RESAMPLING, MODEL SELECTION, & REGULARIZATION

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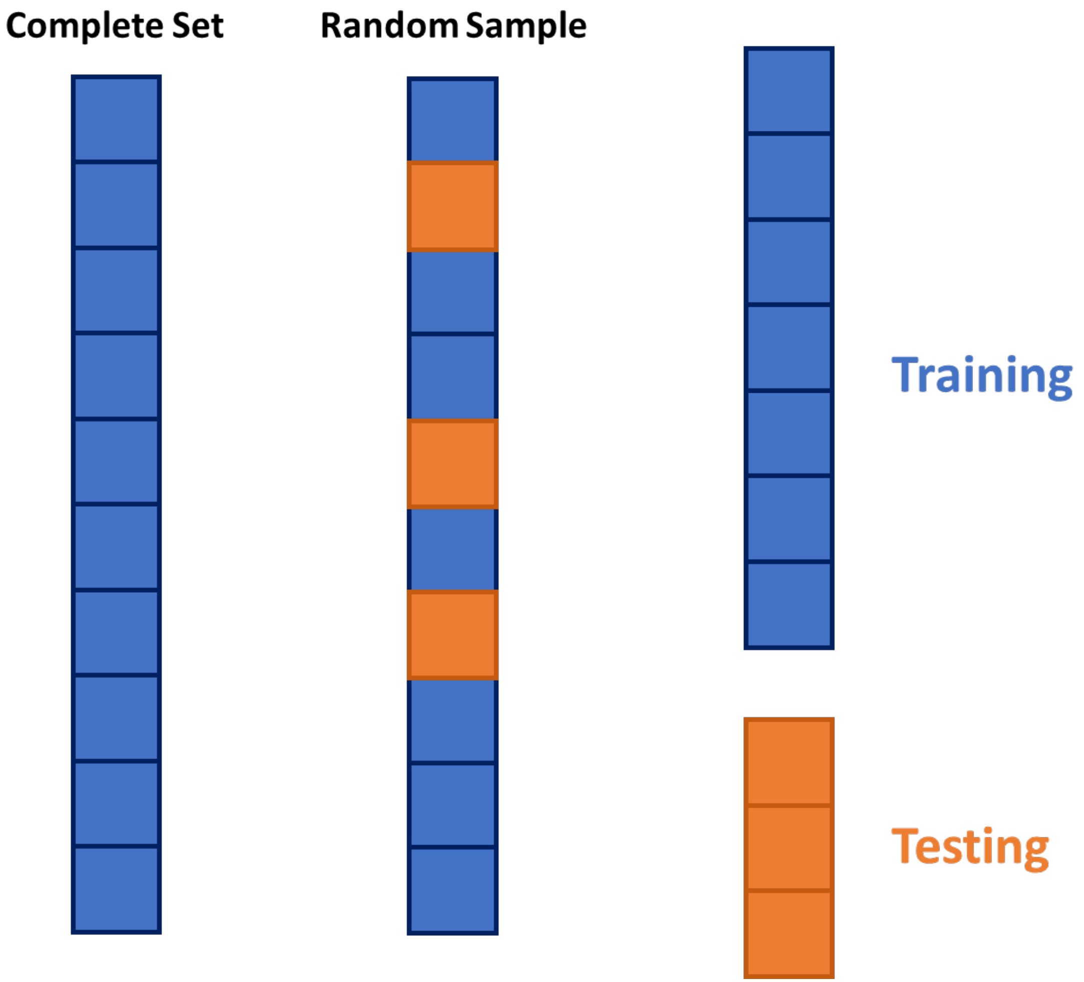
Institute for Advanced Analytics

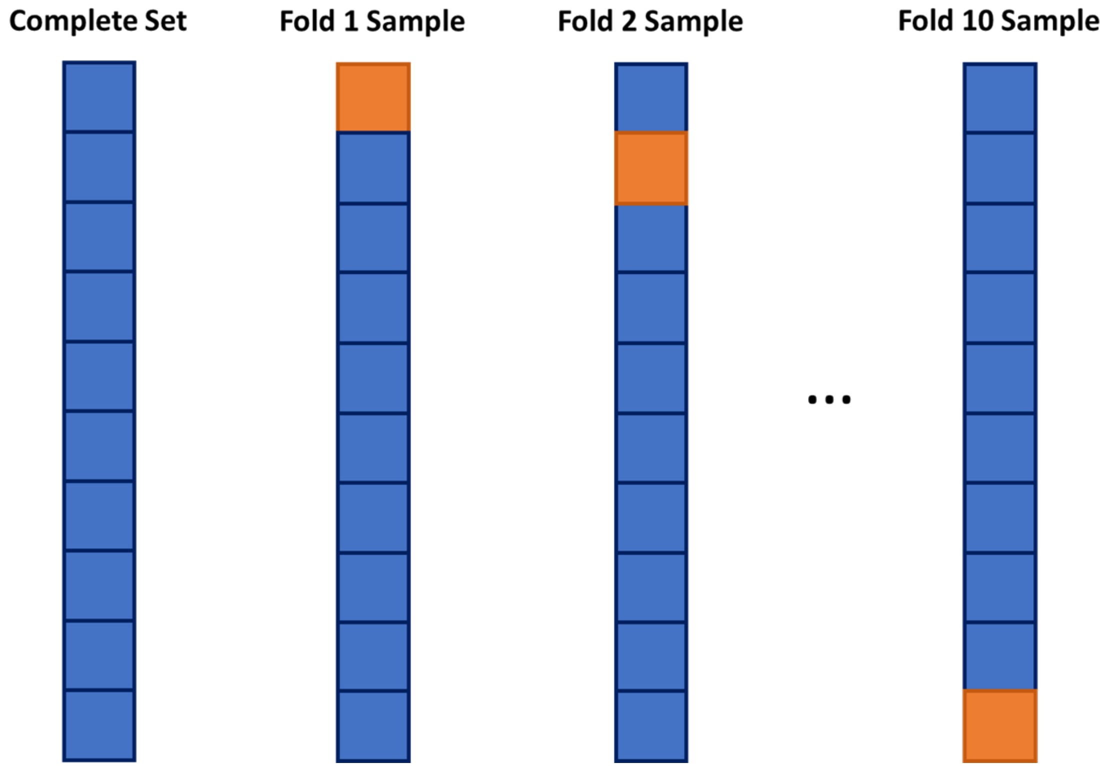
RESAMPLING REVISITED

Training, Validation, Testing



- Split your data into two or three sections of data
  - Training
  - Validation
  - Testing
- Common percentages:
  - 60-20-20
  - 70-20-10
  - 40-40-20
  - Etc.

Cross-Validation



- Divide your data into k-equally sized groups (folds, samples, etc.)
- Model evaluation
  - Average goodness-of-fit across all folds.
- Parameter/Model tuning

Ames Real Estate Data

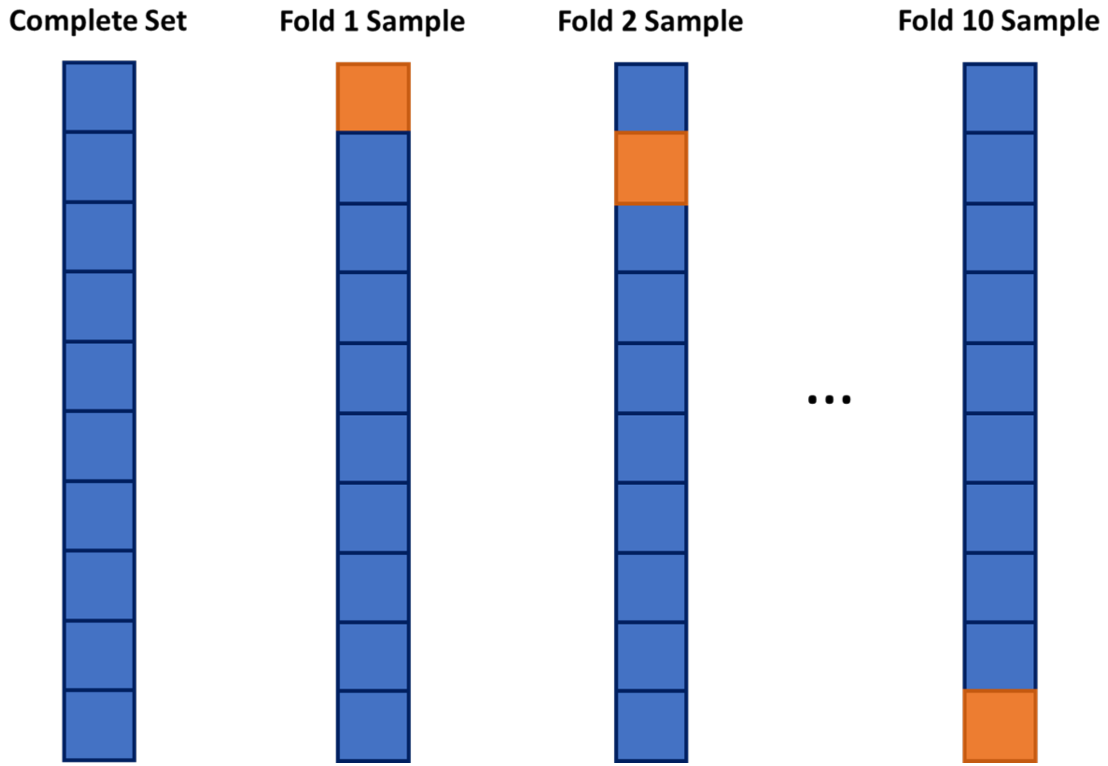
- 2930 homes in Ames, Iowa in the early 2000's.
- Physical attributes of homes along with sales price of home.

Training and Testing Split (No Validation Yet…)

```
ames <- make_ordinal_ames()

ames <- ames %>% mutate(id = row_number())

set.seed(4321)

training <- ames %>% sample_frac(0.7)
testing <- anti_join(ames, training, by = 'id')

training <- training %>%
  select(Sale_Price, Bedroom_AbvGr, Year_Built, Mo_Sold, Lot_Area,
         Street, Central_Air, First_Flr_SF, Second_Flr_SF, Full_Bath,
         Half_Bath, Fireplaces, Garage_Area, Gr_Liv_Area, TotRms_AbvGrd)
```

MODEL SELECTION

Cross-Validation



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Variable Selection in Linear Models

- Linear models contains many different models (linear, logistic, etc.).
- **ALWAYS** start by narrowing a list of reasonable predictor variables through exploratory analysis.

- Explanation/Inference:
  - Forward, Backward, Stepwise

- Prediction:
  - LASSO, Ridge, Elastic Net
  - Potentially provides better predictive models, but at the cost of lack of interpretability

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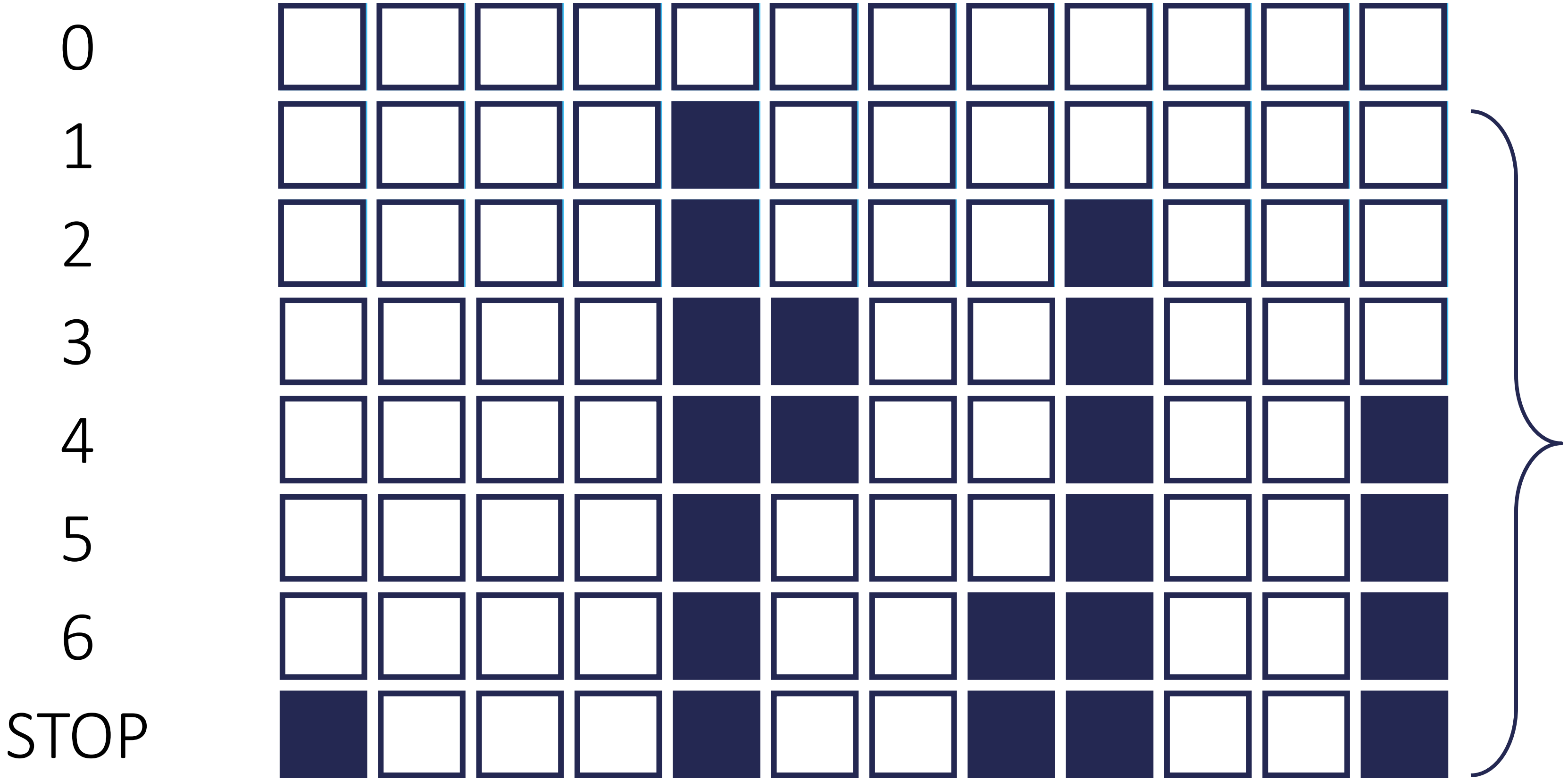
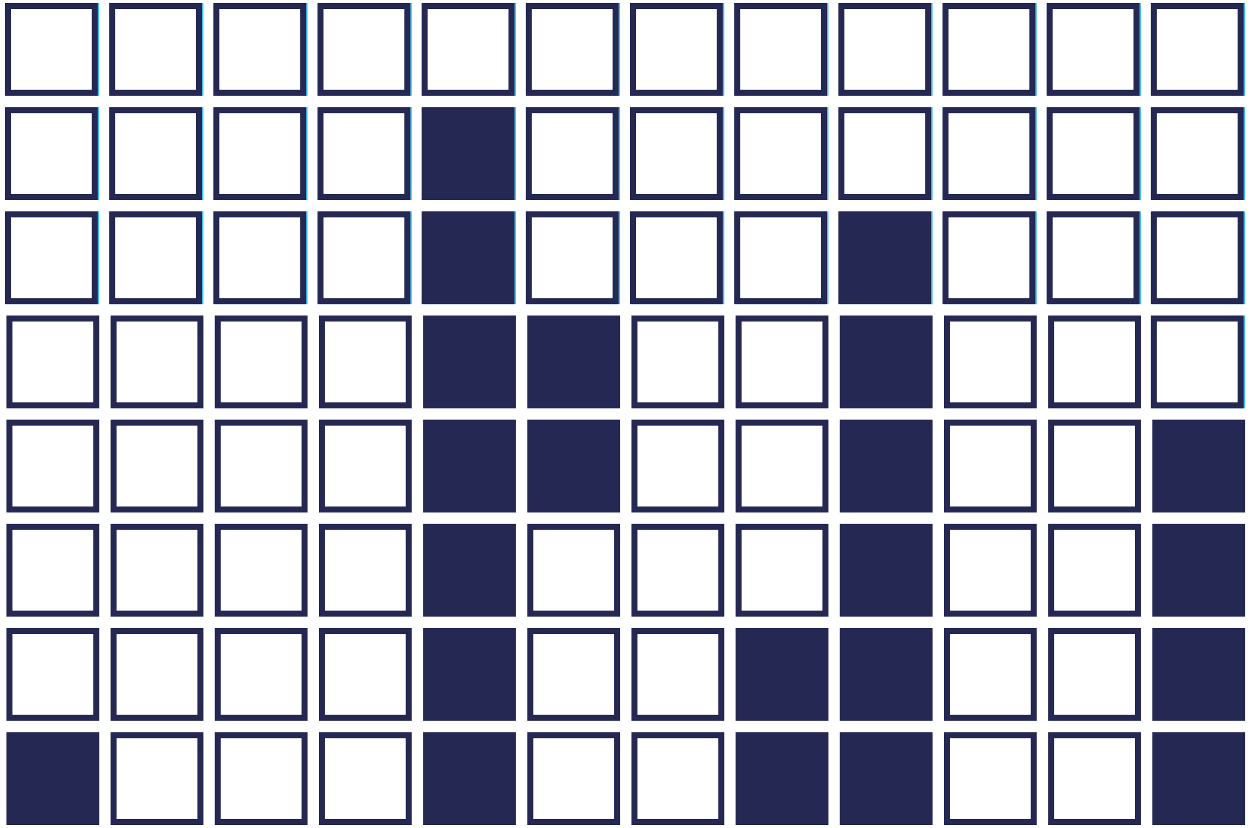
Stepwise Selection through Validation Set



Look at **validation** instead of training for each step. Which is better in **validation set**?

Stepwise Selection through Cross-Validation

0
1
2
3
4
5
6
STOP



Look at **validation** instead of training for each step. Which is better in avg. MSE in **cross-validation**?

Stepwise Selection through Cross-Validation

```
set.seed(9876)

step.model <- train(Sale_Price ~ ., data = training,
                    method = "leapBackward",
                    tuneGrid = data.frame(nvmax = 1:14),
                    trControl = trainControl(method = 'cv', number = 10))
```

From caret package (similar to scikit learn in Python)

Stepwise Selection through Cross-Validation

```
set.seed(9876)

step.model <- train(Sale_Price ~ ., data = training,
                    method = "leapBackward",
                    tuneGrid = data.frame(nvmax = 1:14),
                    trControl = trainControl(method = 'cv', number = 10))
```

Cross validation – 10 fold

2 Views of Parameter Tuning

Classical View

- Use validation to evaluate which model is “best” at each step of the procedure.
- Final model contains variables remaining at end of procedure.
- Example: Age, Income, Credit Score

”Modern” View

- Use validation to evaluate which model is “best” at each step of the procedure.
- Final model contains **same number of variables** as model at end of procedure.
- Example: 3 variable model

2 Views of Parameter Tuning

Classical View

- Combine training and validation.
- Update parameter estimates on the chosen variables (ex: Age, Income, Credit Score).

”Modern” View

- Combine training and validation.
- Do not restrict yourself to any variable, just the number of variables (ex: find best 3 variable model).

Stepwise Selection through Cross-Validation

```
step.model$results
```

```
##    nvmax     RMSE  Rsquared      MAE   RMSESD RsquaredSD    MAESD
## 1      1 61611.97 0.3942384 45180.98 5472.666 0.05620948 2526.312
## 2      2 49940.14 0.6074530 34262.71 7925.632 0.09929920 3450.872
## 3      3 42271.12 0.7153532 28108.76 7112.714 0.07760796 2655.431
## 4      4 41519.38 0.7274272 27291.26 7807.909 0.08250703 2626.796
## 5      5 39709.65 0.7505967 26396.47 7761.820 0.08026905 2621.732
## 6      6 39293.66 0.7556266 26266.02 7486.423 0.07609118 2547.016
## 7      7 39403.58 0.7542579 26256.86 7471.045 0.07604703 2553.544
## 8      8 39436.99 0.7538030 26265.14 7447.858 0.07528998 2562.365
## 9      9 39547.27 0.7525961 26324.07 7624.466 0.07703777 2651.493
## 10    10 39466.09 0.7536853 26281.15 7644.350 0.07719334 2660.940
## 11    11 39395.64 0.7546030 26253.80 7674.807 0.07729593 2706.320
## 12    12 39344.06 0.7552931 26195.33 7685.764 0.07737416 2753.871
## 13    13 39340.86 0.7553046 26182.74 7675.699 0.07725826 2737.195
## 14    14 39347.25 0.7553214 26190.40 7671.560 0.07724606 2724.610
```

```
step.model$bestTune
```

```
##   nvmax
## 6     6
```

Stepwise Selection through Cross-Validation

```
summary(step.model$finalModel)
```

```
## 1 subsets of each size up to 6
## Selection Algorithm: backward
##          Bedroom_AbvGr Year_Built Mo_Sold Lot_Area StreetPave Central_AirY
## 1  ( 1 ) " "           " "        " "     " "      " "        " "
## 2  ( 1 ) " "           " "        " "     " "      " "        " "
## 3  ( 1 ) " "           "*"        " "     " "      " "        " "
## 4  ( 1 ) " "           "*"        " "     " "      " "        " "
## 5  ( 1 ) "*"           "*"        " "     " "      " "        " "
## 6  ( 1 ) "*"           "*"        " "     " "      " "        " "
##          First_Flr_SF Second_Flr_SF Full_Bath Half_Bath Fireplaces Garage_Area
## 1  ( 1 ) "*"          " "           " "       " "       " "        " "
## 2  ( 1 ) "*"          "*"           " "       " "       " "        " "
## 3  ( 1 ) "*"          "*"           " "       " "       " "        " "
## 4  ( 1 ) "*"          "*"           " "       " "       " "        "*"
## 5  ( 1 ) "*"          "*"           " "       " "       " "        "*"
## 6  ( 1 ) "*"          "*"           " "       " "       "*"        "*"
##          Gr_Liv_Area TotRms_AbvGrd
## 1  ( 1 ) " "         " "
## 2  ( 1 ) " "         " "
## 3  ( 1 ) " "         " "
## 4  ( 1 ) " "         " "
## 5  ( 1 ) " "         " "
## 6  ( 1 ) " "         " "
```

"Classical" View of Parameter Tuning

```
final.model1 <- glm(Sale_Price ~ First_Flr_SF + Second_Flr_SF + Year_Built + Garage_Area +
                                  Bedroom_AbvGr + Fireplaces,
                    data = training)

summary(final.model1)


## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)   -1.407e+06  6.439e+04 -21.852  < 2e-16 ***
## First_Flr_SF   1.128e+02  3.236e+00  34.871  < 2e-16 ***
## Second_Flr_SF  8.252e+01  2.812e+00  29.342  < 2e-16 ***
## Year_Built     7.256e+02  3.306e+01  21.945  < 2e-16 ***
## Garage_Area    6.012e+01  5.366e+00  11.203  < 2e-16 ***
## Bedroom_AbvGr -1.265e+04  1.317e+03  -9.607  < 2e-16 ***
## Fireplaces     1.113e+04  1.555e+03   7.157 1.14e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## AIC: 49246
```

“Modern” View of Parameter Tuning

```
empty.model <- glm(Sale_Price ~ 1, data = training)
full.model <- glm(Sale_Price ~ ., data = training)

final.model2 <- step(empty.model, scope = list(lower = formula(empty.model),
                                               upper = formula(full.model)),
                     direction = "both", steps = 6)


summary(final.model2)
```

```
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)    -1.441e+06  6.451e+04 -22.343  < 2e-16 ***
## Gr_Liv_Area     8.116e+01  2.790e+00  29.086  < 2e-16 ***
## Year_Built      7.433e+02  3.313e+01  22.438  < 2e-16 ***
## First_Flr_SF    3.053e+01  2.944e+00  10.370  < 2e-16 ***
## Garage_Area     6.110e+01  5.373e+00  11.372  < 2e-16 ***
## Bedroom_AbvGr  -1.258e+04  1.322e+03  -9.518  < 2e-16 ***
## Fireplaces      1.138e+04  1.558e+03   7.305 3.95e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ‘ 1
##
## AIC: 49257
```

"Modern" View of Parameter Tuning

```
empty.model <- glm(Sale_Price ~ 1, data = training)
full.model <- glm(Sale_Price ~ ., data = training)

final.model2 <- step(empty.model, scope = list(lower = formula(empty.model),
                                               upper = formula(full.model)),
                     direction = "both", steps = 6)


summary(final.model2)
```

```
## Coefficients:
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## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
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```

Different 6 variables!

?

REGULARIZATION

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- Explanation/Inference:
  - Forward, Backward, Stepwise

- Prediction:
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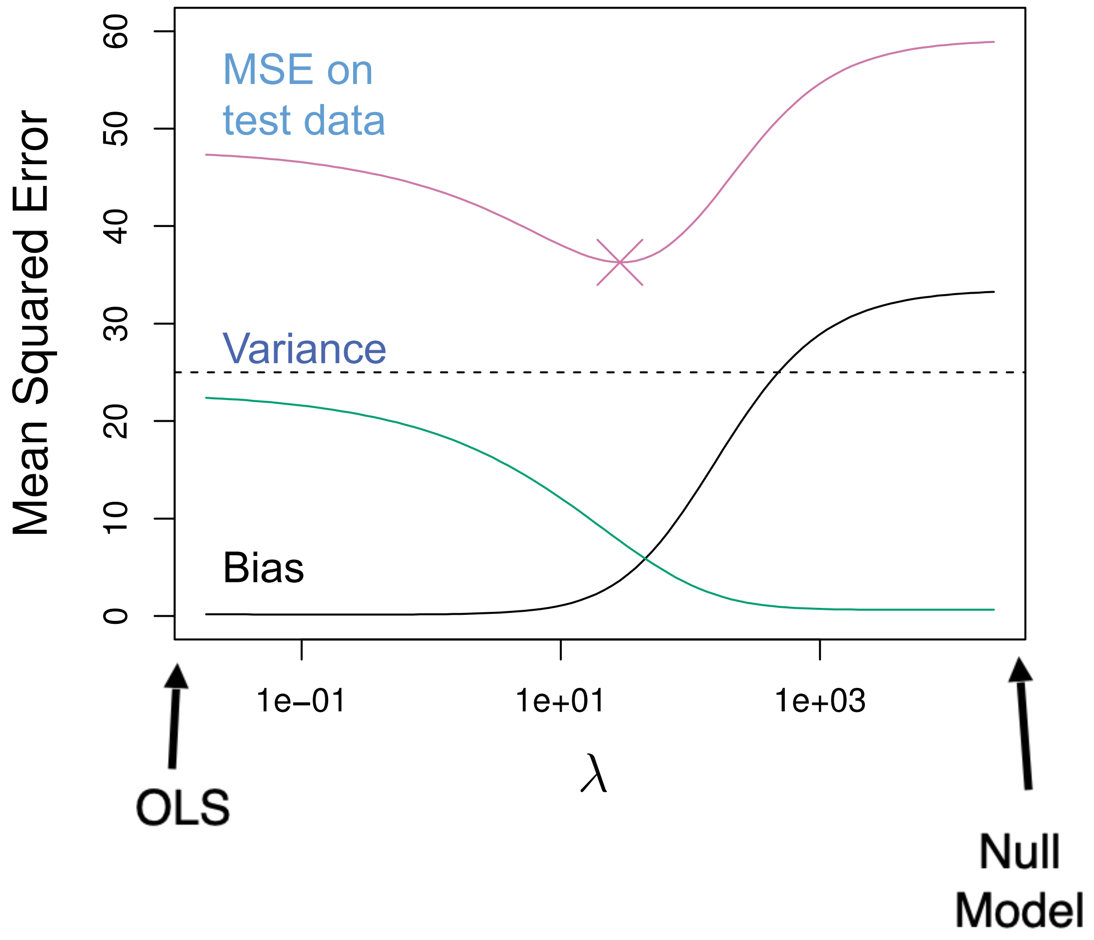
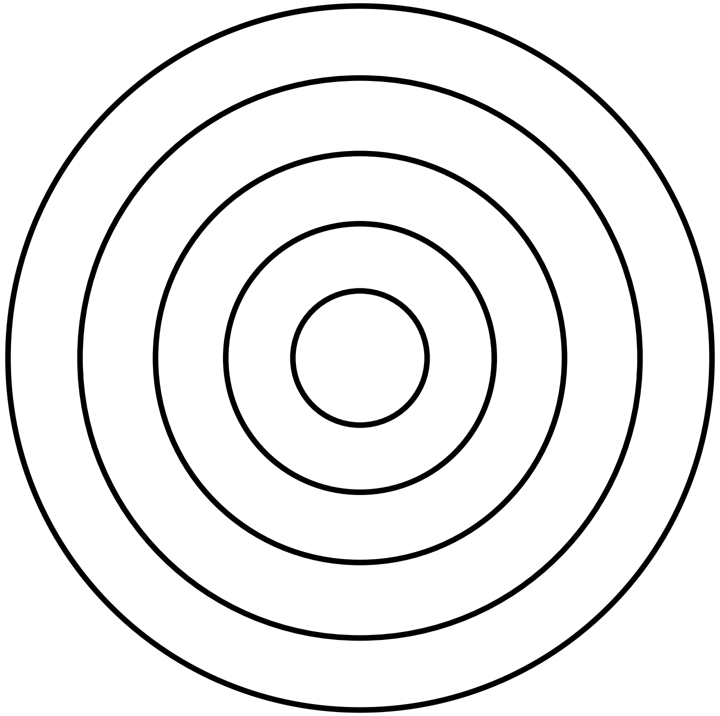
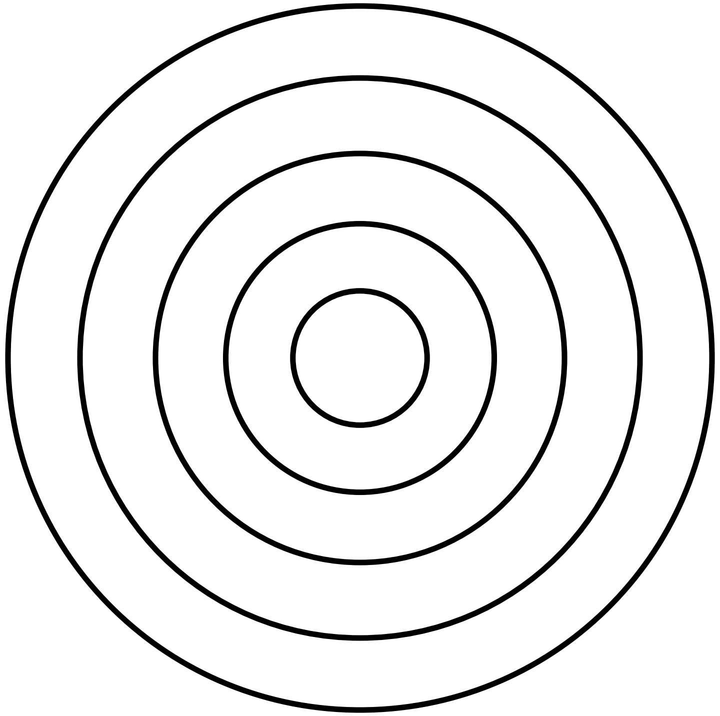
Regularization

- **Regularization** (or penalization / shrinkage) is a common tool to control the complexity/flexibility of a model.
- Adds penalty term to penalize model complexity.
- Model becomes biased, but potentially improve variance of the model.

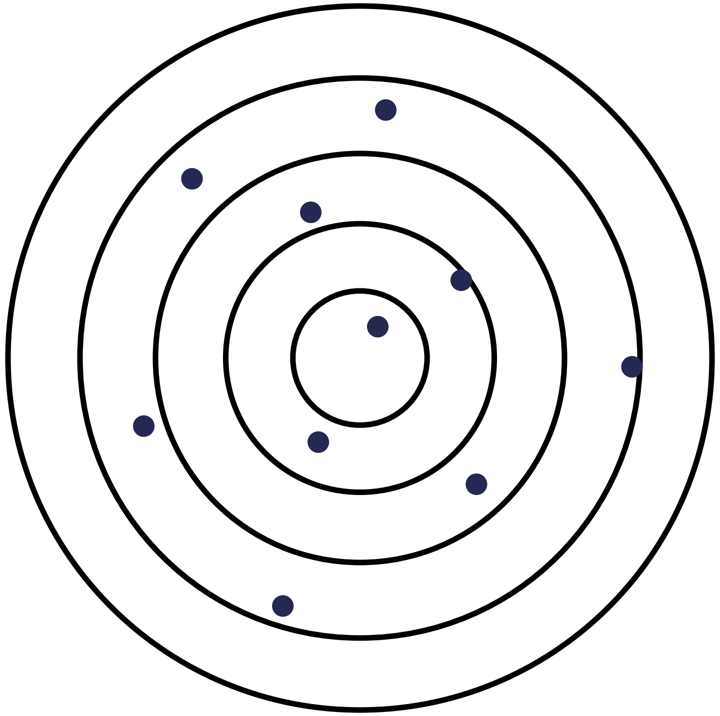


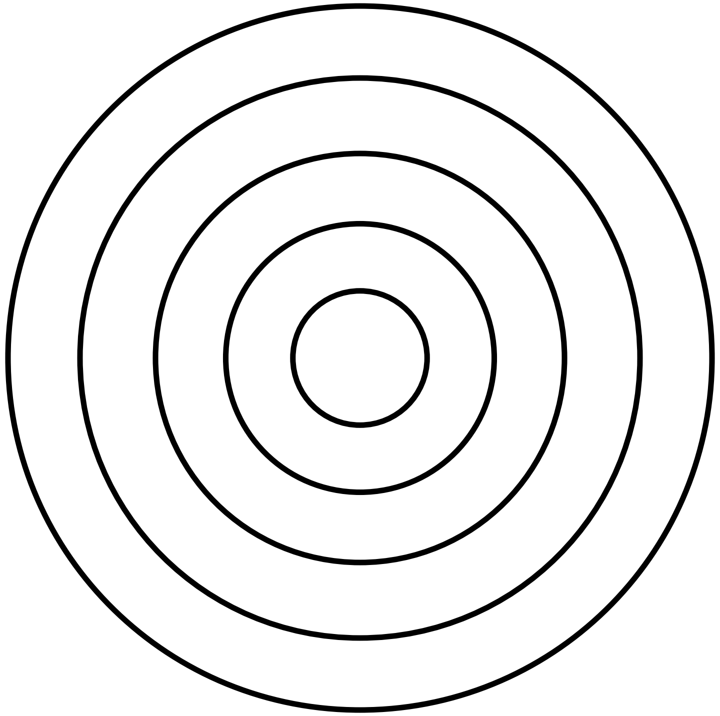
Biased Regression Techniques

Biased Regression Techniques

Unbiased but not precise





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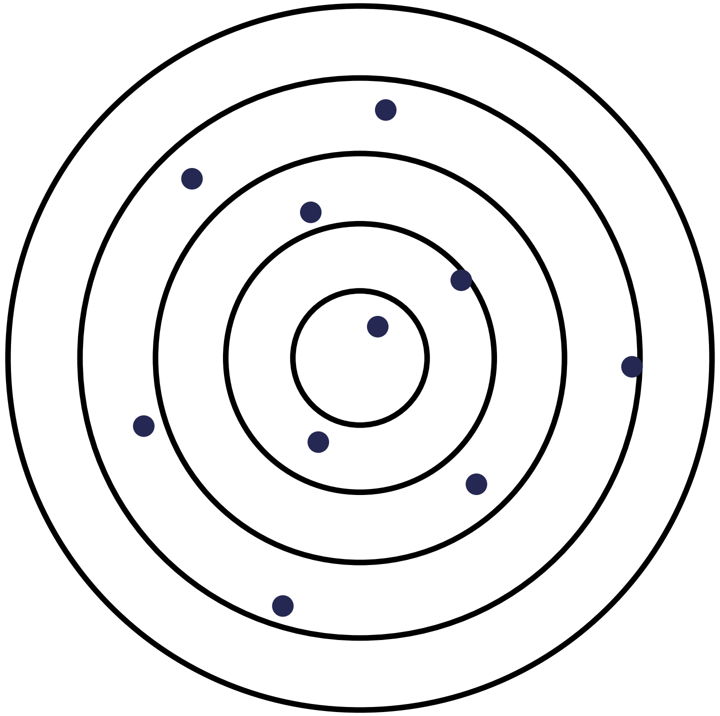

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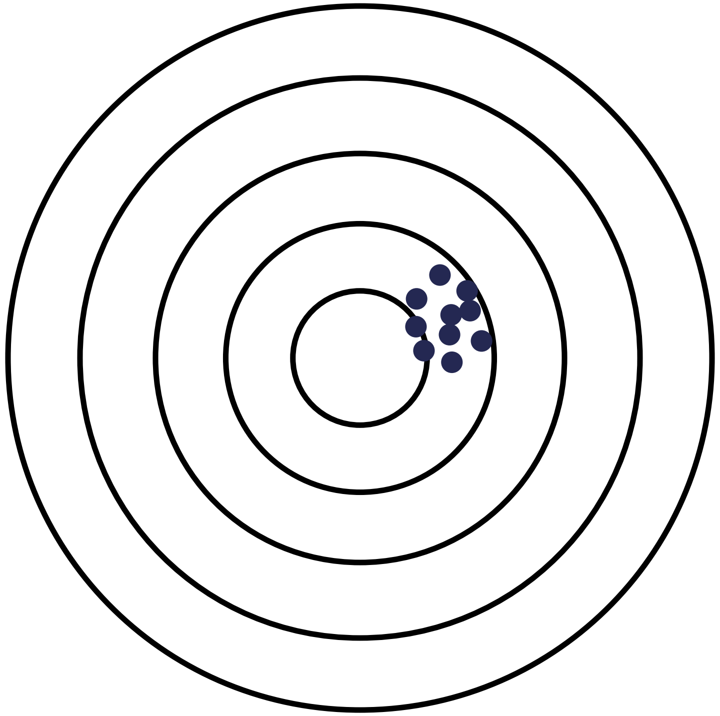

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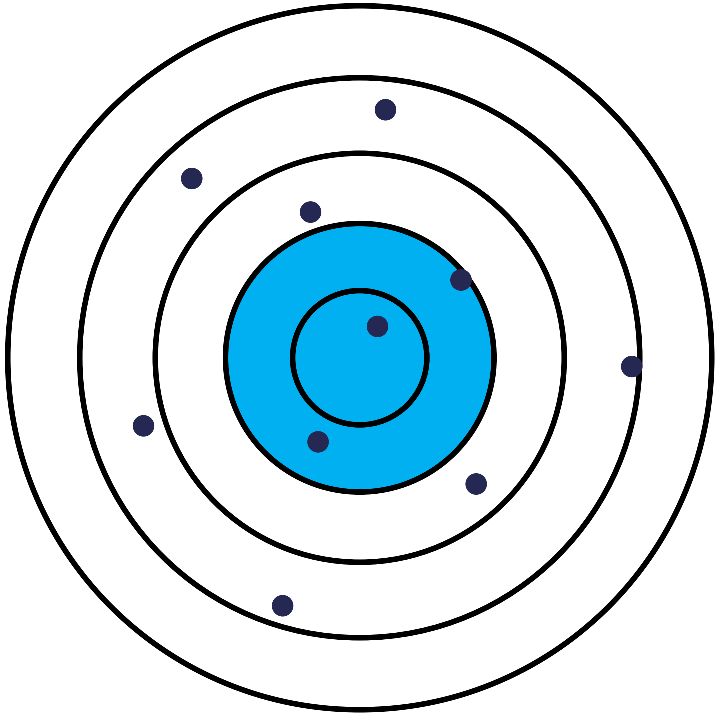

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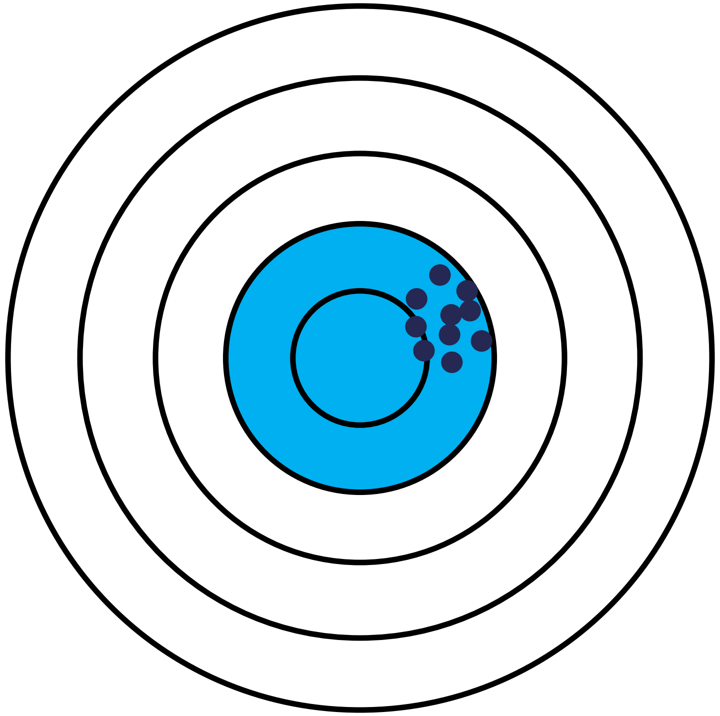


Regularized Regression

- **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:

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

- Regularized regression introduces a penalty term to the minimization:

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

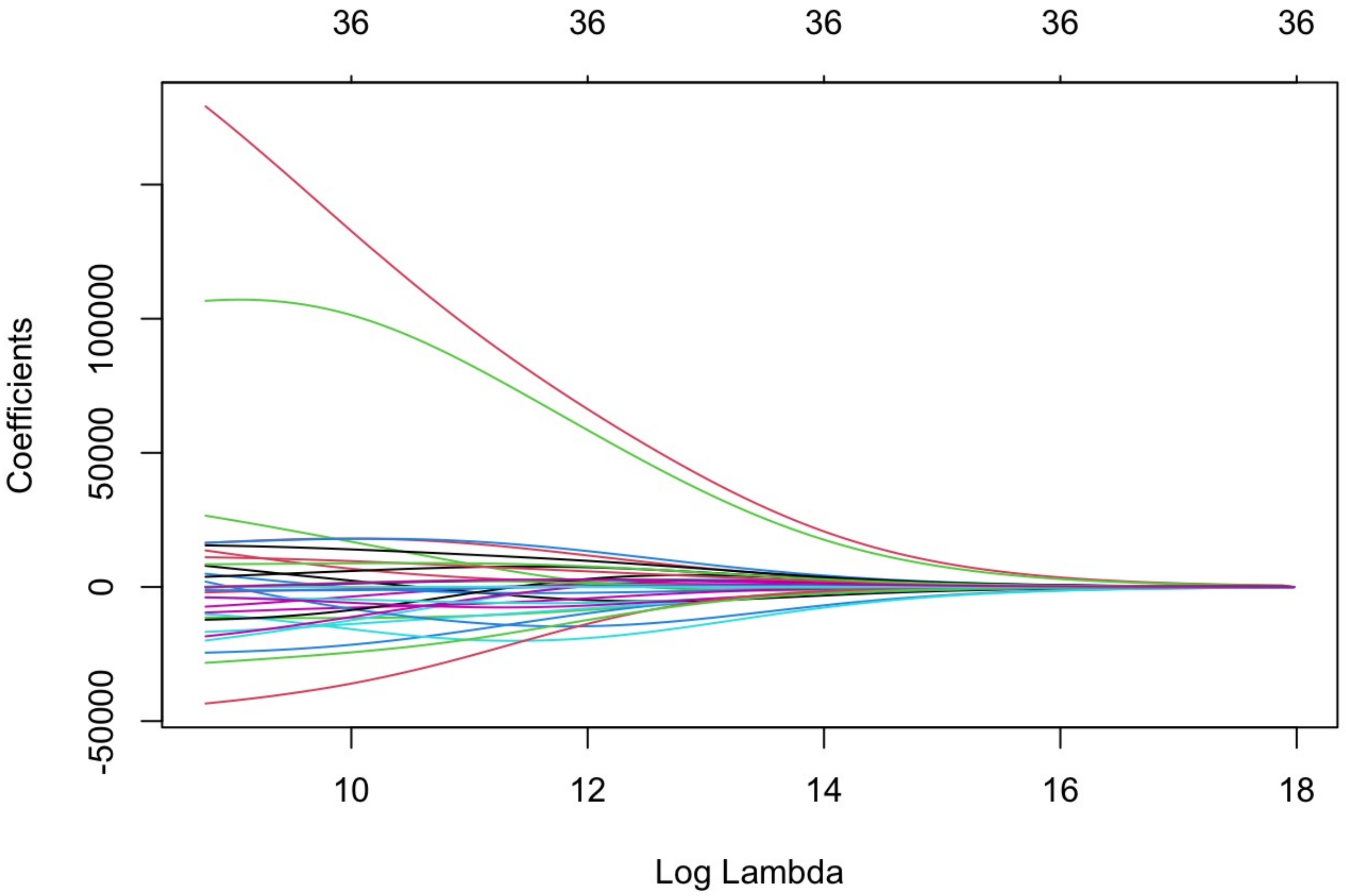
Ridge Regression

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

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

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

Ridge Regression



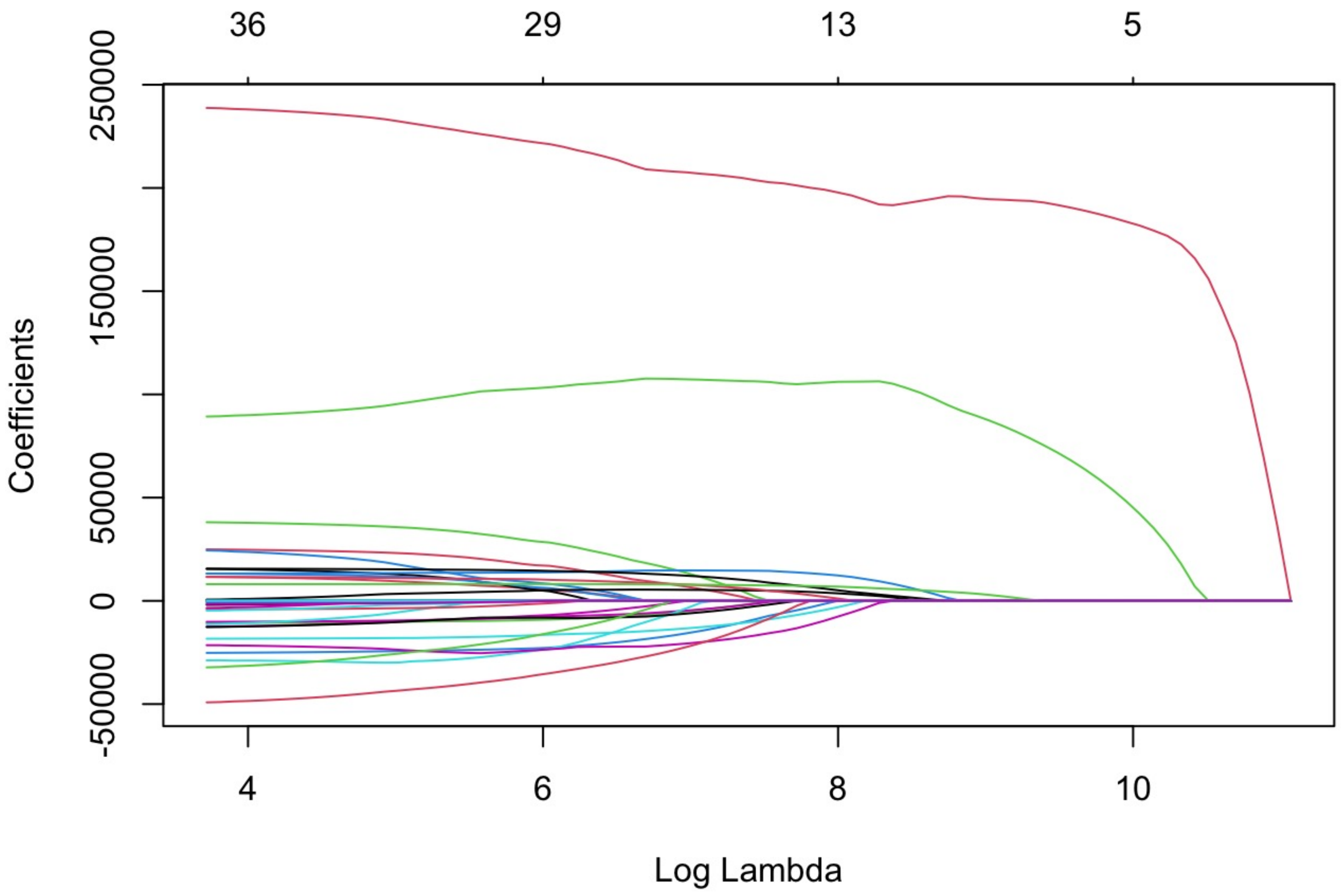
LASSO Regression

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

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

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

LASSO Regression



Differences in Effects

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

Differences in effects are due to differences in penalty.

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

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

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$$\hat{\beta}_{OLS} = (X^TX)^{-1}X^TY \qquad \hat{\beta}_R = (X^TX + \lambda I)^{-1}X^TY \qquad \hat{\beta}_L = (X^TX)^{-1}(X^TY - \lambda I)$$

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

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

Elastic Net

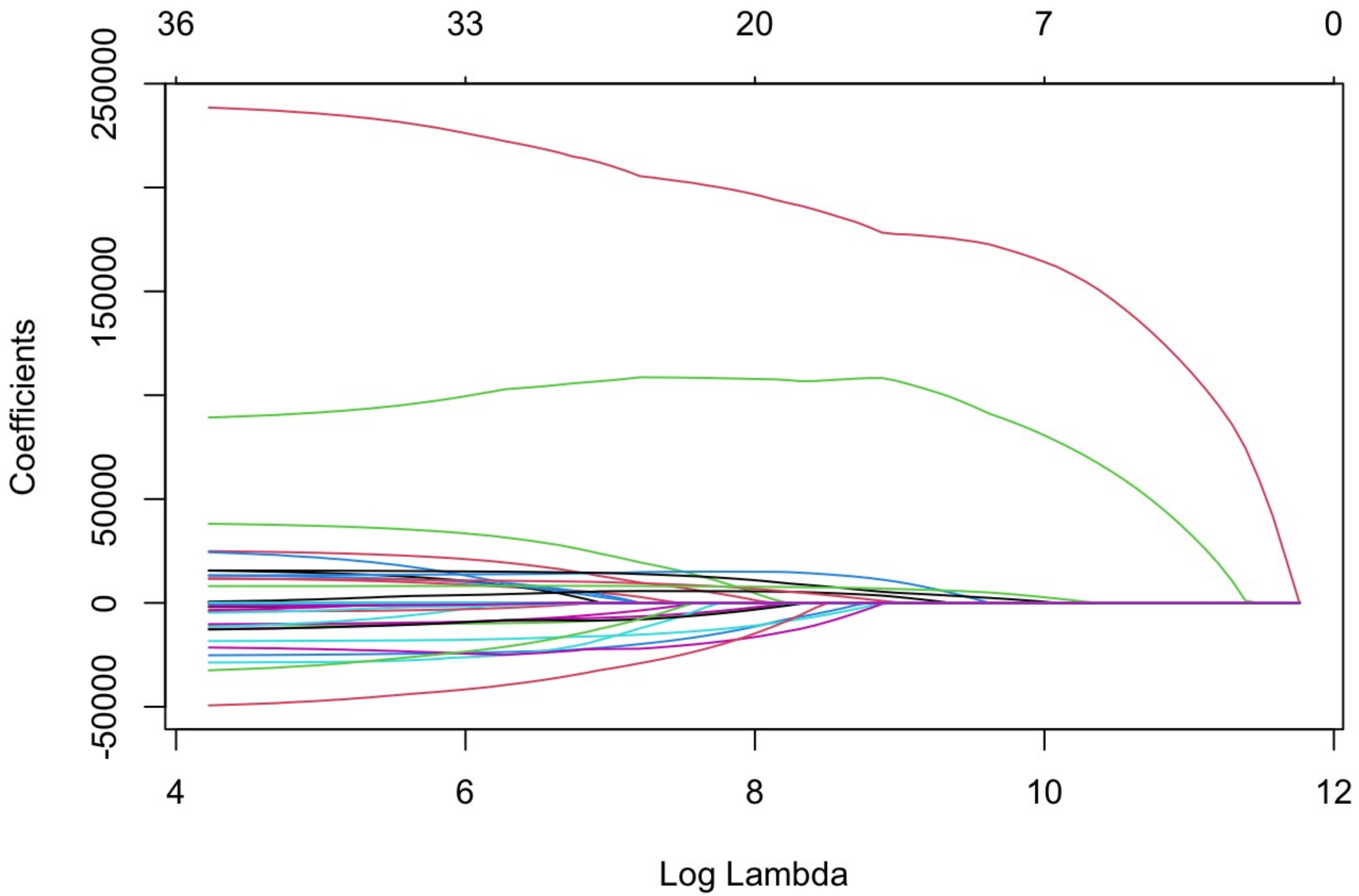
- The `glmnet` function in R takes slightly different approach:

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

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

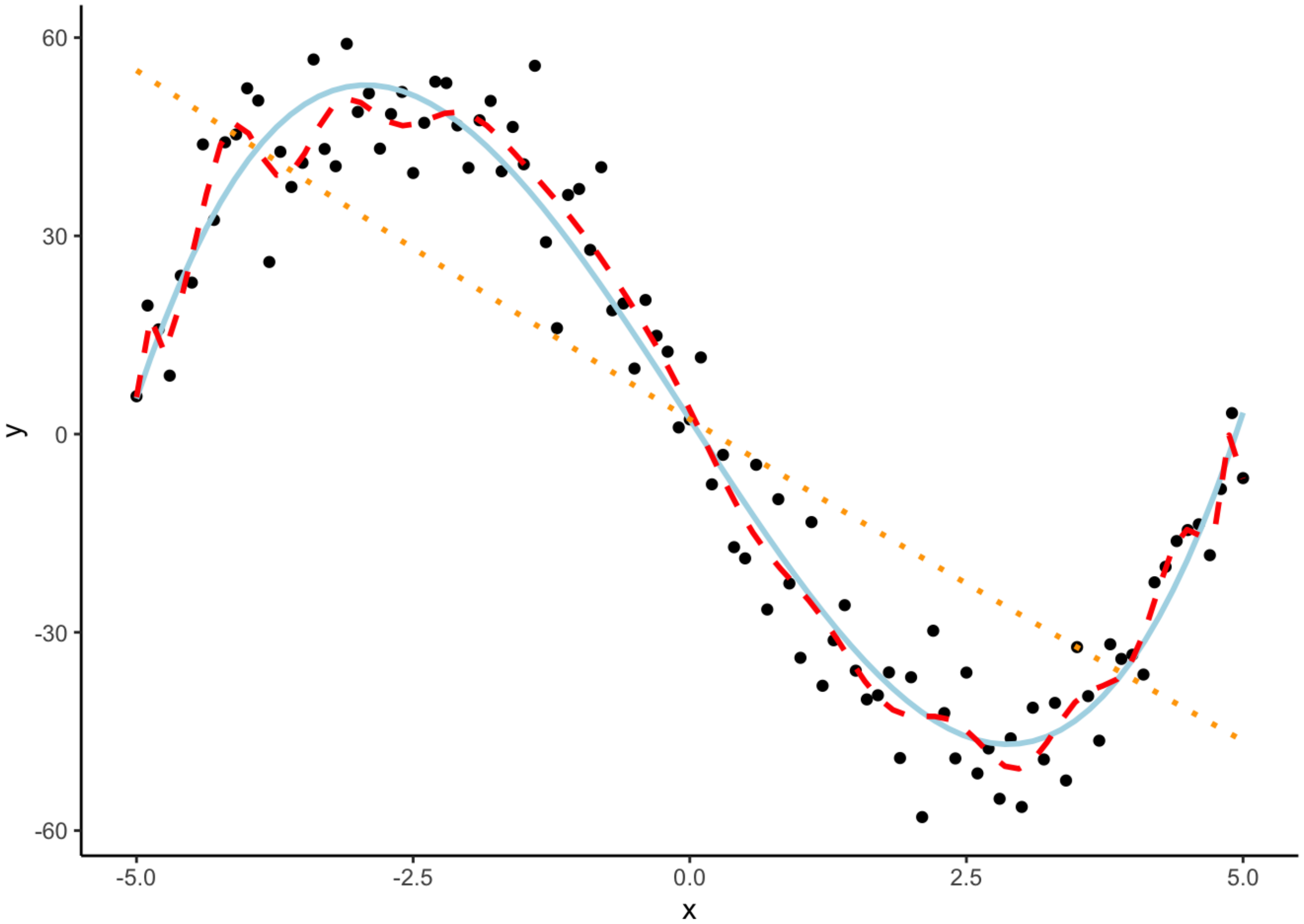
- Any value of `alpha` between 0 and 1 gives a combination of both penalties (elastic net).

Elastic Net Regression



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.

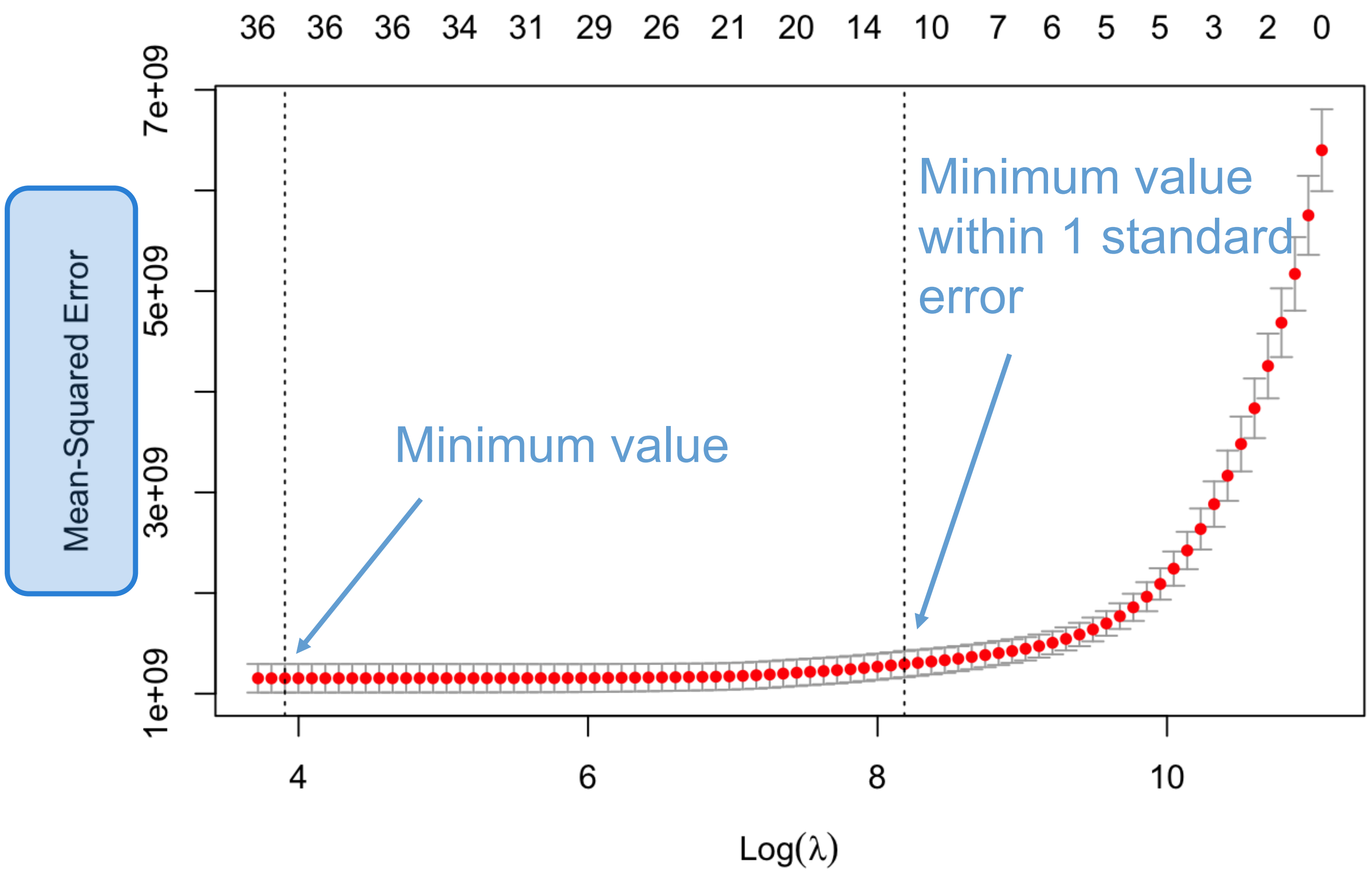


Cross-Validation

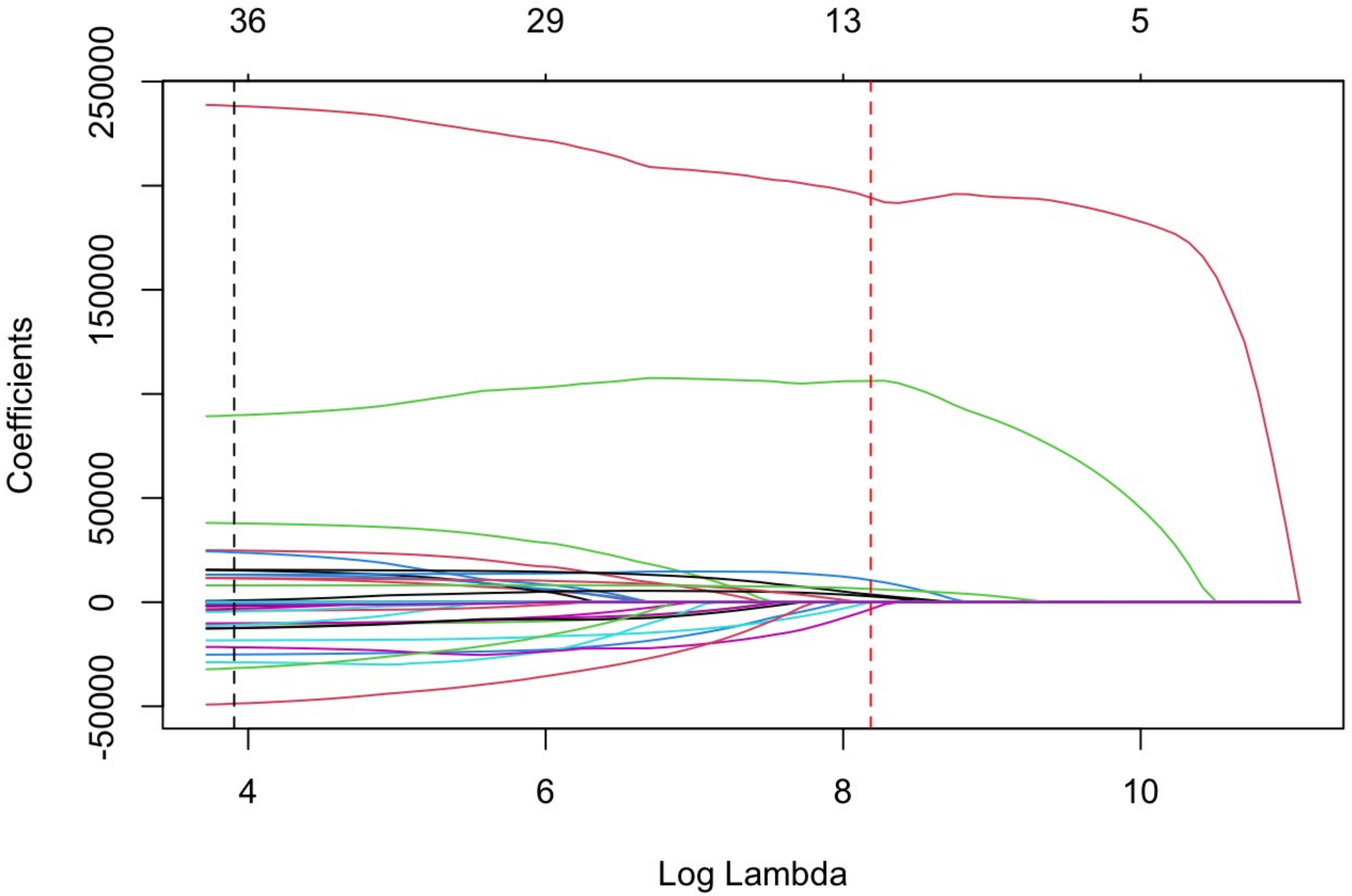
- **Cross-validation** (CV) is common approach to prevent overfitting when tuning a parameter.
- Concept:
  - Split training data into multiple pieces
  - Build model on majority of pieces
  - Evaluate on remaining piece
  - Repeat process with switching out pieces for building and evaluation

LASSO Regression

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



LASSO Regression



Elastic Net Optimization

```
set.seed(5)

en.model <- train(Sale_Price ~ ., data = training,
                  method = "glmnet",
                  tuneGrid = expand.grid(.alpha = seq(0,1, by = 0.05),
                                         .lambda = seq(100,60000, by = 1000)),
                  trControl = trainControl(method = 'cv', number = 10))
```

Defining the parameters we want to tune

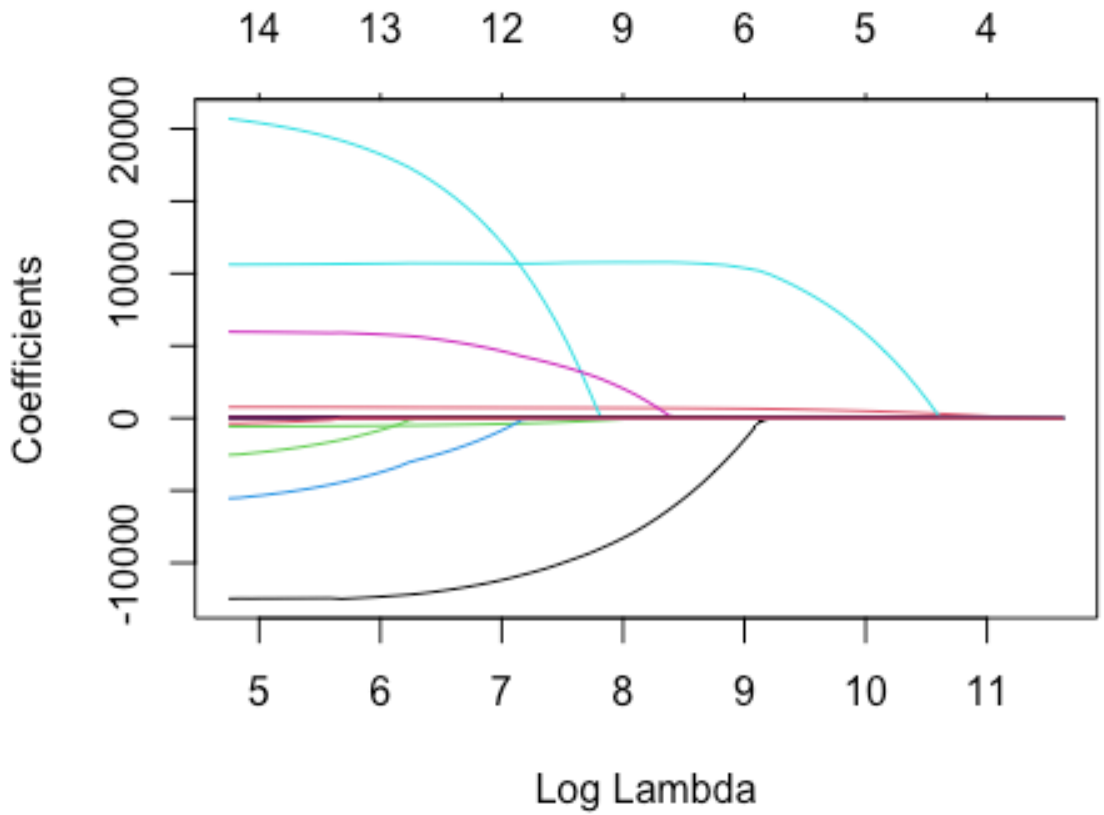
Elastic Net Optimization

```
en.model
```

```
## glmnet
##
## 2051 samples
##   14 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1847, 1846, 1846, 1846, 1846, 1845, ...
## Resampling results across tuning parameters:
##
##   alpha  lambda  RMSE      Rsquared   MAE
##   0.00     100   39425.23  0.7549646  26190.91
##   0.00    1100   39425.23  0.7549646  26190.91
##   0.00    2100   39425.23  0.7549646  26190.91
…
##   1.00   56100   78334.99  0.5086181  57328.76
##   1.00   57100   78607.53  0.4385170  57550.28
##   1.00   58100   78616.60        NaN  57557.27
##   1.00   59100   78616.60        NaN  57557.27
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were alpha = 0.5 and lambda = 100.
```

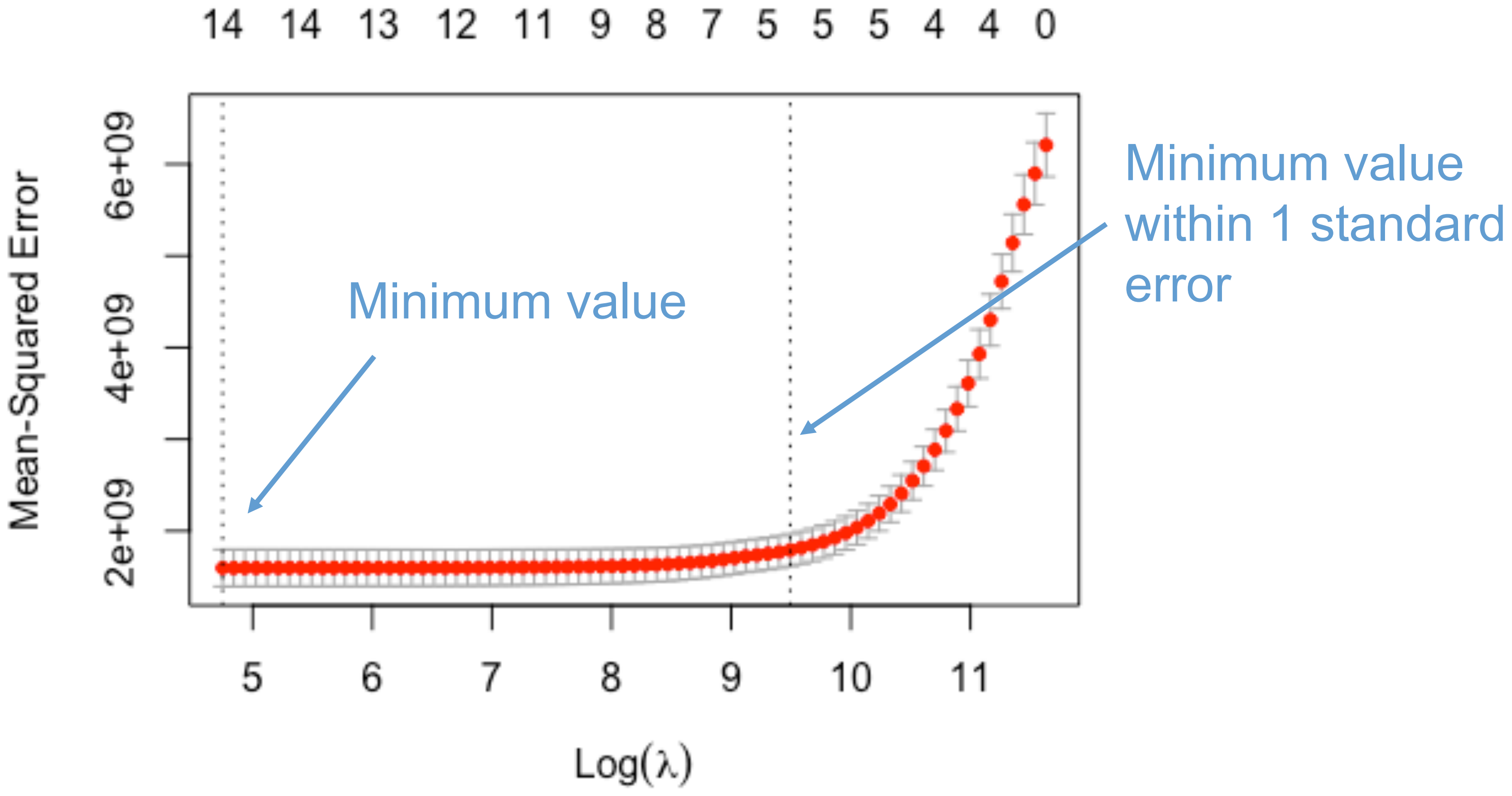
Elastic Net Optimization

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

ames_en <- glmnet(x = train_x,  y = train_y,
                  alpha = 0.5)

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



Elastic Net Optimization

```
set.seed(5)
ames_en_cv <- cv.glmnet(x = train_x,  y = train_y,  alpha = 0.5)

plot(ames_en_cv)
```



Elastic Net Optimization

```
ames_en_cv$lambda.min
## [1] 115.4119
```

Similar to our value of 100

```
ames_en_cv$lambda.1se
## [1] 13269.57
```