

Supervised Learning

Regularization

June 28th, 2021

Previously...

We talked about variable selection in the linear model context:

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p$$

Why would we attempt to select a **subset** of the p variables?

- *To improve prediction accuracy*
 - Eliminating uninformative predictors can lead to lower variance in the test-set MSE, at the expense of a slight increase in bias
- *To improve model interpretability*
 - Eliminating uninformative predictors is obviously a good thing when your goal is to tell the story of how your predictors are associated with your response.

Remember the bias-variance tradeoff:

$$\text{MSE} = (\text{Bias})^2 + \text{Variance}$$

- Introduce bias but decrease variance to improve predictions

Shrinkage methods: Ridge regression

Remember: linear regression estimates coefficients by minimizing:

$$\text{RSS} = \sum_i^n (Y_i - \beta_0 - \sum_j^p \hat{\beta}_j x_{ij})^2$$

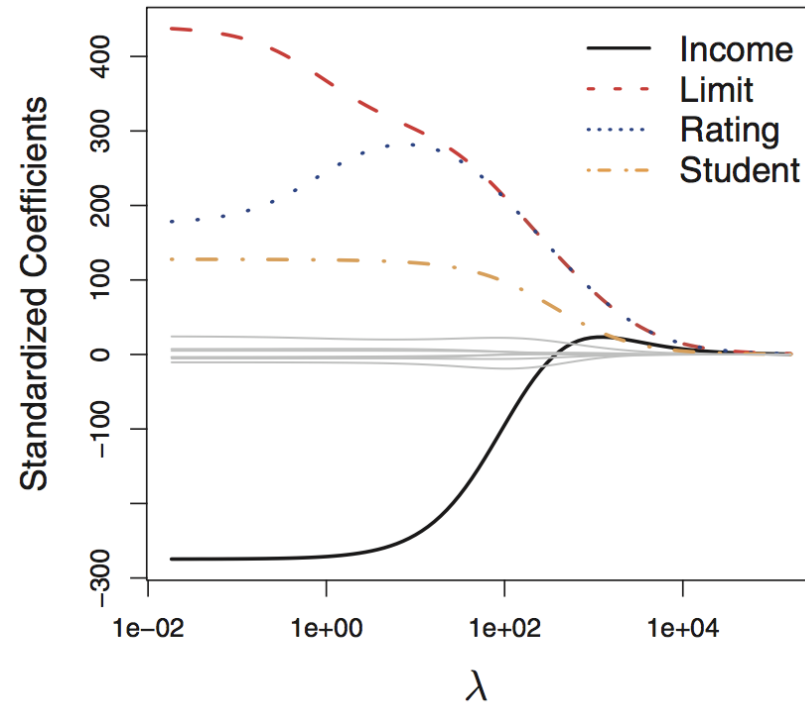
Ridge regression introduces a **shrinkage penalty** $\lambda \geq 0$ by minimizing:

$$\sum_i^n (Y_i - \beta_0 - \sum_j^p \beta_j x_{ij})^2 + \lambda \sum_j^p \beta_j^2 = \text{RSS} + \lambda \sum_j^p \beta_j^2$$

- as λ increases \Rightarrow flexibility of models decreases
 - **increases bias, but decreases variance**
- for fixed value of λ , ridge regression fits only a single model
 - need to use cross-validation to **tune** λ

Shrinkage methods: Ridge regression

For example: note how the magnitude of the coefficient for Income trends as $\lambda \rightarrow \infty$



The coefficient **shrinks towards zero**, but never actually reaches it

- Income is always a variable in the learned model, regardless of the value of λ

Shrinkage methods: Lasso regression

Ridge regression **keeps all variables**

But we may believe there is a **sparse** solution

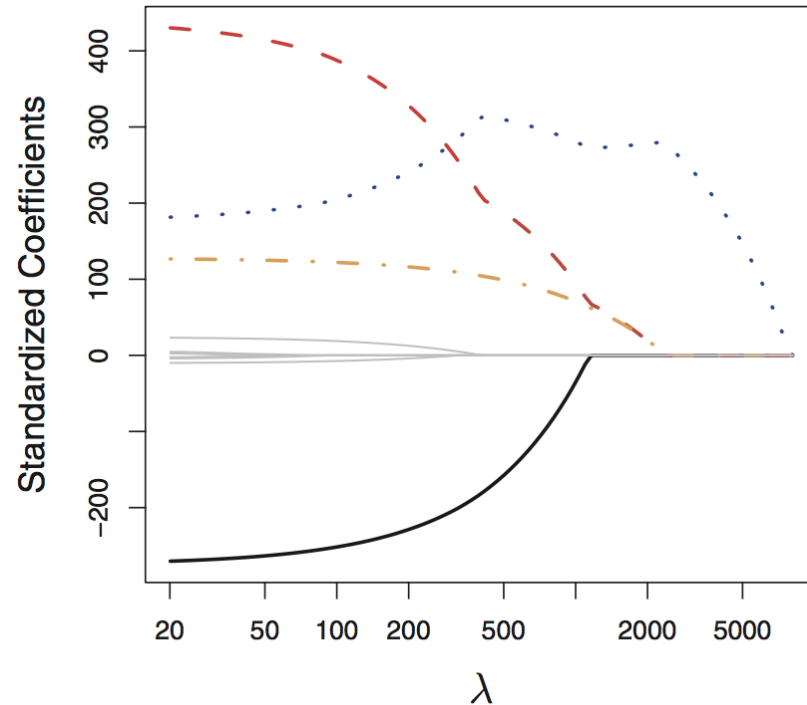
Lasso enables variable selection with λ by minimizing:

$$\sum_i^n (Y_i - \beta_0 - \sum_j^p \beta_j X_{ij})^2 + \lambda \sum_j^p |\beta_j| = \text{RSS} + \lambda \sum_j^p |\beta_j|$$

- Lasso uses an ℓ_1 ("ell 1") penalty
- as λ increases \Rightarrow flexibility of models decreases
 - **increases bias, but decreases variance**
- Can handle the $p > n$ case, i.e. more variables than observations!

Shrinkage methods: Lasso regression

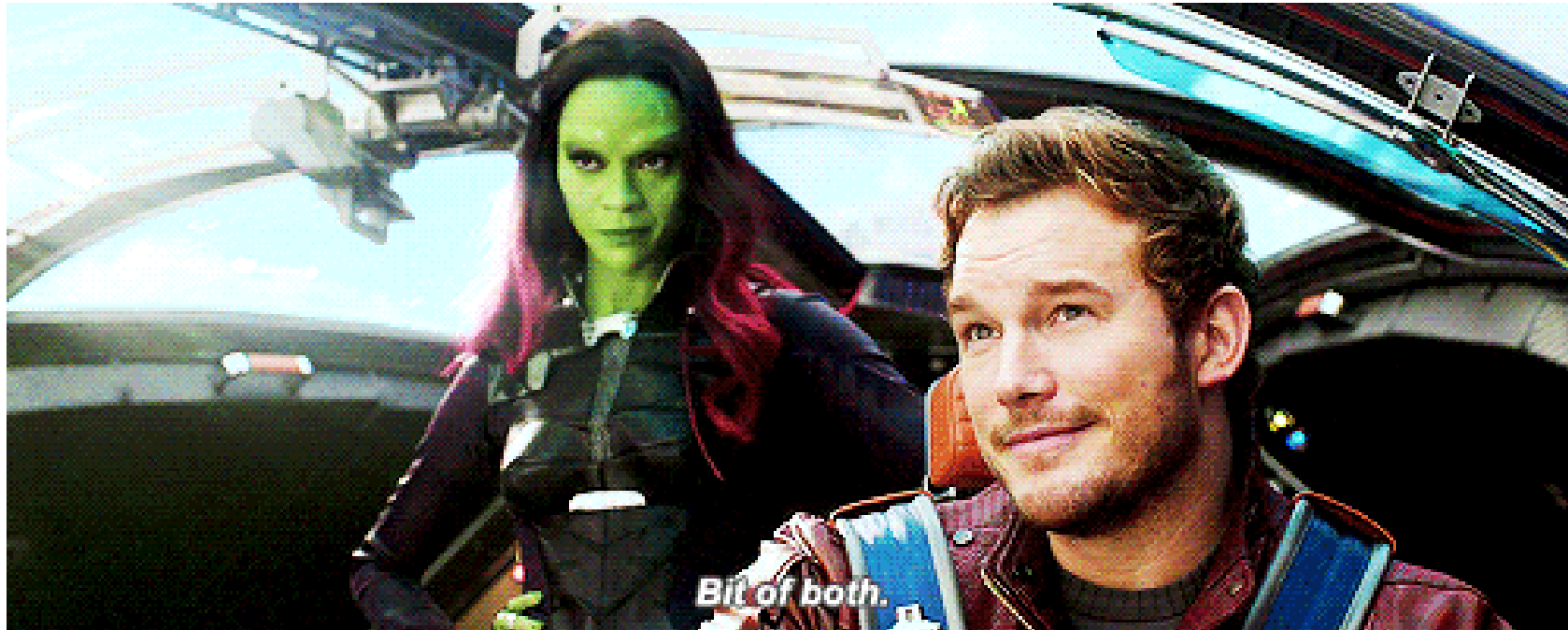
Lasso regression **performs variable selection** yielding **sparse** models



The coefficient shrinks towards and **eventually equals zero** at $\lambda \approx 1000$

- if the optimum value of λ is larger, then Income would NOT be included in the learned model

Which do we use?



Best of both worlds? Elastic net

$$\sum_i^n \left(Y_i - \beta_0 - \sum_j^p \beta_j X_{ij} \right)^2 + \lambda \left[(1 - \alpha) \|\beta\|_2^2 / 2 + \alpha \|\beta\|_1 \right]$$

- $\|\beta\|_1$ is the ℓ_1 norm: $\|\beta\|_1 = \sum_j^p |\beta_j|$
- $\|\beta\|_2$ is the ℓ_2 , Euclidean, norm: $\|\beta\|_2 = \sqrt{\sum_j^p \beta_j^2}$
- Ridge penalty: $\lambda \cdot (1 - \alpha) / 2$
- Lasso penalty: $\lambda \cdot \alpha$
- α controls the **mixing** between the two types, ranges from 0 to 1
 - $\alpha = 1$ returns lasso
 - $\alpha = 0$ return ridge

Caveats to consider...

- For either ridge, lasso, or elastic net: **you should standardize your data**
- Common convention: within each column, compute then subtract off the sample mean, and compute the divide off the sample standard deviation:

$$\tilde{x}_{ij} = \frac{x_{ij} - \bar{x}_j}{s_{x,j}}$$

- `glmnet` package does this by default and reports coefficients on the original scale
- λ and α are **tuning parameters**
- Have to select appropriate values based on test data / cross-validation
- When using `glmnet`, the `cv.glmnet()` function will perform the cross-validation for you

Example data: NFL teams summary

Created dataset using `nflfastR` summarizing NFL team performances from 1999 to 2020

```
library(tidyverse)
nfl_teams_data <- read_csv("http://www.stat.cmu.edu/cmsac/sure/2021/materials/data/regression_pro
nfl_model_data <- nfl_teams_data %>%
  mutate(score_diff = points_scored - points_allowed) %>%
  # Only use rows with air yards
  filter(season >= 2006) %>%
  dplyr::select(-wins, -losses, -ties, -points_scored, -points_allowed, -season, -team)
```

Introduction to glmnet

We will use the `glmnet` package for ridge, lasso, and elastic net

```
library(glmnet)
```

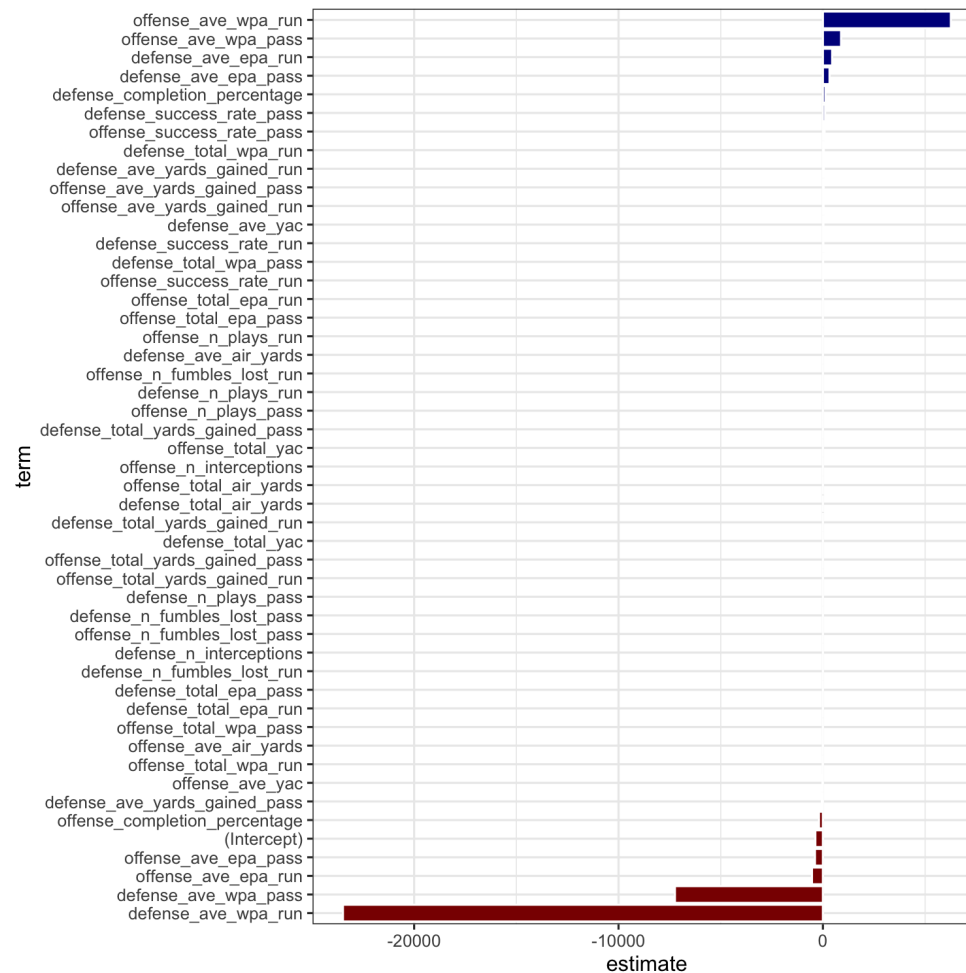
- could use the `model.matrix()` function (which converts factors to 0-1 dummy variables!)

```
model_x <- nfl_model_data %>%  
  dplyr::select(-score_diff) %>%  
  as.matrix()  
model_y <- nfl_model_data$score_diff  
# model_x <- model.matrix(score_diff ~ ., nfl_model_data)[, -1]
```

Initial model with `lm()`

- What do the initial regression coefficients look like?
- Use **broom** to tidy model output for plotting

```
init_reg_fit <- lm(score_diff ~ ., nfl_model_  
library(broom)  
tidy(init_reg_fit) %>%  
  mutate(coef_sign = as.factor(sign(estimate)  
    term = fct_reorder(term, estimate))  
  ggplot(aes(x = term, y = estimate, fill = c  
    geom_bar(stat = "identity", color = "white"  
    scale_fill_manual(values = c("darkred", "da  
      guide = FALSE) +  
    coord_flip() + theme_bw()
```

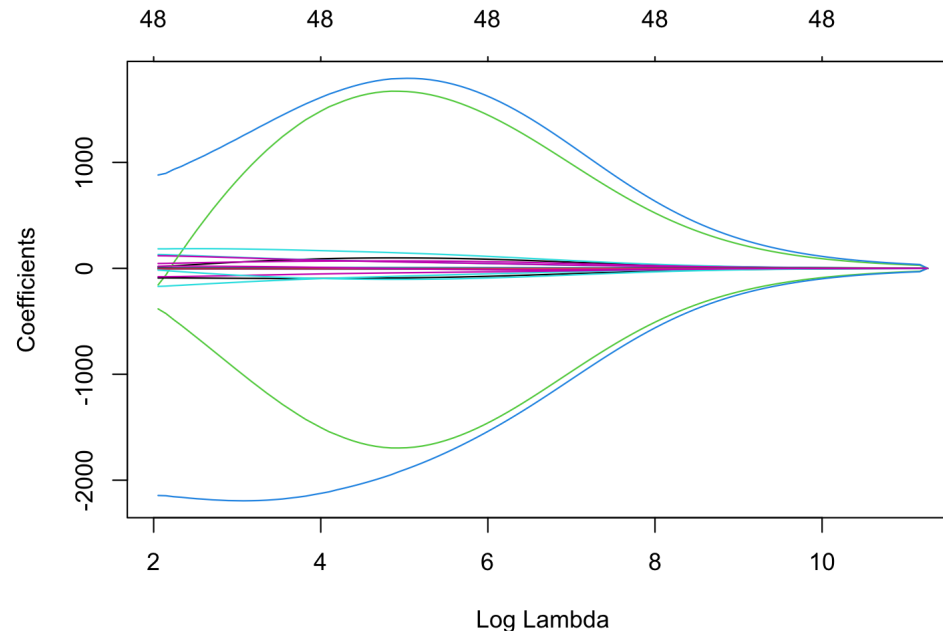


Ridge regression example

Perform ridge regression using `glmnet` with `alpha = 0` (more on that later)

By default it standardizes your predictors and fits model across a range of λ values (can plot these!)

```
init_ridge_fit <- glmnet(model_x, model_y, alpha = 0)  
plot(init_ridge_fit, xvar = "lambda")
```

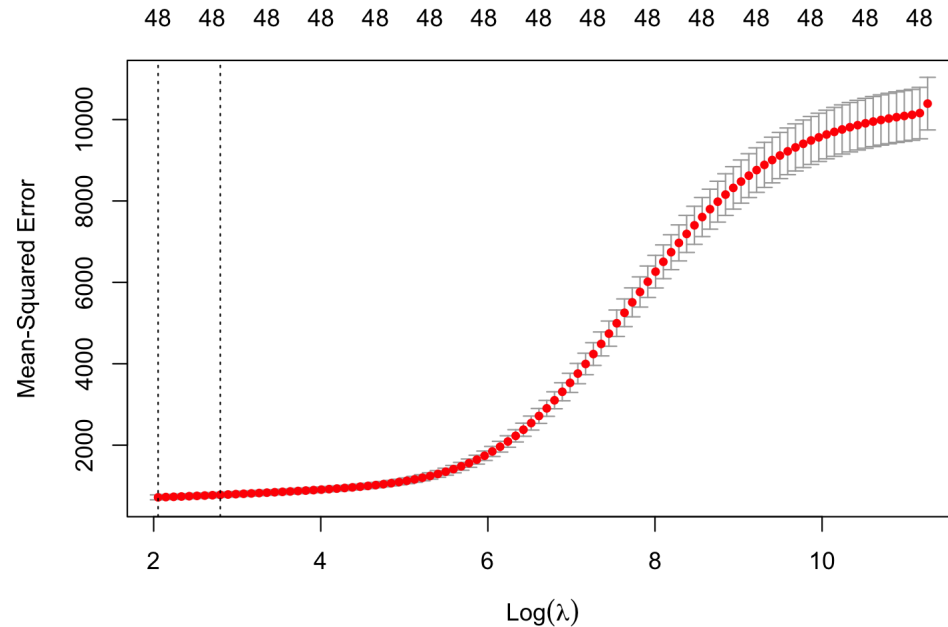


Ridge regression example

We use cross-validation to select λ with `cv.glmnet()` which uses 10-folds by default

- specify ridge regression with `alpha = 0`

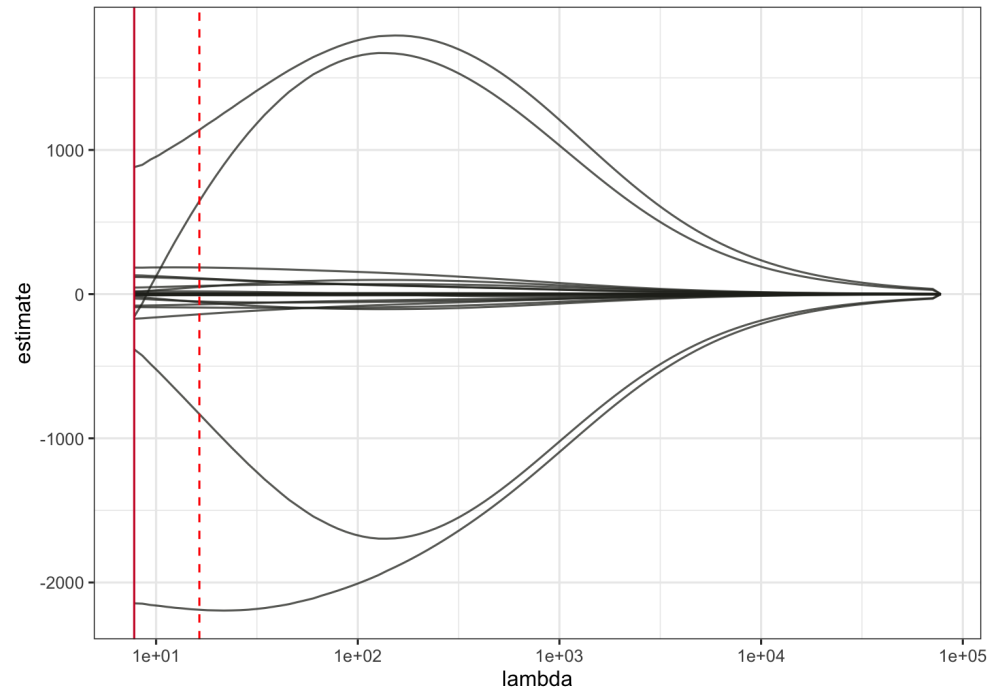
```
fit_ridge_cv <- cv.glmnet(model_x, model_y, alpha = 0)  
plot(fit_ridge_cv)
```



Tidy ridge regression

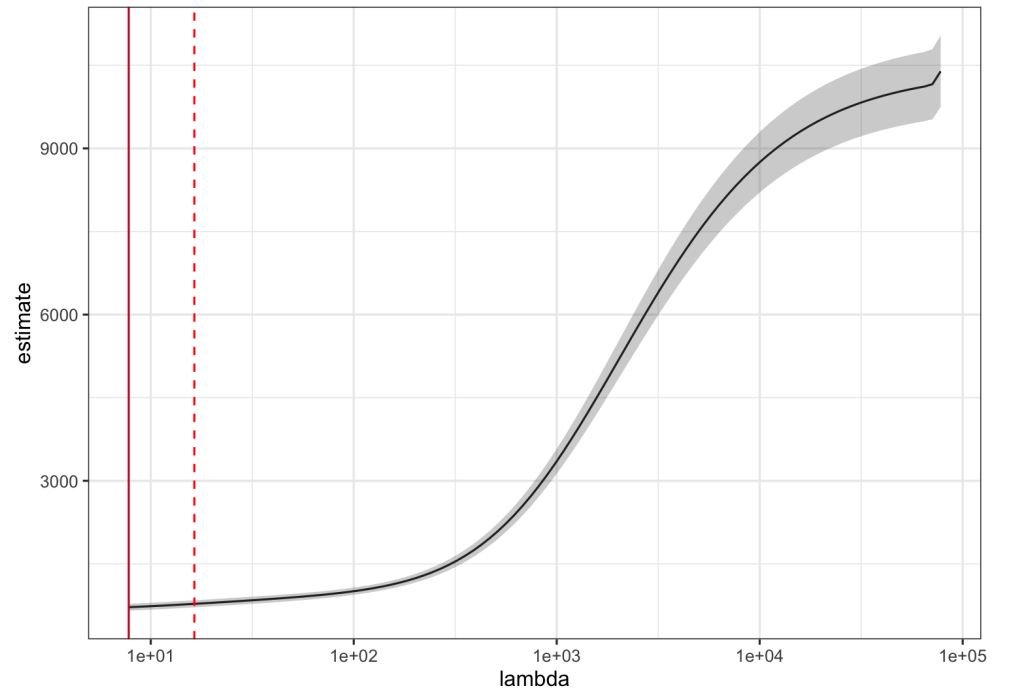
```
tidy_ridge_coef <- tidy(fit_ridge_cv$glmnet.f  
tidy_ridge_coef %>%  
  ggplot(aes(x = lambda, y = estimate,  
             group = term)) +  
  scale_x_log10() +  
  geom_line(alpha = 0.75) +  
  geom_vline(xintercept =  
             fit_ridge_cv$lambda.min) +  
  geom_vline(xintercept =  
             fit_ridge_cv$lambda.1se,  
             linetype = "dashed", color = "red")  
  theme_bw()
```

- Could easily add color with legend for variables...



Tidy ridge regression

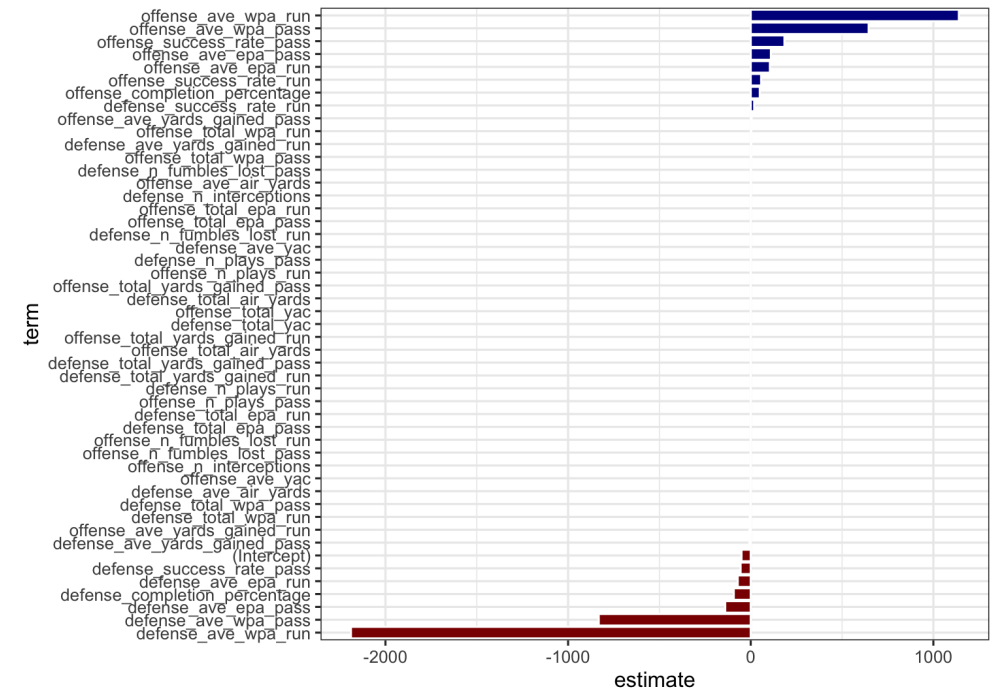
```
tidy_ridge_cv <- tidy(fit_ridge_cv)
tidy_ridge_cv %>%
  ggplot(aes(x = lambda, y = estimate)) +
  geom_line() + scale_x_log10() +
  geom_ribbon(aes(ymin = conf.low,
                 ymax = conf.high), alpha =
  geom_vline(xintercept =
              fit_ridge_cv$lambda.min) +
  geom_vline(xintercept =
              fit_ridge_cv$lambda.1se,
              linetype = "dashed", color = "red"
  theme_bw()
```



Ridge regression coefficients

Coefficients using the **1 standard error rule** λ

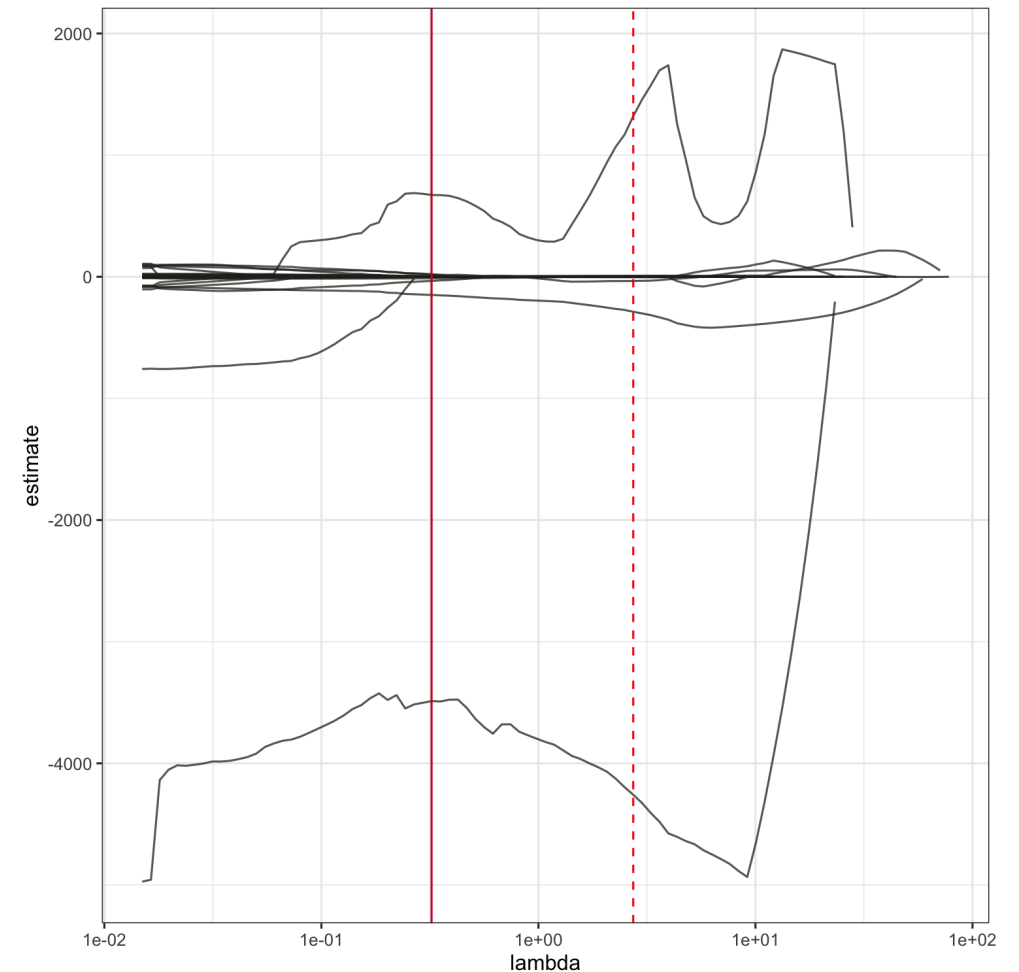
```
tidy_ridge_coef %>%  
  filter(lambda == fit_ridge_cv$lambda.1se) %  
  mutate(coef_sign = as.factor(sign(estimate))  
         term = fct_reorder(term, estimate))  
ggplot(aes(x = term, y = estimate, fill = c  
geom_bar(stat = "identity", color = "white"  
scale_fill_manual(values = c("darkred", "da  
coord_flip() + theme_bw()
```



Lasso regression example

Similar syntax to ridge but specify $\alpha = 1$:

```
fit_lasso_cv <- cv.glmnet(model_x, model_y,  
                          alpha = 1)  
tidy_lasso_coef <- tidy(fit_lasso_cv$glmnet.f  
tidy_lasso_coef %>%  
  ggplot(aes(x = lambda, y = estimate,  
             group = term)) +  
  scale_x_log10() +  
  geom_line(alpha = 0.75) +  
  geom_vline(xintercept =  
             fit_lasso_cv$lambda.min) +  
  geom_vline(xintercept =  
             fit_lasso_cv$lambda.1se,  
             linetype = "dashed", color = "red")  
  theme_bw()
```

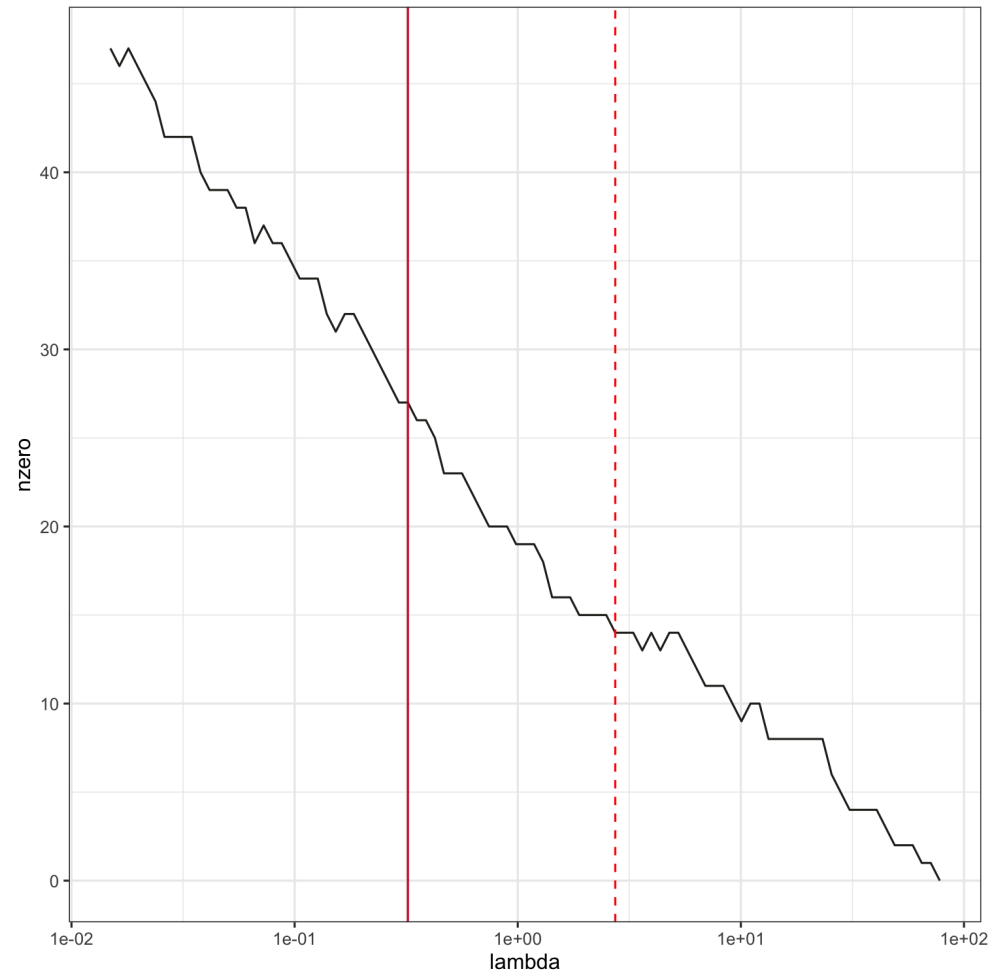


Lasso regression example

Number of non-zero predictors by λ

```
tidy_lasso_cv <- tidy(fit_lasso_cv)
tidy_lasso_cv %>%
  ggplot(aes(x = lambda, y = nzero)) +
  geom_line() +
  geom_vline(xintercept = fit_lasso_cv$lambda
    geom_vline(xintercept = fit_lasso_cv$lambda
      linetype = "dashed", color = "red"
    scale_x_log10() + theme_bw()
```

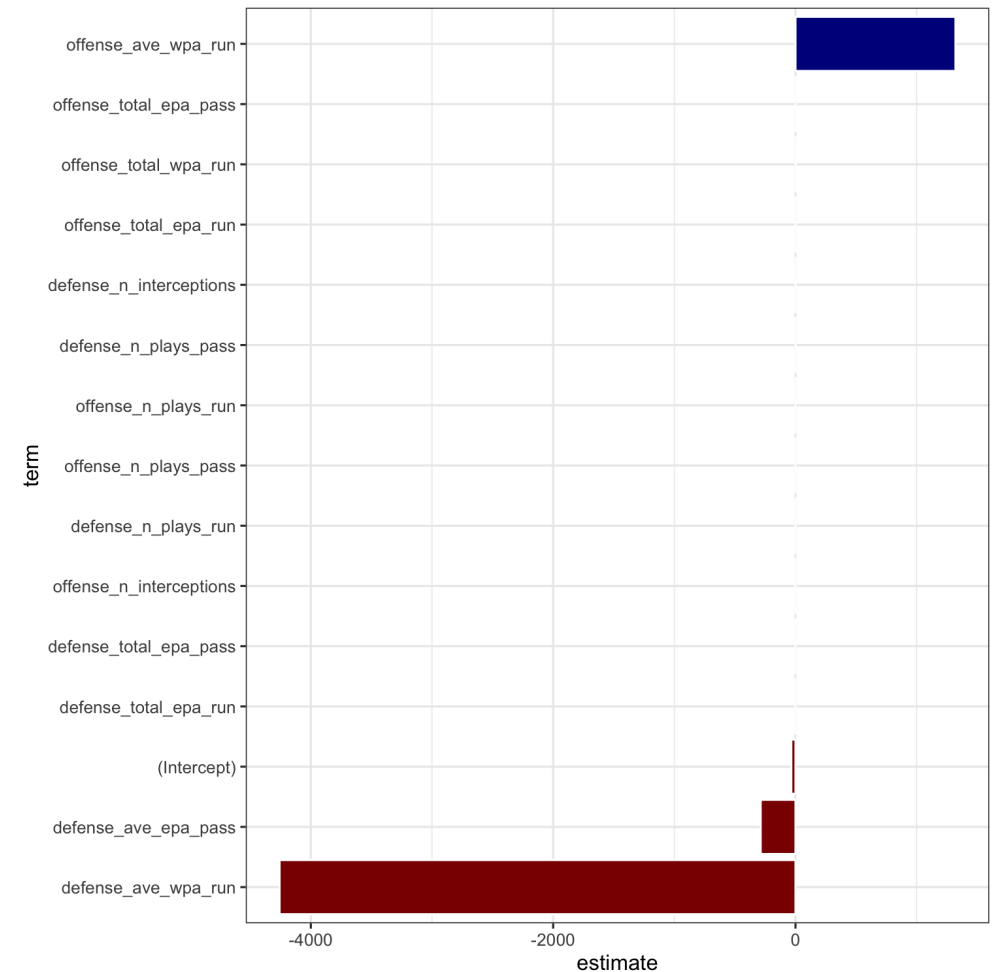
Reduction in variables using **1 standard error rule**
 λ



Lasso regression example

Coefficients using the **1 standard error rule** λ

```
tidy_lasso_coef %>%  
  filter(lambda == fit_lasso_cv$lambda.1se) %  
  mutate(coef_sign = as.factor(sign(estimate))  
         term = fct_reorder(term, estimate))  
  ggplot(aes(x = term, y = estimate,  
            fill = coef_sign)) +  
  geom_bar(stat = "identity", color = "white"  
  scale_fill_manual(values = c("darkred", "darkblue"  
                             guide = FALSE) +  
  coord_flip() +  
  theme_bw()
```



Elastic net example

Need to tune both λ and α - can do so manually with our own folds

```
set.seed(2020)
fold_id <- sample(rep(1:10, length.out = nrow(model_x)))
```

Then use cross-validation with these folds for different candidate alpha values:

```
cv_en_25 <- cv.glmnet(model_x, model_y, foldid = fold_id, alpha = .25)
cv_en_50 <- cv.glmnet(model_x, model_y, foldid = fold_id, alpha = .5)
cv_ridge <- cv.glmnet(model_x, model_y, foldid = fold_id, alpha = 0)
cv_lasso <- cv.glmnet(model_x, model_y, foldid = fold_id, alpha = 1)
```

Can see which one had the lowest CV error among its candidate λ values:

```
which.min(c(min(cv_en_25$cvm), min(cv_en_50$cvm), min(cv_ridge$cvm), min(cv_lasso$cvm)))
```

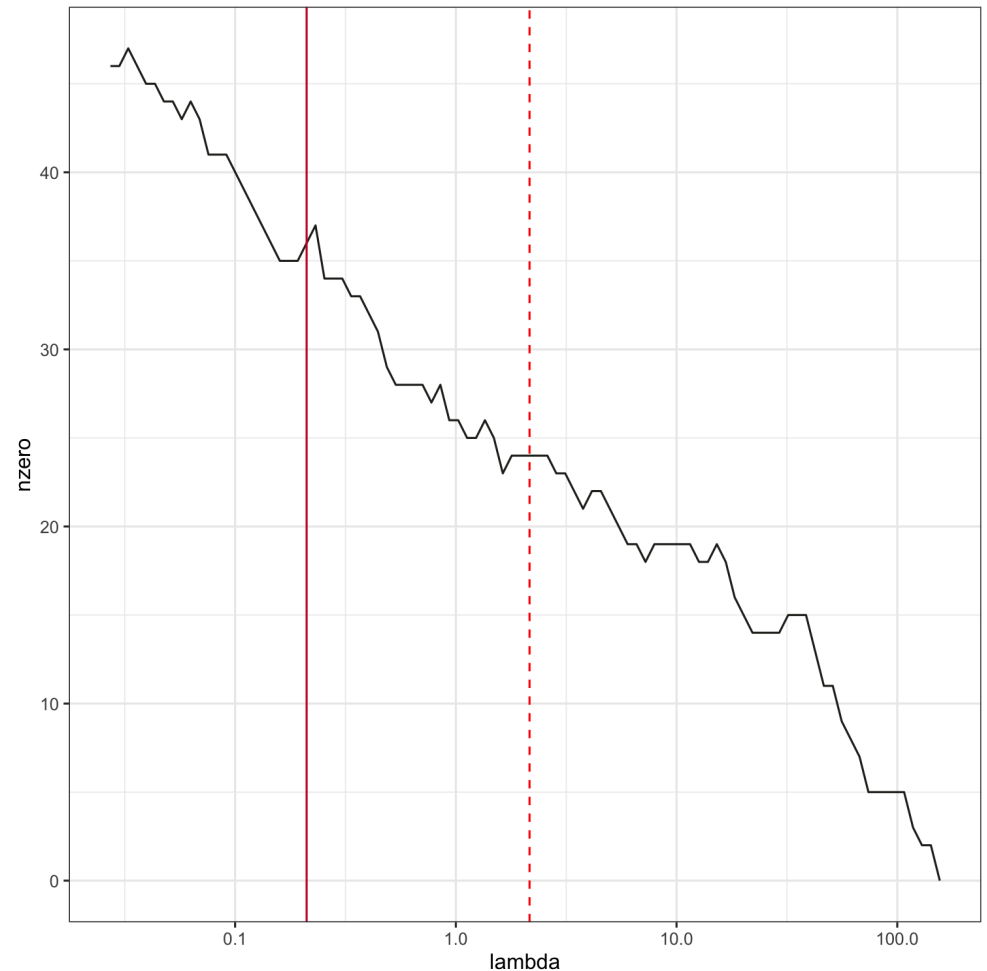
```
## [1] 2
```

Elastic net example

Can view same type of summary

```
tidy(cv_en_50) %>%  
  ggplot(aes(x = lambda, y = nzero)) +  
    geom_line() +  
    geom_vline(xintercept = cv_en_50$lambda.min,  
               geom_vline(xintercept = cv_en_50$lambda.1se  
                           linetype = "dashed",  
                           color = "red")) +  
    scale_x_log10() +  
    theme_bw()
```

- More relaxed than lasso for variable entry



Comparison of models based on holdout performance

```
set.seed(2020)
nfl_model_data <- nfl_model_data %>% mutate(test_fold = sample(rep(1:5, length.out = n()))))
holdout_predictions <-
  map_dfr(unique(nfl_model_data$test_fold),
    function(holdout) {
      # Separate test and training data:
      test_data <- nfl_model_data %>% filter(test_fold == holdout)
      train_data <- nfl_model_data %>% filter(test_fold != holdout)

      # Repeat for matrices
      test_x <- as.matrix(dplyr::select(test_data, -score_diff))
      train_x <- as.matrix(dplyr::select(train_data, -score_diff))

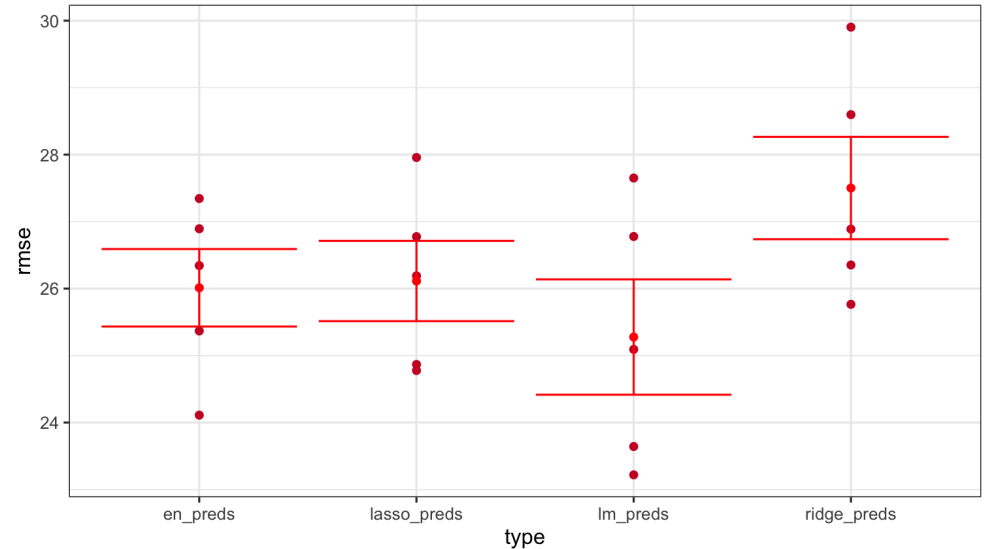
      # Train models:
      lm_model <- lm(score_diff ~ ., data = train_data)
      ridge_model <- cv.glmnet(train_x, train_data$score_diff, alpha = 0)
      lasso_model <- cv.glmnet(train_x, train_data$score_diff, alpha = 1)
      en_model <- cv.glmnet(train_x, train_data$score_diff, alpha = .5)

      # Return tibble of holdout results:
      tibble(lm_preds = predict(lm_model, newdata = test_data),
        ridge_preds = as.numeric(predict(ridge_model, newx = test_x)),
        lasso_preds = as.numeric(predict(lasso_model, newx = test_x)),
        en_preds = as.numeric(predict(en_model, newx = test_x)),
        test_actual = test_data$score_diff, test_fold = holdout)
    })
```

Predictions compared to λ m?

Compute RMSE across folds with std error intervals

```
holdout_predictions %>%  
  pivot_longer(lm_preds:en_preds,  
               names_to = "type", values_to =  
  group_by(type, test_fold) %>%  
  summarize(rmse =  
             sqrt(mean((test_actual - test_p  
ggplot(aes(x = type, y = rmse)) +  
  geom_point() + theme_bw() +  
  stat_summary(fun = mean, geom = "point",  
              color = "red") +  
  stat_summary(fun.data = mean_se, geom = "er  
            color = "red")
```



In this case λ m actually "beat" regularization, but within intervals