Regularization Tutorial

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https://colab.research.google.com/drive/1NW12Nv8Kf_U1Mlr0jyoJrC0NF8y2EasR?usp=sharing

Motivation: In statistics, there are two critical characteristics of estimators to be considered: the bias and the variance:

Bias measures the accuracy of the estimates.

Variance measures the spread, or uncertainty, in these estimates.

Regularization - the aproach which reduces the variance at the cost of introducing some bias. (Almost always beneficial for the predictive performance of the model.)

Load libraries, get data & set seed for reproducibility

```r
set.seed(222)    # seed for reproducibility
library(glmnet)  # for ridge regression
```

```
## Loading required package: Matrix

## Loaded glmnet 4.0-2
```

```r
library(dplyr)   # for data cleaning
```

```
##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```r
library(psych)   # for function tr() to compute trace of a matrix
data("mtcars") #loading data
```

RIDGE REGRESSION

```r
#1. RIDGE REGRESSION
#->decreasing model complexity while keeping all variables in the model

#first, centering:
# Center y, X will be standardized in the modelling function
```

```r
#(ridge regression assumes the predictors are standardized and the response is centered)
y <- mtcars %>% select(mpg) %>% scale(center = TRUE, scale = FALSE) %>% as.matrix()
X <- mtcars %>% select(-mpg) %>% as.matrix()
```

In Ridge Regression, the OLS loss function is augmented in such a way that we not only minimize the sum of squared residuals but also penalize the size of parameter estimates, in order to shrink them towards zero.

Choice of Regularization Parameter:

There are two ways we could tackle this issue. A more traditional approach would be to choose lambda such that some information criterion, e.g., AIC or BIC, is the smallest.

A more machine learning-like approach is to perform cross-validation and select the value of lambda that minimizes the cross-validated sum of squared residuals (or some other measure).

The former approach emphasizes the model's fit to the data, while the latter is more focused on its predictive performance.

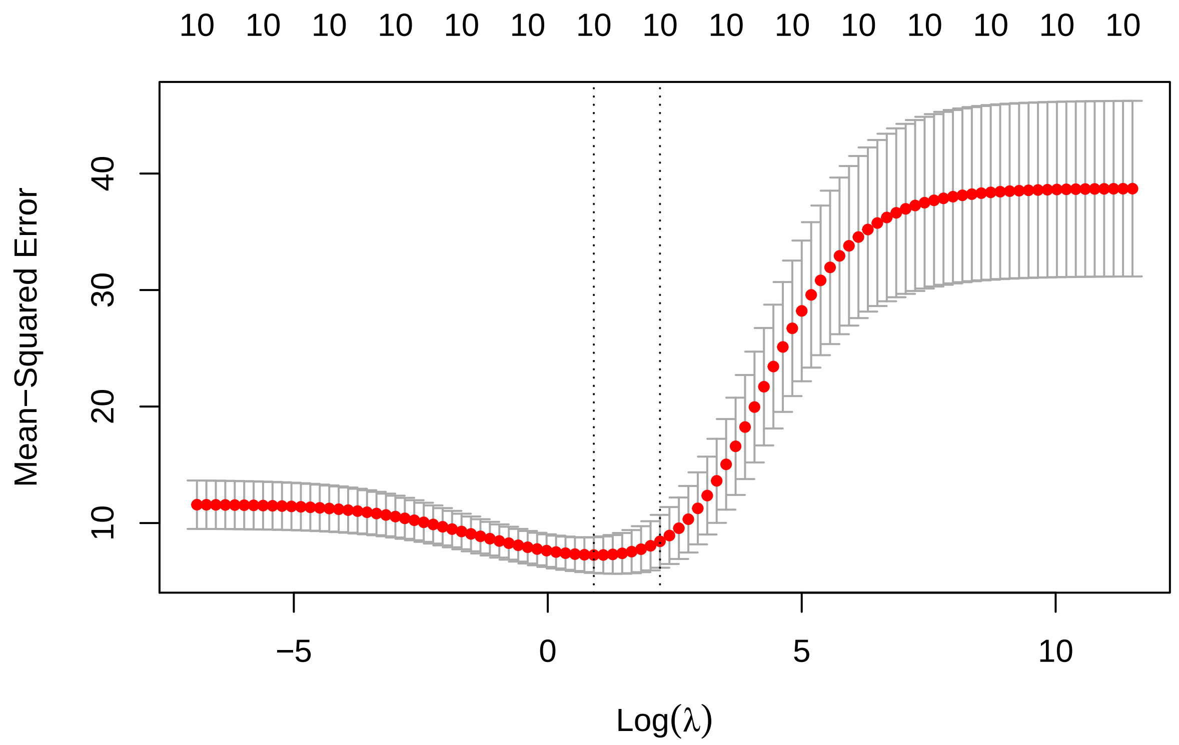
Perform 10-fold cross-validation to select lambda:

```r
lambdas_to_try <- 10^seq(-3, 5, length.out = 100)
#10-fold cross-validation to select lambda

# Setting alpha = 0 implements ridge regression
ridge_cv <- cv.glmnet(X, y, alpha = 0, lambda = lambdas_to_try,
                      standardize = TRUE, nfolds = 10)
#function cv.glmnet does k-fold cross-validation for glmnet,
#produces a plot, and returns a value for lambda



# Plot cross-validation results
plot(ridge_cv)
```



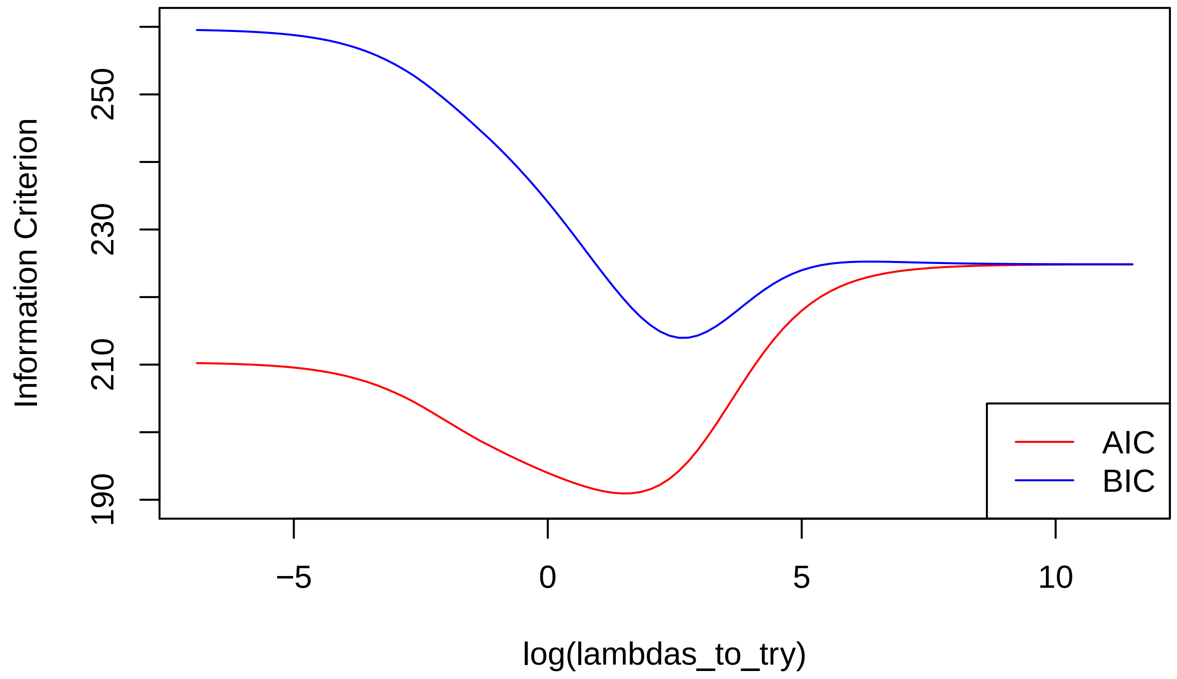
```r
# Best cross-validated lambda
lambda_cv <- ridge_cv$lambda.min
# Fit final model, get its sum of squared residuals and multiple R-squared
model_cv <- glmnet(X, y, alpha = 0, lambda = lambda_cv, standardize = TRUE)
y_hat_cv <- predict(model_cv, X)
ssr_cv <- t(y - y_hat_cv) %*% (y - y_hat_cv) #compute a sum of squared residuals
rsq_ridge_cv <- cor(y, y_hat_cv)^2 #Multiple R squared
```

Use information criteria to select lambda:

```r
X_scaled <- scale(X)
aic <- c()
bic <- c()
for (lambda in seq(lambdas_to_try)) {
  # Run model
  model <- glmnet(X, y, alpha = 0, lambda = lambdas_to_try[lambda], standardize = TRUE)
  # Extract coefficients and residuals (remove first row for the intercept)
  betas <- as.vector((as.matrix(coef(model))[-1, ]))
  resid <- y - (X_scaled %*% betas)
  # Compute hat-matrix and degrees of freedom
  ld <- lambdas_to_try[lambda] * diag(ncol(X_scaled))
  H <- X_scaled %*% solve(t(X_scaled) %*% X_scaled + ld) %*% t(X_scaled)
  df <- tr(H)
  # Compute information criteria
  aic[lambda] <- nrow(X_scaled) * log(t(resid) %*% resid) + 2 * df
  bic[lambda] <- nrow(X_scaled) * log(t(resid) %*% resid) + 2 * df * log(nrow(X_scaled))
}

# Plot information criteria against tried values of lambdas
```

```r
plot(log(lambdas_to_try), aic, col = "red", type = "l",
     ylim = c(190, 260), ylab = "Information Criterion")
lines(log(lambdas_to_try), bic, col = "blue")
legend("bottomright", lwd = 1, col = c("red", "blue"), legend = c("AIC", "BIC"))
```



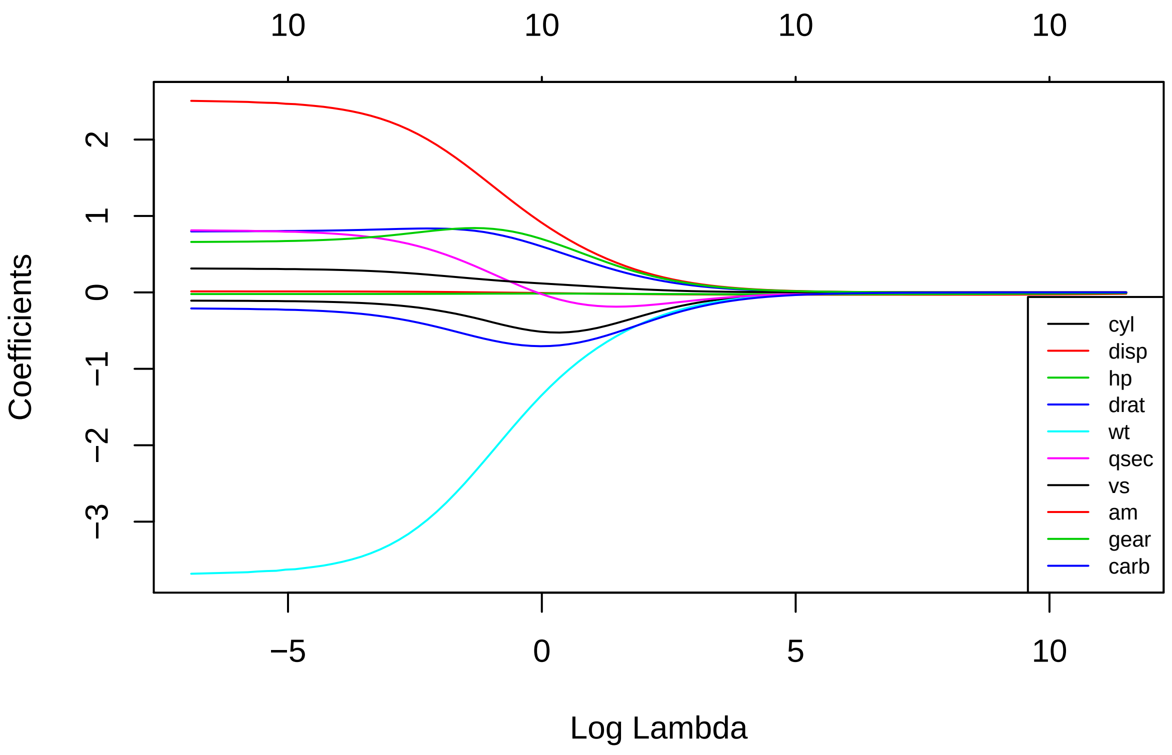
```r
# Optimal lambdas according to both criteria
lambda_aic <- lambdas_to_try[which.min(aic)]
lambda_bic <- lambdas_to_try[which.min(bic)]

# Fit final models, get their sum of squared residuals and multiple R-squared
model_aic <- glmnet(X, y, alpha = 0, lambda = lambda_aic, standardize = TRUE)
y_hat_aic <- predict(model_aic, X)
ssr_aic <- t(y - y_hat_aic) %*% (y - y_hat_aic)
rsq_ridge_aic <- cor(y, y_hat_aic)^2

model_bic <- glmnet(X, y, alpha = 0, lambda = lambda_bic, standardize = TRUE)
y_hat_bic <- predict(model_bic, X)
ssr_bic <- t(y - y_hat_bic) %*% (y - y_hat_bic)
rsq_ridge_bic <- cor(y, y_hat_bic)^2
```

See how increasing lambda shrinks the coefficients :

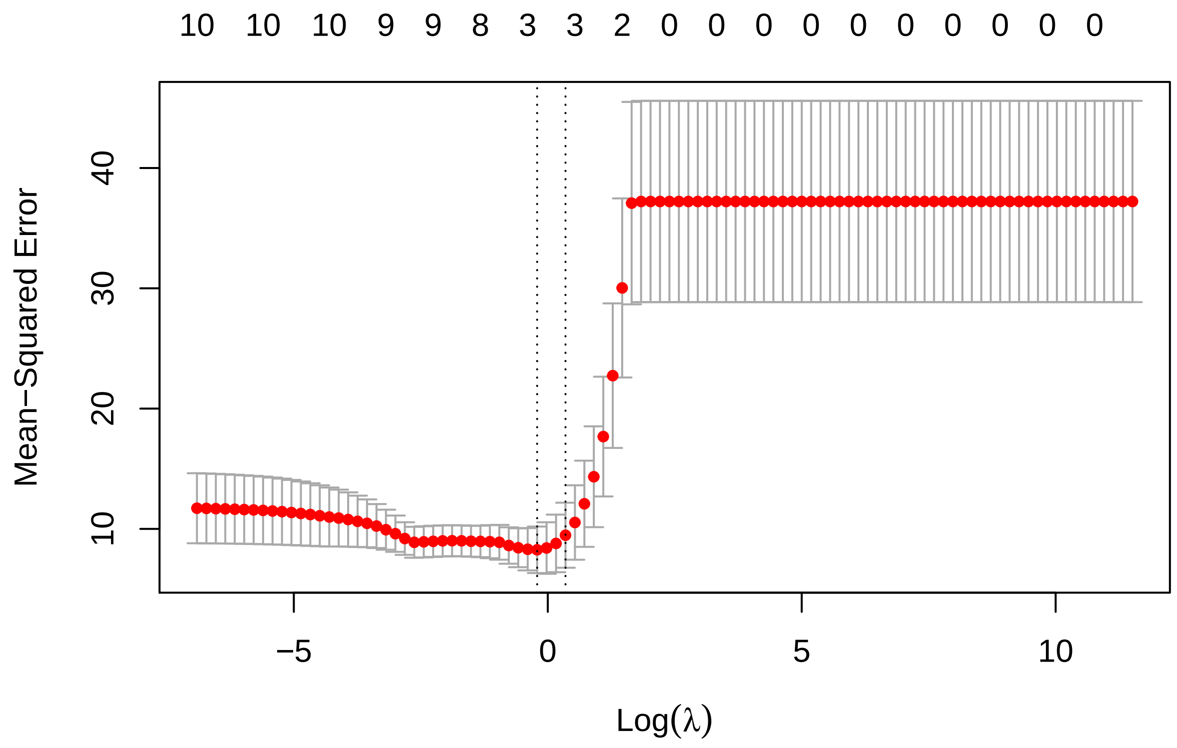
```r
# Each line shows coefficients for one variables, for different lambdas.
# The higher the lambda, the more the coefficients are shrinked towards zero.
res <- glmnet(X, y, alpha = 0, lambda = lambdas_to_try, standardize = FALSE)
plot(res, xvar = "lambda")
legend("bottomright", lwd = 1, col = 1:6, legend = colnames(X), cex = .7)
```



LASSO REGRESSION

Lasso = Least Absolute Shrinkage and Selection Operator, is quite similar conceptually to ridge regression. It also adds a penalty for non-zero coefficients, but unlike ridge regression which penalizes sum of squared coefficients (the so-called L2 penalty), lasso penalizes the sum of their absolute values (L1 penalty). As a result, for high values of lambda, many coefficients are exactly zeroed under lasso, which is never the case in ridge regression.

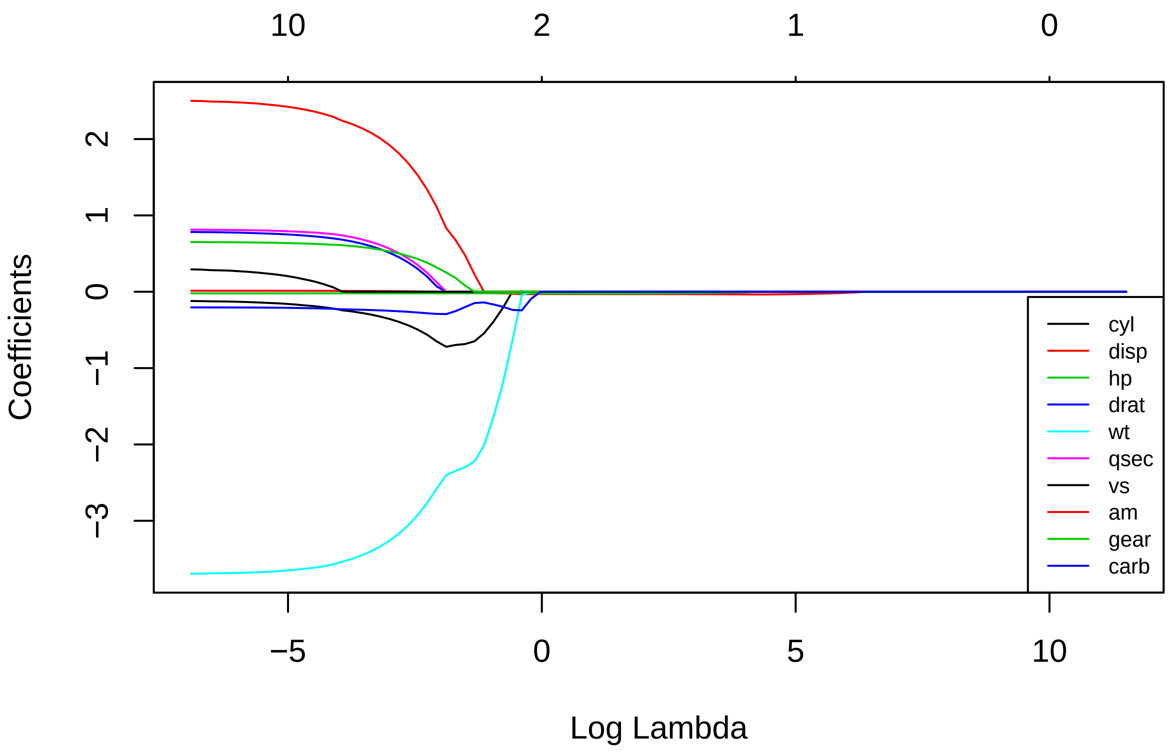
```r
# Perform 10-fold cross-validation to select lambda
lambdas_to_try <- 10^seq(-3, 5, length.out = 100)
# Setting alpha = 1 implements lasso regression
#(you can re-use the glmnet() function, but with the alpha parameter set to 1)
lasso_cv <- cv.glmnet(X, y, alpha = 1, lambda = lambdas_to_try,
                      standardize = TRUE, nfolds = 10)
# Plot cross-validation results
plot(lasso_cv)
```



```r
# Best cross-validated lambda
lambda_cv <- lasso_cv$lambda.min
# Fit final model, get its sum of squared residuals and multiple R-squared
model_cv <- glmnet(X, y, alpha = 1, lambda = lambda_cv, standardize = TRUE)
y_hat_cv <- predict(model_cv, X)#predict  data
ssr_cv <- t(y - y_hat_cv) %*% (y - y_hat_cv) #compute a sum of squared residuals
rsq_lasso_cv <- cor(y, y_hat_cv)^2 #Multiple R squared
#(actually can be viewed as the correlation between response and the fitted values.
```

See how increasing lambda shrinks the coefficients:

```r
# Each line shows coefficients for one variables, for different lambdas.
# The higher the lambda, the more the coefficients are shrinked towards zero.
res <- glmnet(X, y, alpha = 1, lambda = lambdas_to_try, standardize = FALSE)
plot(res, xvar = "lambda")
legend("bottomright", lwd = 1, col = 1:6, legend = colnames(X), cex = .7)
```



Let us compare the multiple R-squared of various models we have estimated:

RIDGE VS. LASSO

```
rsq <- cbind("R-squared" = c(rsq_ridge_cv, rsq_ridge_aic, rsq_ridge_bic, rsq_lasso_cv))
rownames(rsq) <- c("ridge cross-validated", "ridge AIC", "ridge BIC", "lasso cross_validated")
print(rsq)
```

```
##                       R-squared
## ridge cross-validated 0.8536968
## ridge AIC             0.8496310
## ridge BIC             0.8412011
## lasso cross_validated 0.8424217
```

Some more general considerations about how ridge and lasso compare:

- Often neither one is overall better.
- Lasso can set some coefficients to zero, thus performing variable selection, while ridge regression cannot.
- Both methods allow to use correlated predictors, but they solve multicollinearity issue differently:
- In ridge regression, the coefficients of correlated predictors are similar;
- In lasso, one of the correlated predictors has a larger coefficient, while the rest are (nearly) zeroed.
- Lasso tends to do well if there are a small number of significant parameters and the others are close to zero (ergo: when only a few predictors actually influence the response).
- Ridge works well if there are many large parameters of about the same value (ergo: when most predictors impact the response).

(However, in practice, we don't know the true parameter values, so the previous two points are somewhat theoretical. Just run cross-validation to select the more suited model for a specific case)

(optional task)

ELASTIC NET

Elastic Net first emerged as a result of critique on lasso, whose variable selection can be too dependent on data and thus unstable. The solution is to combine the penalties of ridge regression and lasso to get the best of both worlds:

Check multiple R-squared:

```r
y_hat_enet <- predict(elastic_net_model, X)
y_hat_enet
```

```
##           Mazda RX4       Mazda RX4 Wag          Datsun 710      Hornet 4 Drive
##          2.05551135          1.74280776          6.28216492          0.52249594
##   Hornet Sportabout             Valiant          Duster 360           Merc 240D
##         -3.27605721          0.15274583         -5.58554614          2.91074947
##            Merc 230            Merc 280           Merc 280C          Merc 450SE
##          3.20191054         -0.23145256         -0.15061543         -4.52522390
##           Merc 450SL         Merc 450SLC  Cadillac Fleetwood Lincoln Continental
##         -3.98074275         -4.00295948         -8.12176404         -8.41163995
##   Chrysler Imperial            Fiat 128         Honda Civic      Toyota Corolla
##         -8.22108855          7.26534418          8.46202739          8.05969802
##       Toyota Corona    Dodge Challenger         AMC Javelin          Camaro Z28
##          3.86926293         -3.30051536         -2.67542264         -5.50883573
##    Pontiac Firebird           Fiat X1-9       Porsche 914-2        Lotus Europa
##         -4.13174939          7.59060420          6.05949380          6.85211961
##      Ford Pantera L        Ferrari Dino       Maserati Bora          Volvo 142E
##         -1.83268991         -0.04290647         -6.03188981          5.00416337
```

```r
rsq_enet <- cor(y, y_hat_enet)^2
rsq_enet
```

```
##          [,1]
## mpg 0.8570287
```