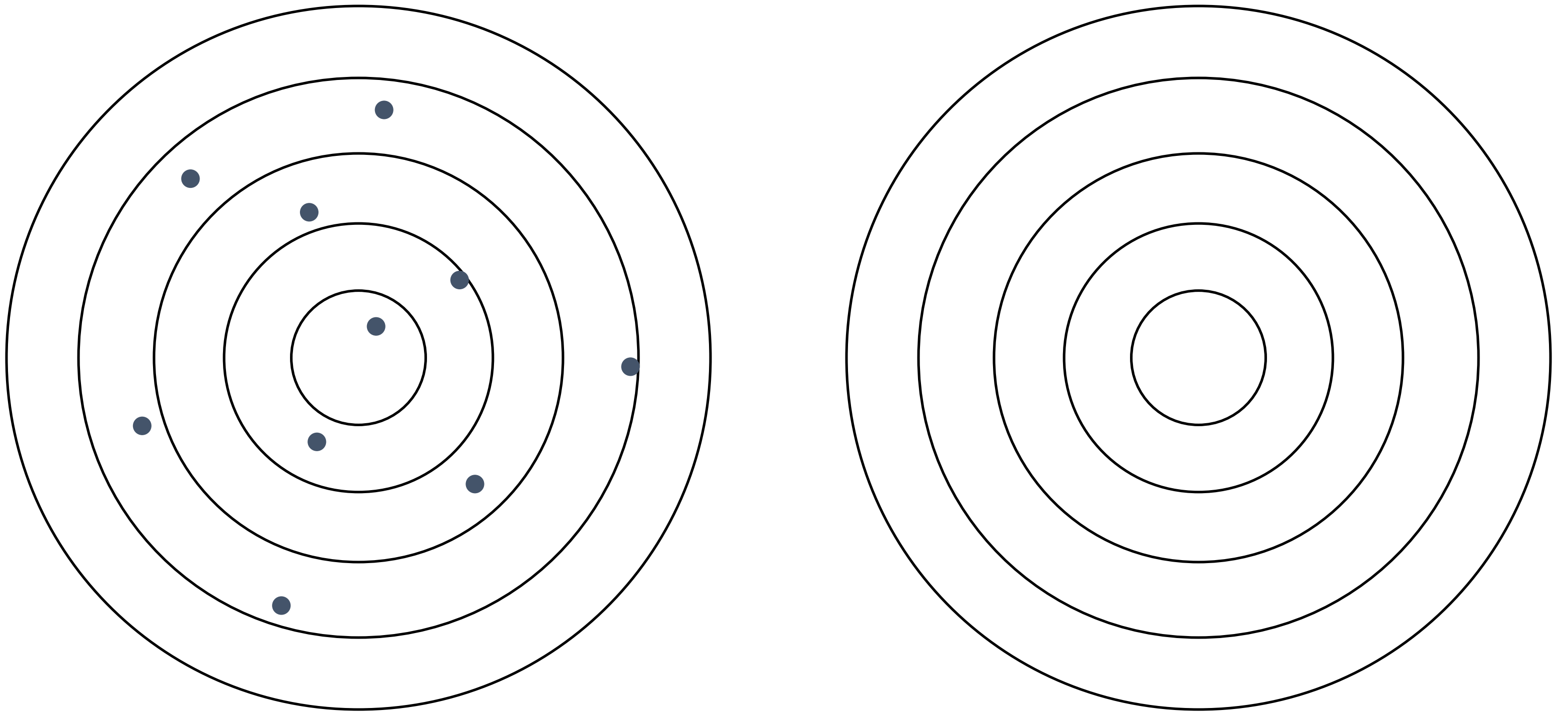
Biased Regression Techniques





Biased Regression Techniques

Unbiased but not precise



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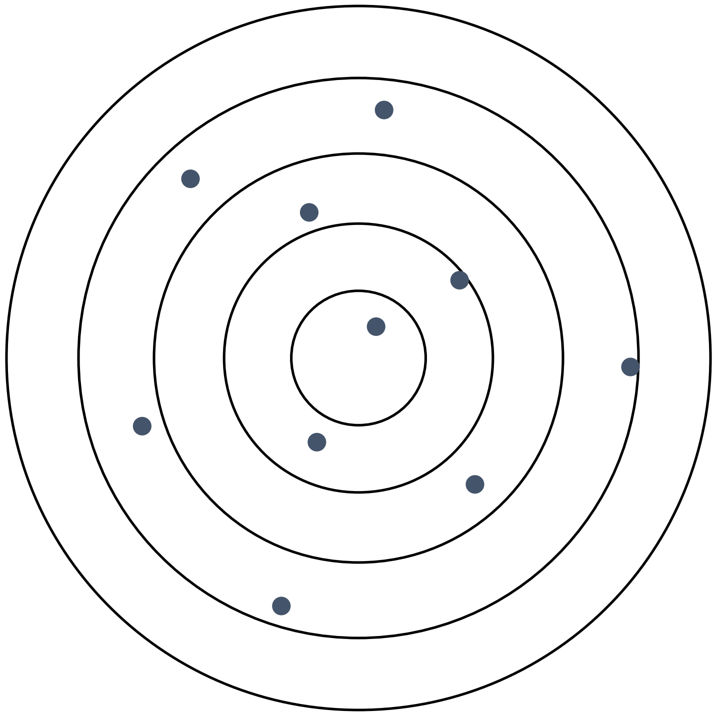
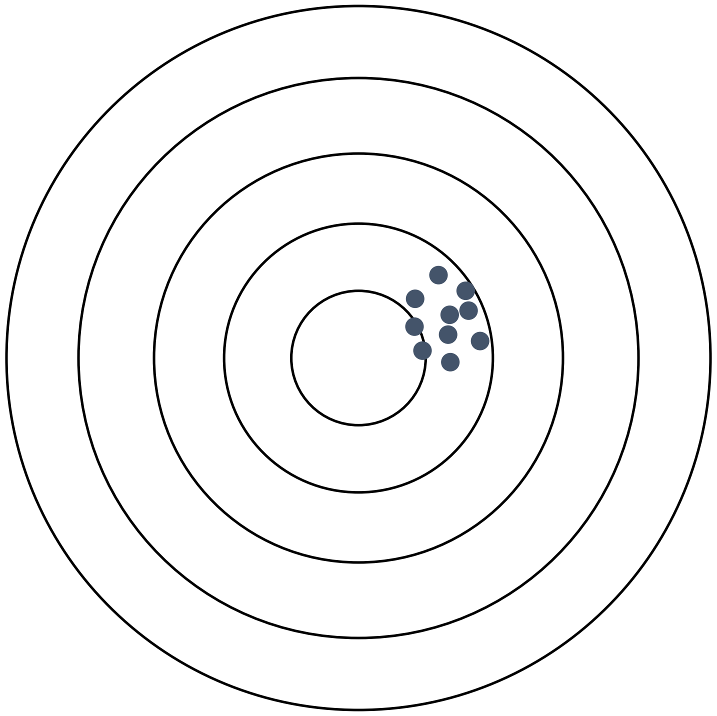


Biased but precise



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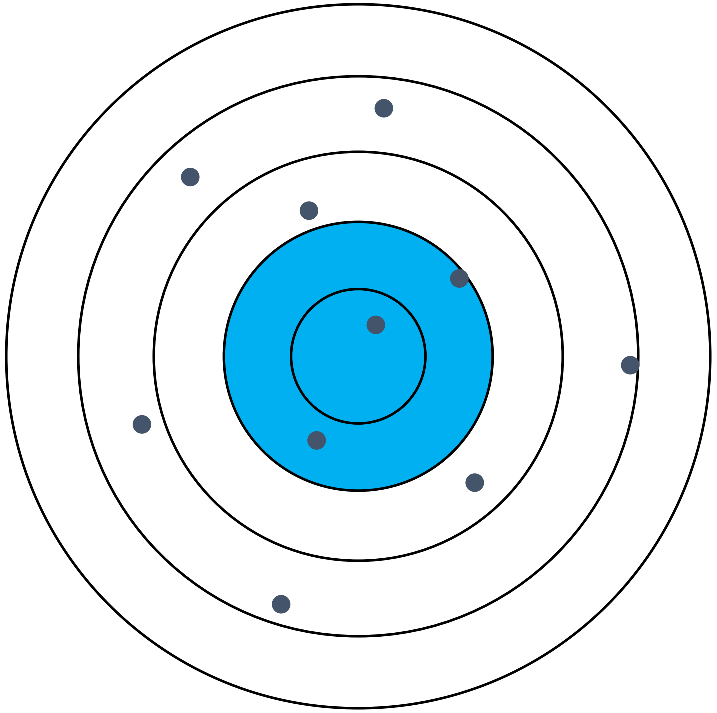
Unbiased but not precise



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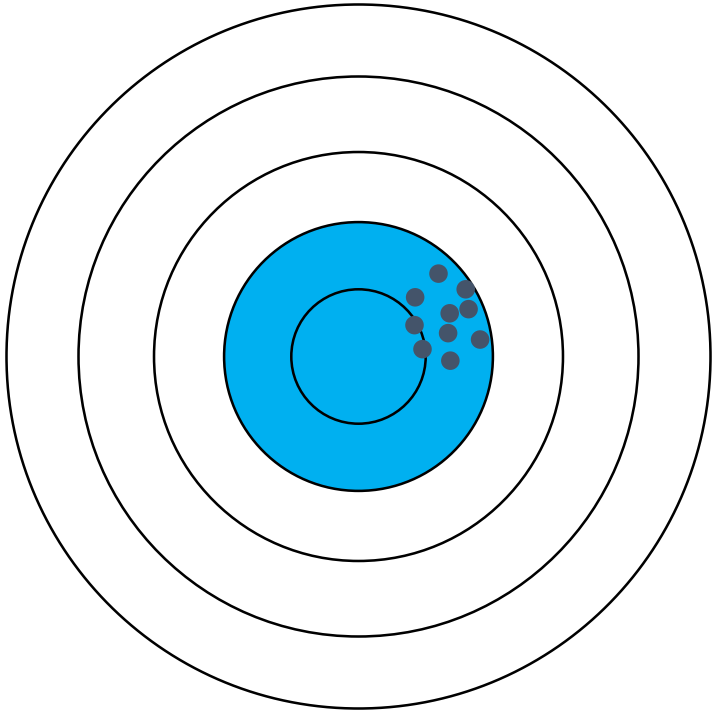

Regularized Regression

- **Regularized regression** (or penalized / shrinkage regression) puts constraints on the estimated coefficients in our model and *shrink* these estimates to 0.

- Coefficients become biased, but potentially improve variance of the model.

- 3 Common Approaches – Ridge, LASSO, Elastic Net

Penalties in Models

- OLS regression minimizes the sum of squared errors:

$$\min\left(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2\right) = \min(SSE)$$

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- Regularized regression introduces a penalty term to the minimization:

$$\min\left(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + Penalty\right) = \min(SSE + Penalty)$$

?

Regularized Regression

RIDGE REGRESSION

Penalties in Models

- Ridge regression introduces an “L_2” penalty term to the minimization:

$$\min\left(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda\sum_{j=1}^{p}\hat{\beta}_j^2\right) = \min\left(SSE + \lambda\sum_{j=1}^{p}\hat{\beta}_j^2\right)$$

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- Penalty is controlled by **tuning parameter**, λ.
  - If $\lambda = 0$, then OLS.
  - As $\lambda \to \infty$, coefficients shrink to 0.

Ridge Regression

```r
train_reg <- train %>%
              dplyr::select(Sale_Price, Lot_Area, Street,
                            Bldg_Type, House_Style, Overall_Qual,
                            Roof_Style, Central_Air, First_Flr_SF,
                            Second_Flr_SF, Full_Bath, Half_Bath,
                            Fireplaces, Garage_Area, Gr_Liv_Area,
                            TotRms_AbvGrd) %>%
              replace(is.na(.), 0)
train_x <- model.matrix(Sale_Price ~ ., data = train_reg)[, -1]
train_y <- train_reg$Sale_Price
```

Ridge Regression

```
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train_x <- model.matrix(Sale_Price ~ ., data = train_reg)[, -1]
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```

Ridge Regression

```
test_reg <- test %>%
              dplyr::select(Sale_Price, Lot_Area, Street,
                            Bldg_Type, House_Style, Overall_Qual,
                            Roof_Style, Central_Air, First_Flr_SF,
                            Second_Flr_SF, Full_Bath, Half_Bath,
                            Fireplaces, Garage_Area, Gr_Liv_Area,
                            TotRms_AbvGrd) %>%
              replace(is.na(.), 0)
test_x <- model.matrix(Sale_Price ~ ., data = test_reg)[, -1]
test_y <- test_reg$Sale_Price
```

Ridge Regression

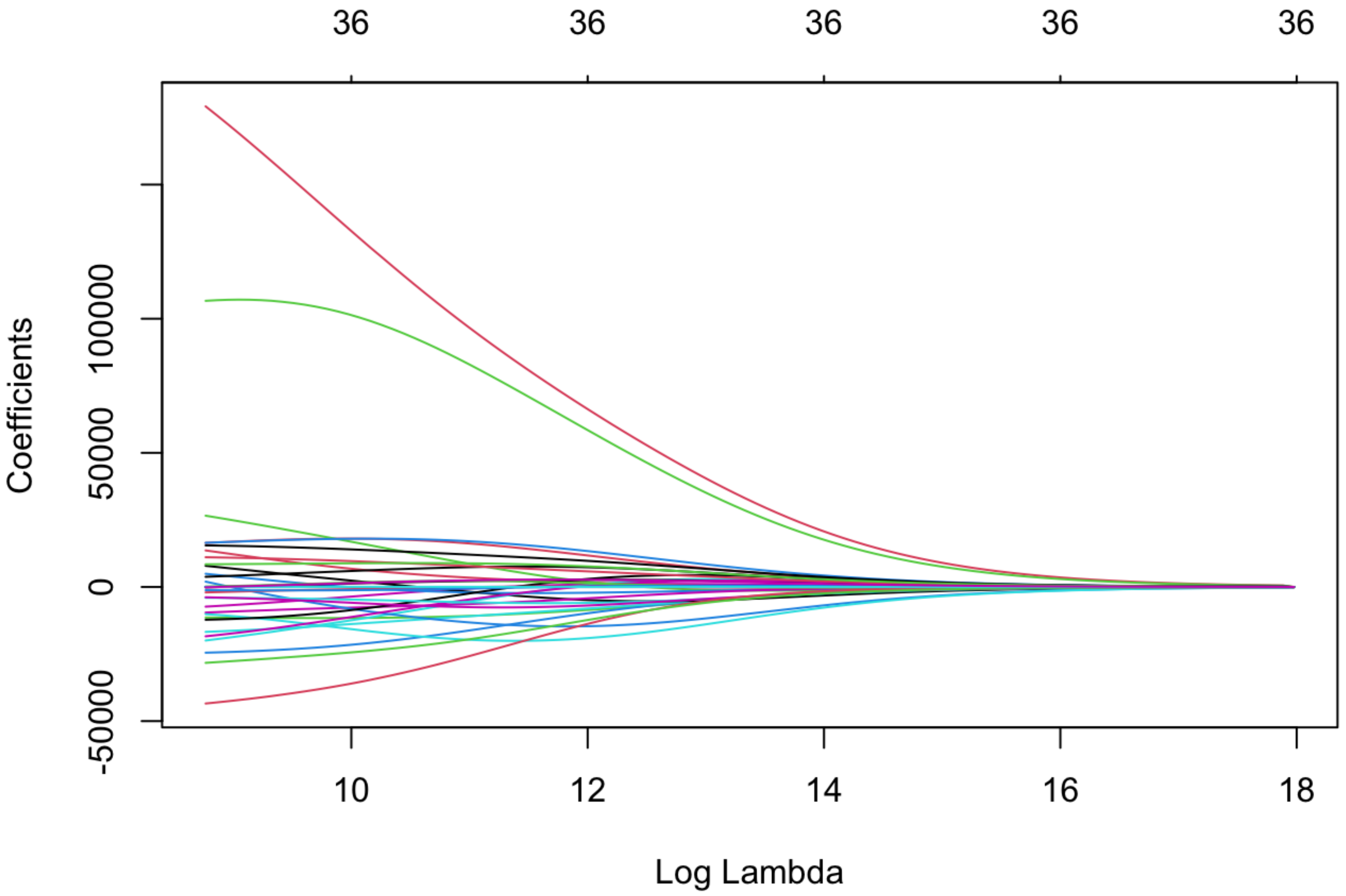
```r
library(glmnet)

ames_ridge <- glmnet(x = train_x, y = train_y, alpha = 0)

plot(ames_ridge, xvar = "lambda")
```

Ridge Regression

```
library(glmnet)
ames_ridge <- glmnet(x = train_x, y = train_y, alpha = 0)
plot(ames_ridge, xvar = "lambda")
```

Option to use ridge penalty

Ridge Regression



Regularized Regression

LASSO REGRESSION

Penalties in Models

- Least absolute shrinkage and selection operator (LASSO) regression introduces an "L_1" penalty term to the minimization:

$$\min\left(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{p} |\hat{\beta}_j|\right) = \min\left(SSE + \lambda \sum_{j=1}^{p} |\hat{\beta}_j|\right)$$

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- Penalty is controlled by **tuning parameter**, λ.
  - If $\lambda = 0$, then OLS.
  - As $\lambda \to \infty$, coefficients shrink to 0.

Differences in Effects

- Penalty is controlled by **tuning parameter**, λ.
  - If $\lambda = 0$, then OLS.
  - As $\lambda \to \infty$, coefficients shrink to 0.

Ridge regression approaches 0 asymptotically.

LASSO can have coefficients equal to 0
(variable removed from model).

Differences in Effects

- Penalty is controlled by **tuning parameter**, λ.
  - If $\lambda = 0$, then OLS.
  - As $\lambda \to \infty$, coefficients shrink to 0.

Differences in effects are due to differences in penalty.

When solving the system of equations for the different penalties we get the following:

$$\hat{\beta}_{OLS} = \left(X^T X\right)^{-1} X^T Y \qquad \hat{\beta}_R = \left(X^T X + \lambda I\right)^{-1} X^T Y \qquad \hat{\beta}_L = \left(X^T X\right)^{-1} \left(X^T Y - \lambda I\right)$$

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As $\lambda \to \infty$, $\hat{\beta}_R$ gets infinitely close to 0

Differences in Effects

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  - If $\lambda = 0$, then OLS.
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If $\lambda = X^T Y$, $\hat{\beta}_L$ can actually equal 0

LASSO Regression

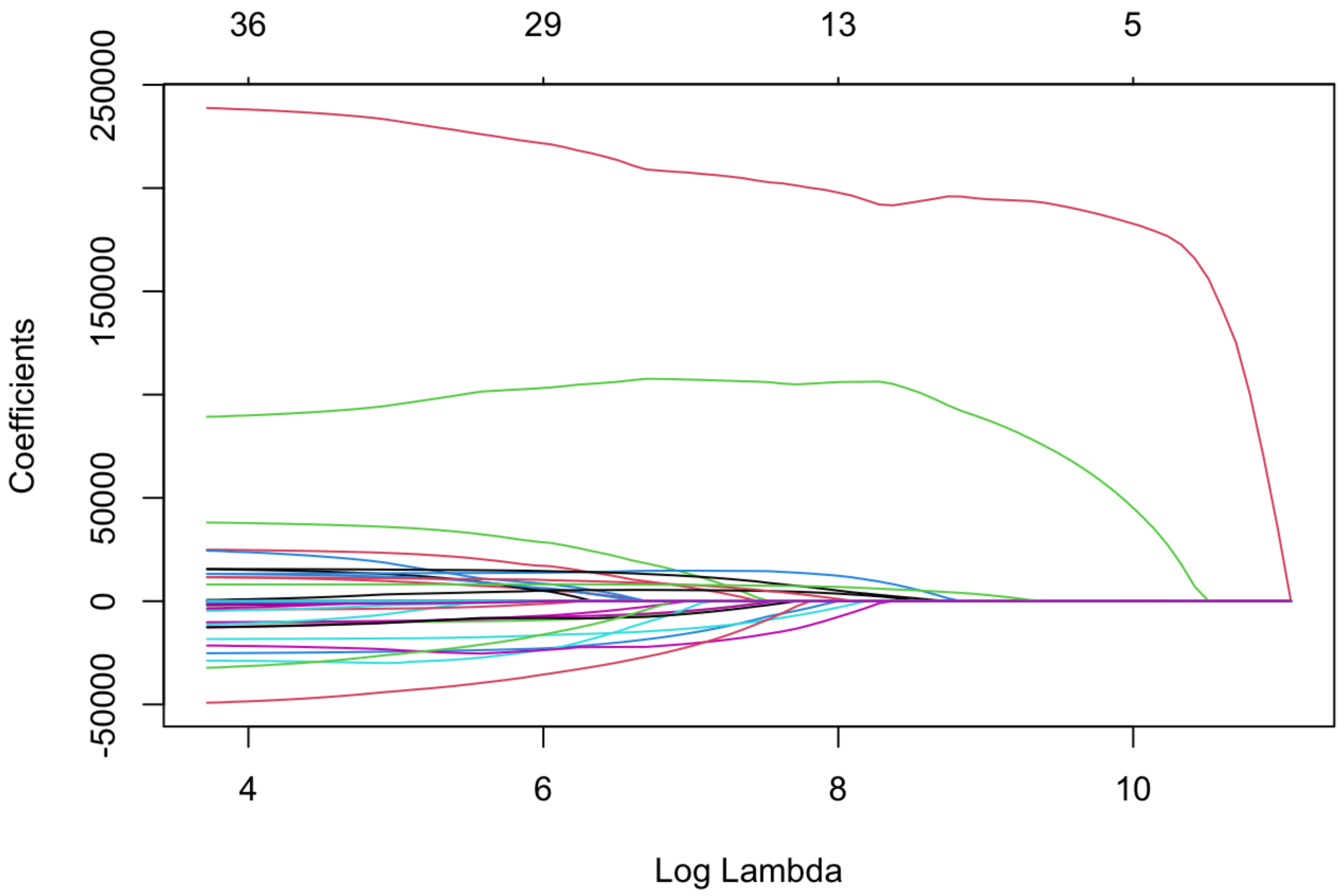
```
library(glmnet)
ames_lasso <- glmnet(x = train_x, y = train_y, alpha = 1)
plot(ames_lasso, xvar = "lambda")
```

LASSO Regression

```r
library(glmnet)
ames_lasso <- glmnet(x = train_x, y = train_y, alpha = 1)
plot(ames_lasso, xvar = "lambda")
```

Option to use LASSO penalty

LASSO Regression



Regularized Regression

ELASTIC NET REGRESSION

Penalties in Models

- Both ridge and LASSO have advantages and disadvantages.
  - LASSO does variable selection.
  - Ridge keeps all variables (LASSO drops arbitrarily)

- Elastic net regression combines both penalty terms in the minimization:

$$\min\left(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda_1 \sum_{j=1}^{p}|\hat{\beta}_j| + \lambda_2 \sum_{j=1}^{p}\hat{\beta}_j^2\right)$$

Penalties in Models

- The `glmnet` function in R takes slightly different approach:

$$\min\left(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda\left[\alpha\sum_{j=1}^{p}\left|\hat{\beta}_j\right| + (1-\alpha)\sum_{j=1}^{p}\hat{\beta}_j^2\right]\right)$$

Penalties in Models

- The `glmnet` function in R takes slightly different approach:

$$\min\left(\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 + \lambda\left[\alpha\sum_{j=1}^{p}\left|\hat{\beta}_j\right| + (1-\alpha)\sum_{j=1}^{p}\hat{\beta}_j^2\right]\right)$$

Why R has the "`alpha = `" option.

- Any value of `alpha` between 0 and 1 gives a combination of both penalties (elastic net).

Elastic Net Regression

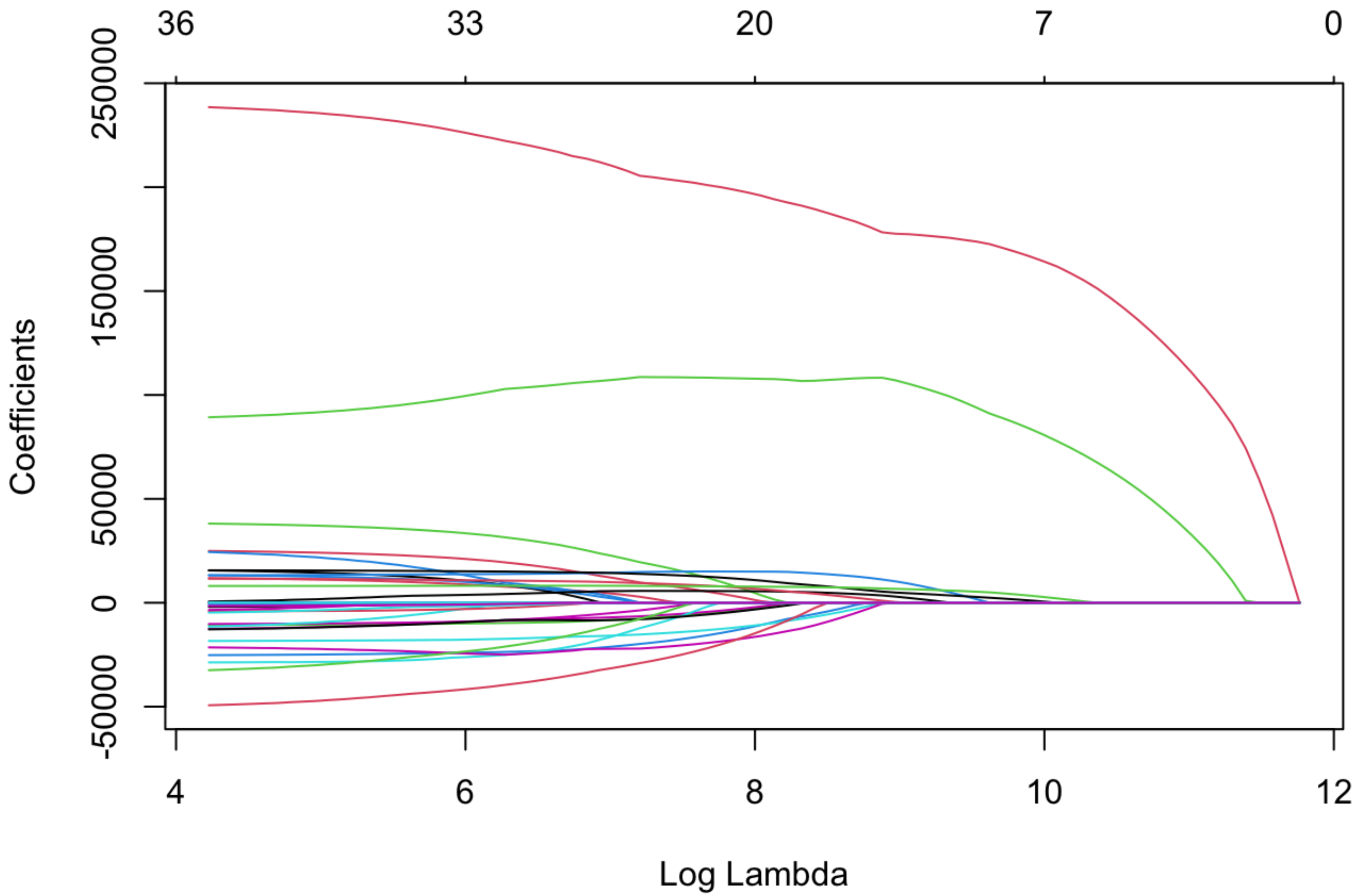
```r
library(glmnet)
ames_en <- glmnet(x = train_x, y = train_y, alpha = 0.5)
plot(ames_en, xvar = "lambda")
```

Elastic Net Regression

```
library(glmnet)
ames_en <- glmnet(x = train_x, y = train_y, alpha = 0.5)
plot(ames_en, xvar = "lambda")
```

Use elastic net since value between 0 and 1.

Elastic Net Regression



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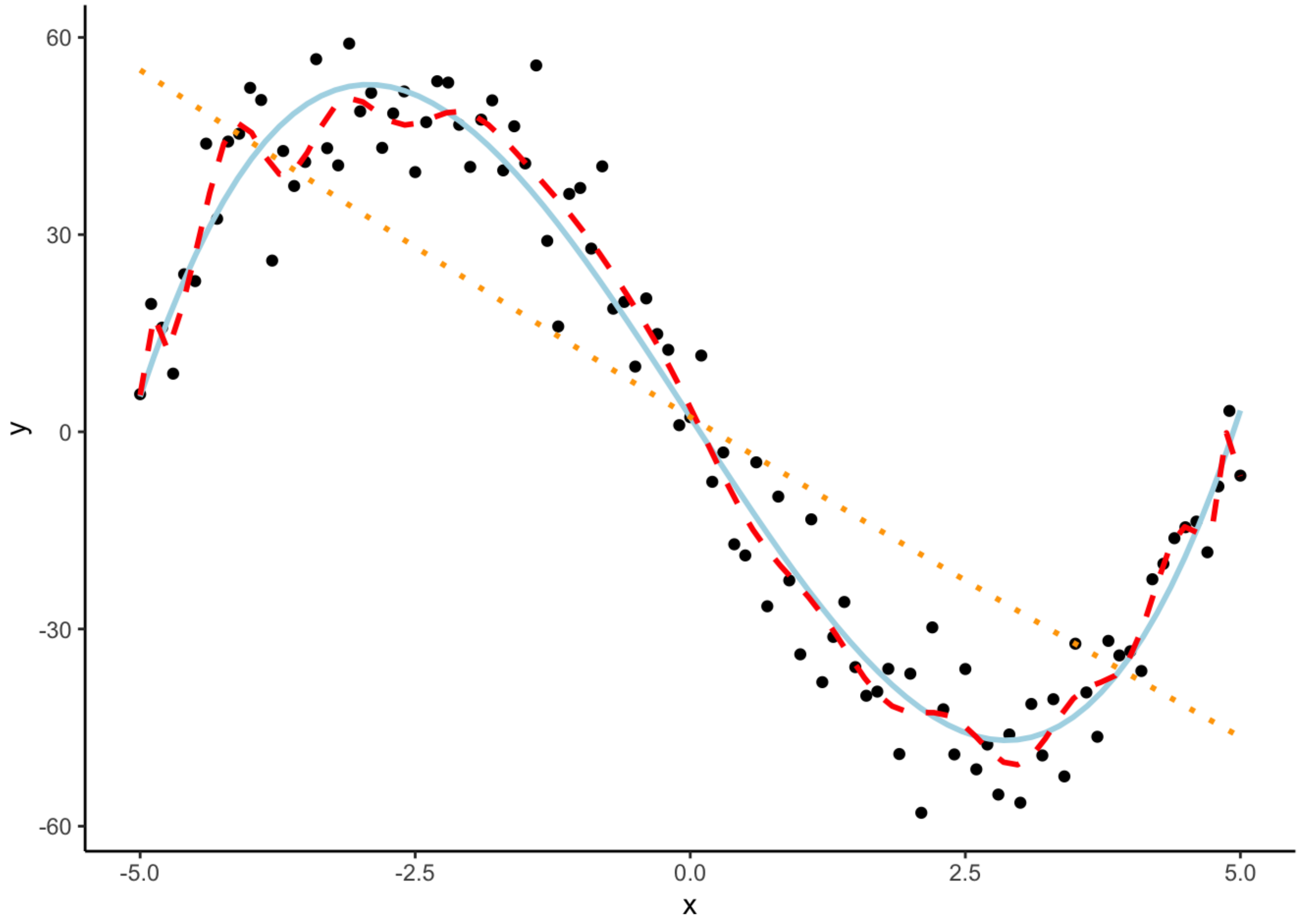
Optimizing Penalties

Fear of Overfitting

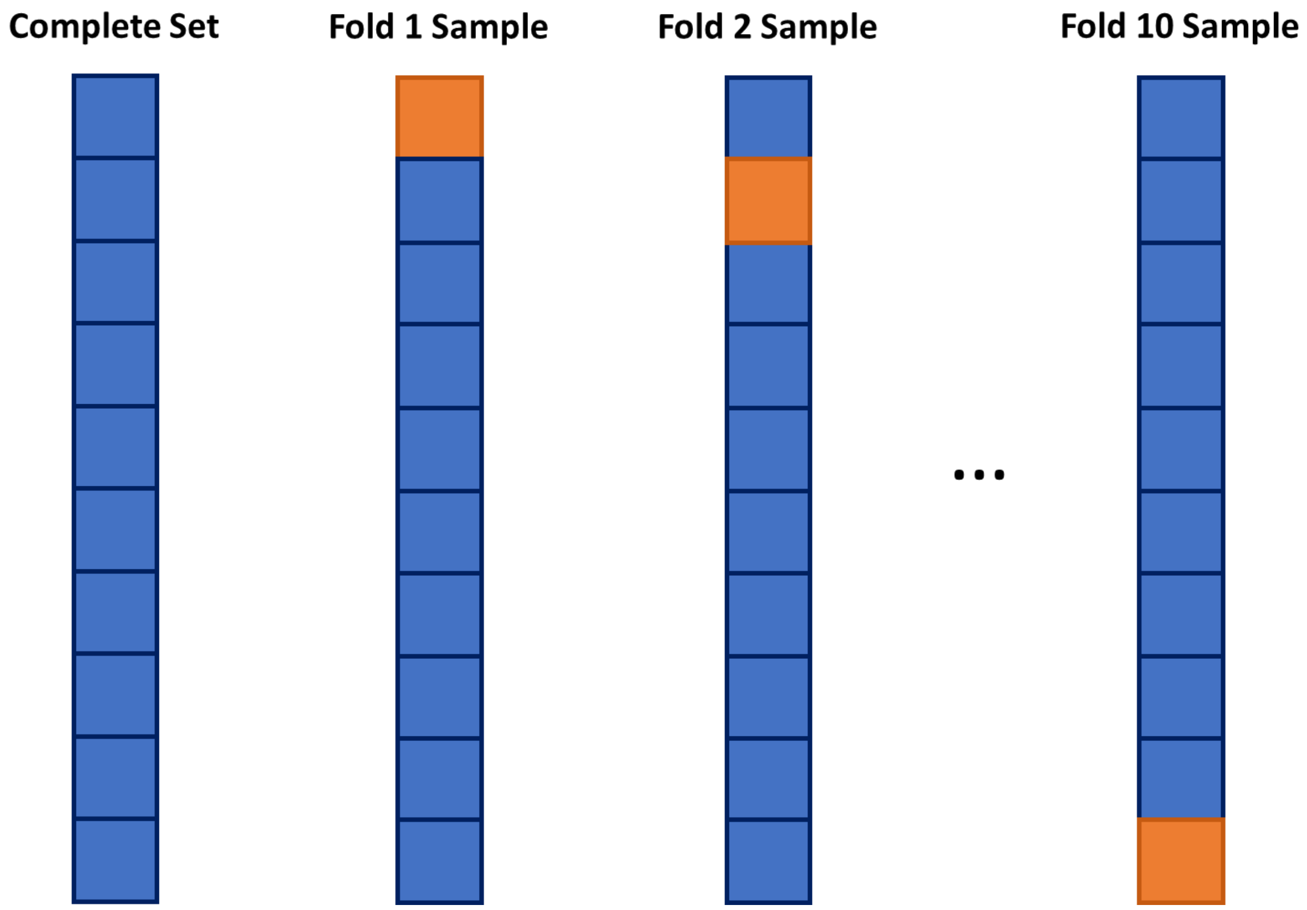
- Need to select λ for any of the regularized regression approaches.
- Don't want to minimize variance to the point of overfitting our model to the training data.



Cross-Validation

- **Cross-validation** (CV) is common approach to prevent overfitting when tuning a parameter.
- Concept:
  - Split training data into multiple pieces
  - Build model on majority of pieces
  - Evaluate on remaining piece
  - Repeat process with switching out pieces for building and evaluation

k-fold Cross-Validation

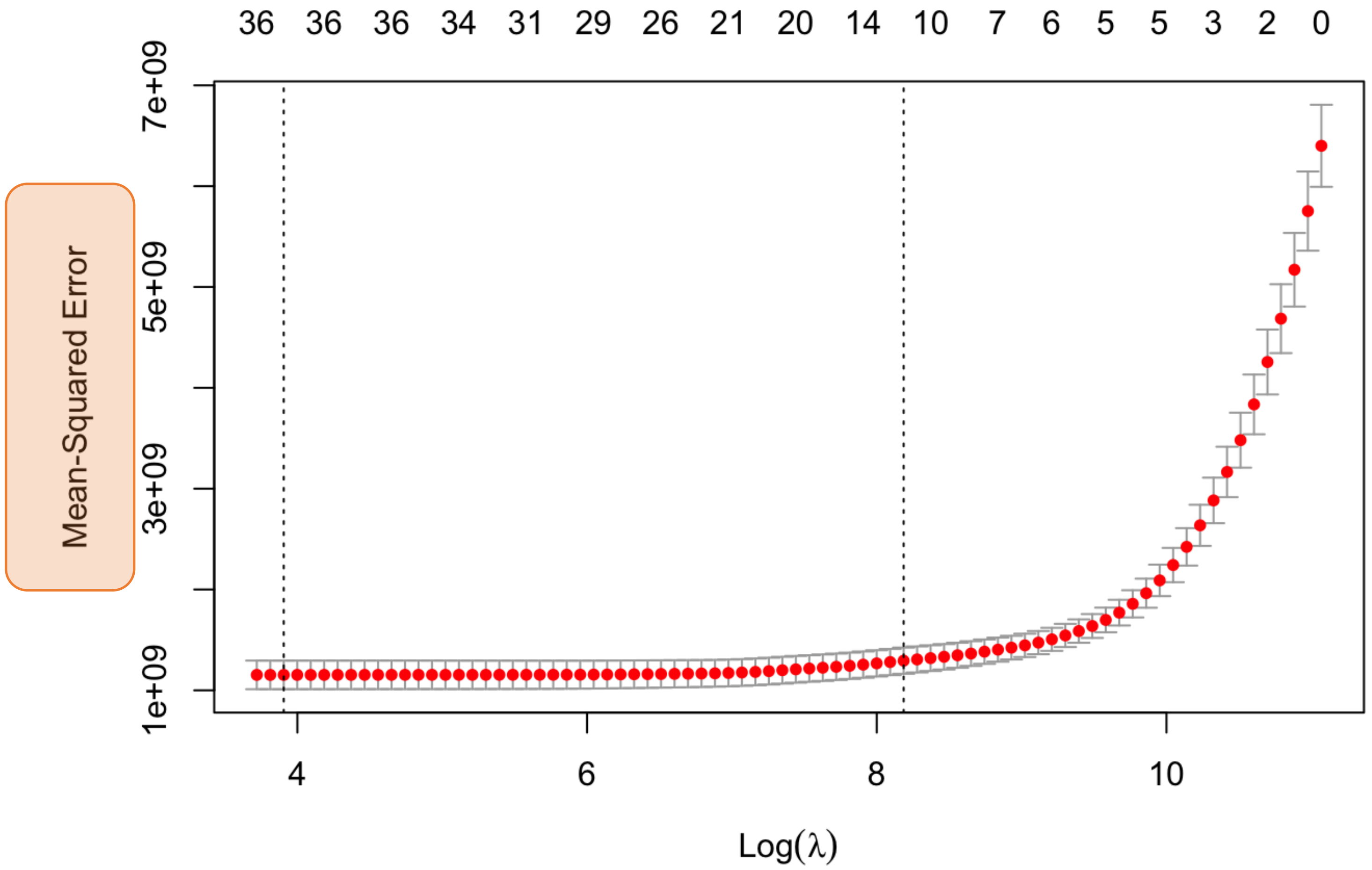


LASSO Regression

```
ames_lasso_cv <- cv.glmnet(x = train_x, y = train_y, alpha = 1)
plot(ames_lasso_cv)
```

LASSO Regression

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$



LASSO Regression

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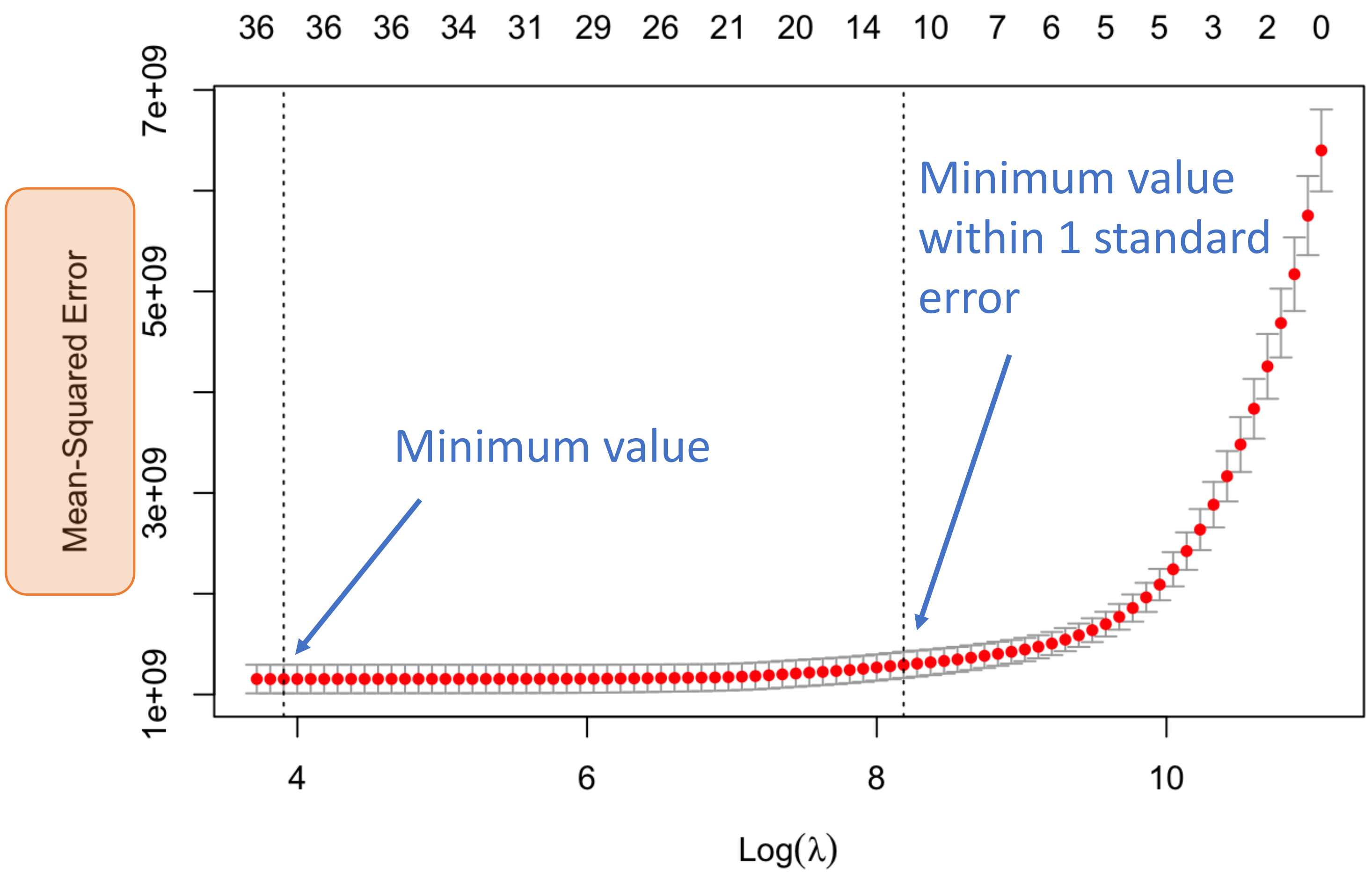
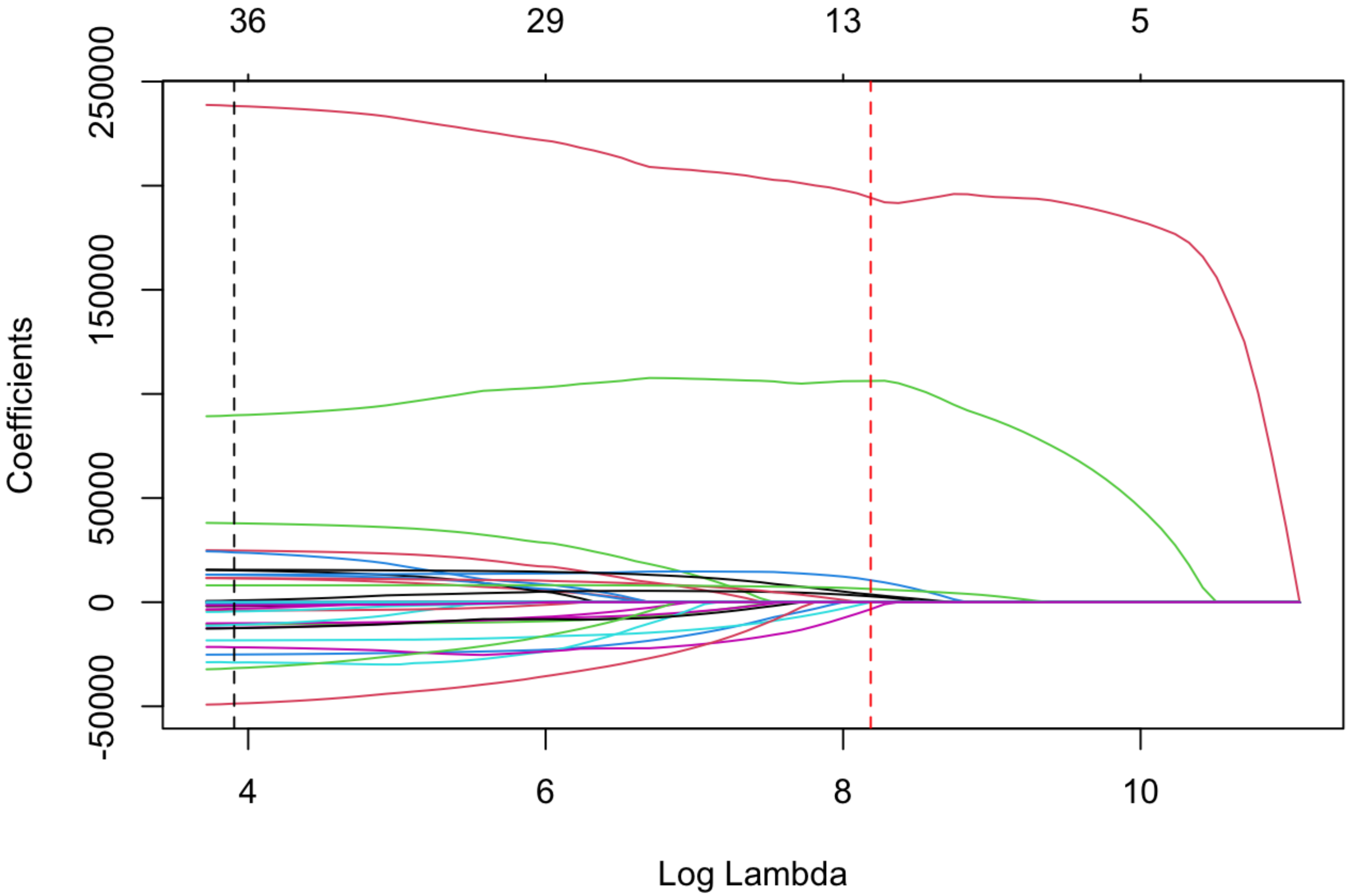


LASSO Regression

```
plot(ames_lasso, xvar = "lambda")
abline(v = log(ames_lasso_cv$lambda.1se), col = "red", lty = "dashed")
abline(v = log(ames_lasso_cv$lambda.min), col = "black", lty = "dashed")
```

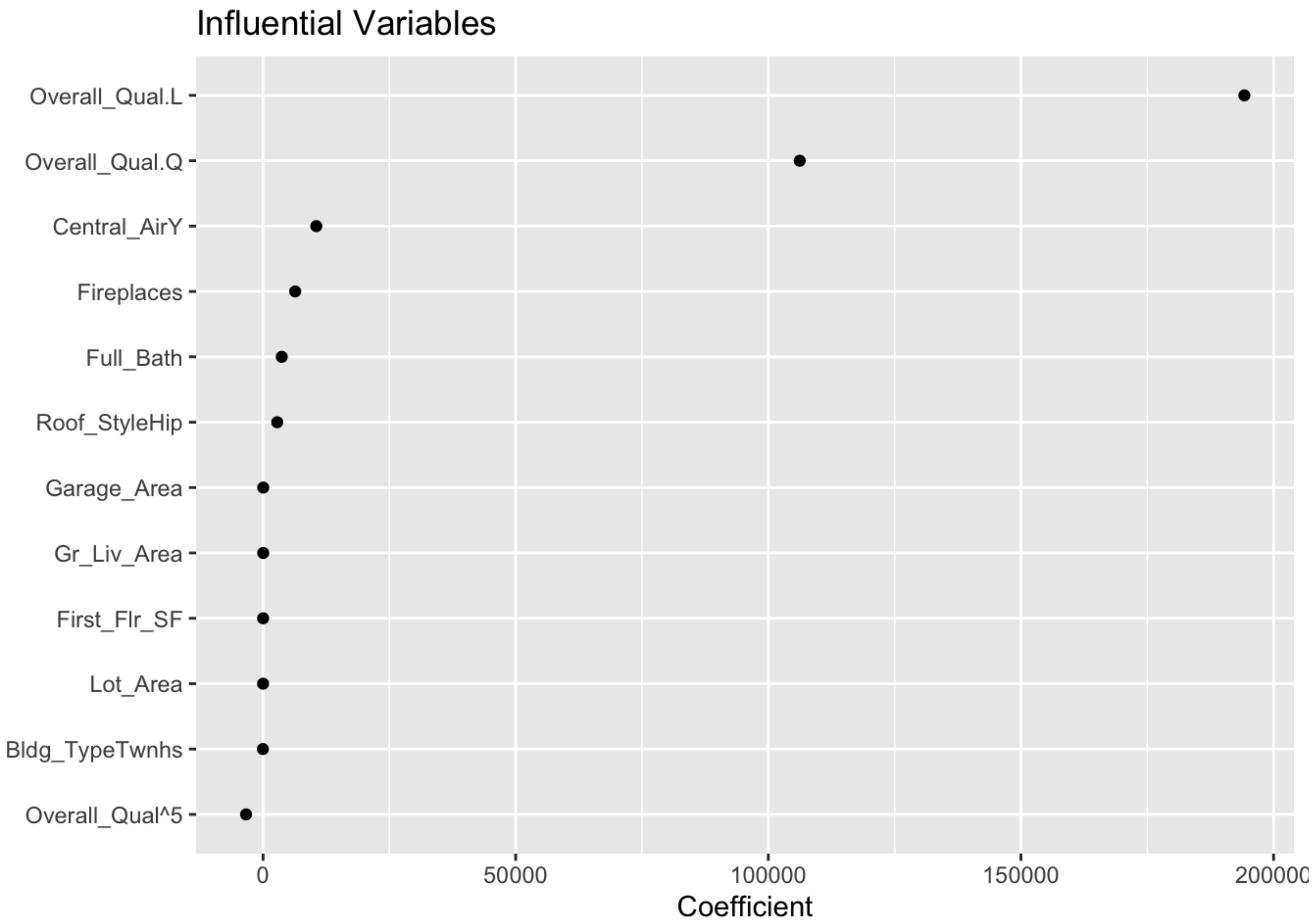
LASSO Regression



Important Variables

```r
coef(ames_lasso, s = ames_lasso_cv$lambda.1se) %>%
  broom::tidy() %>%
  filter(row != "(Intercept)") %>%
  ggplot(aes(value, reorder(row, value))) +
    geom_point() +
    ggtitle("Influential Variables") +
    xlab("Coefficient") +
    ylab(NULL)
```

Important Variables



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Model Comparisons

Comparing Models

- The model results in a formula or rules.
- The data require modifications:
  - Derived inputs
  - Transformations
  - Missing value imputation

- To score/compare, you **do not rerun the algorithm**!
- Apply score code (equations) obtained from the final model to the test data for comparing.

Comparing Models

- Test dataset is for comparing final models and reporting final metrics.
- **DO NOT GO BACK AFTER TO REBUILD MODEL!**
- **DO NOT JUST BUILD 1000's OF MODELS TO COMPARE IN THE TEST SET!**
- We do not want to fit to the test dataset as it is our honest assessment of how good our models can do.

Model Metrics

- Root MSE (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

- Mean Absolute Error (MAE):

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

- Mean Absolute Percentage Error (MAPE):

$$MAPE = 100 \times \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$$

Model Metrics

- Root MSE (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Problems:

- Not easily interpretable

- Mean Absolute Error (MAE):

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

Problems:

- Not scale invariant

- Mean Absolute Percentage Error (MAPE):

$$MAPE = 100 \times \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$$

Problems:

- Not symmetric

Predictions

```r
test$pred_lm <- predict(ames_lm, newdata = test)
head(test$pred_lm)
```

```
##        1        2        3        4        5        6
## 142107.3 142107.3 228909.6 142107.3 142107.3 142107.3
```

```r
test_reg$pred_lasso <- predict(ames_lasso, s = ames_lasso_cv$lambda.1se, newx = test_x)
head(test_reg$pred_lasso)
```

```
##        1        2        3        4        5        6
## 156677.8 172432.5 239922.1 105713.6 200908.8 124913.5
```

Predictions – MAPE

```
test %>%
  mutate(lm_APE = 100*abs((Sale_Price - pred_lm)/Sale_Price)) %>%
  dplyr::summarise(MAPE_lm = mean(lm_APE))
```

```
##   MAPE_lm
##     <dbl>
## 1    23.2
```

```
test_reg %>%
  mutate(lasso_APE = 100*abs((Sale_Price - pred_lasso)/Sale_Price)) %>%
  dplyr::summarise(MAPE_lasso = mean(lasso_APE))
```

```
##   MAPE_lasso
##        <dbl>
## 1       13.4
```

?