Lecture 16: Regularization/Shrinkage Methods Big Data and Machine Learning for Applied Economics Econ 4676

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Agenda

- 1 Recap & Implementation
 - K-Fold Cross Validation
- 2 Regularization
 - Lasso
 - Ridge
 - Extension
 - Demo Regularization
- 3 Further Readings

Overfit and out of Sample Prediction

- ML we care about prediction out of sample
- Overfit: complex models predict very well inside a sample but "bad" outside
- Choose the right complexity level
- ► Trade off Bias/Variance
- Challenge: accept some bias to decrease variance

Motivation

- Estimating test error: two approaches
 - 1 We can directly estimate the test error, using either a validation set approach or a cross-validation approach
 - 2 We can indirectly estimate test error by making an adjustment to the training error to account for overfitting.
 - ightharpoonup AIC, BIC, C_p and Adjusted R^2
 - These techniques adjust the training error for the model size, and can be used to select among a set of models with different numbers of variables.
 - ► AIC and BIC are very closely related to classical notions of hypothesis testing.

Demo: Prelogomenon

```
#Load the required packages
library("McSpatial") #loads the package
library("dplyr") #for data wrangling
library("caret") #ML
data(matchdata) #loads the data set
matchdata <- matchdata %>% mutate(price=exp(lnprice)) %>% select(-lnprice)
#transforms log prices to standard prices
set.seed(123) #set the seed for replication purposes
str(matchdata) #compact display
## 'data.frame':
                 3204 obs. of 18 variables:
## $ vear : num 1995 1995 1995 2005 1995 ...
## $ lnland : num 8.23 8.63 8.7 8.63 8.63 ...
## $ lnbldg : num 6.98 7.02 7.22 6.87 7.2 ...
## $ rooms : int 5 5 5 4 6 7 7 6 4 6 ...
## $ bedrooms : int 3 3 3 2 3 3 4 3 2 3 ...
## $ bathrooms: num 1 1.5 1.5 1 1 2 1 2 1.5 1.5 ...
## $ centair : int 0 1 1 0 1 0 1 1 1 1 ...
## $ fireplace: int 0 0 0 0 0 1 0 0 0 0 ...
## $ brick : num 1 1 1 1 1 1 1 1 1 ...
## $ garage1 : num 1 0 0 1 0 1 0 0 1 0 ...
## $ garage2 : num 0 1 1 0 1 0 1 0 0 0 ...
## $ dcbd : num 13.6 13.5 13.6 13.5 13.6 ...
## $ rr : num 0 0 0 0 0 0 0 0 0 ...
## $ vrbuilt : num 1953 1952 1952 1949 1953 ...
## $ carea : Factor w/ 11 levels "Albany Park",..: 3 3 3 3 3 3 3 3 3 3 ...
## $ latitude : num 42 42 42 42 42 ...
## $ longitude: num -87.8 -87.8 -87.8 -87.8 -87.8 ...
## $ price : num 170750 168000 192500 398000 215000 ...
```

Demo: K-fold CV

```
model2 <- train(price ~ bedrooms, # model to fit</pre>
                         data = matchdata.
                         trControl = trainControl(method = "cv", number = 10),
                         # Method: crossvalidation, 10 folds
                         method = "lm")# specifying regression model
model2
## Linear Regression
## 3204 samples
     1 predictor
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 2883, 2884, 2884, 2883, 2884, 2885, ...
## Resampling results:
##
             Rsquared
    RMSE
                        MAE
    147308.8 0.01385314 122117.8
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Demo: K-fold CV

```
model2 <- train(price ~ bedrooms+bathrooms+ rooms+centair+fireplace+brick+
                        lnland+lnbldg+garage1+garage2+
                        dcbd+ rr +
                        yrbuilt+ factor(year) +
                        carea+ latitude+longitude,
                        data = matchdata.
                        trControl = trainControl(method = "cv", number = 10).
                        method = "lm")
```

model2

```
## Linear Regression
## 3204 samples
    17 predictor
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 2883, 2884, 2884, 2883, 2883, 2884, ...
## Resampling results:
##
    RMSE
              Rsquared MAE
    74297.54 0.7490674 48170.37
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Model Subset Selection

- \blacktriangleright We have M_k models
- ▶ We want to find the model that best predicts out of sample
- We have a number of ways to go about it
 - Best Subset Selection
 - Stepwise Selection
 - ► Forward selection
 - Backward selection

Best Subset Selection

$$y = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p + u \tag{1}$$

- **I** Estimate **all** possible models with k = 0, 1, ..., p predictors.
- 2 Compute the prediction error using cross validation
- 3 Pick the one with the smallest prediction error

Caret is usually the solution but it doesn't have everything =(

Linear Regression with Backwards Selection	leapBackward	Regression	leaps	nvmax
Linear Regression with Forward Selection	leapForward	Regression	leaps	nvmax
Linear Regression with Stepwise Selection	leapSeq	Regression	leaps	nvmax

Note: https://topepo.github.io/caret/available-models.html

```
require("leaps")
class(matchdata$carea)
## [1] "factor"
class(matchdata$year)
## [1] "numeric"
matchdata$year<-factor(matchdata$year)</pre>
best<-regsubsets(price ~ ., method="exhaustive",data = matchdata)</pre>
summary(best)
```

```
## Subset selection object
## Call: regsubsets.formula(price ~ ., method = "exhaustive", data = matchdata)
## 26 Variables (and intercept)
## Selection Algorithm: exhaustive
            year2005 lnland lnbldg rooms bedrooms bathrooms centair fireplace
            brick garage1 garage2 dcbd rr yrbuilt careaEdgewater careaEdison Park
                                                    11 --- 11
```

```
careaForest Glen careaJefferson Park careaLincoln Square
careaNorth Park careaNorwood Park careaRogers Park careaUptown
                                                      11 🛊 11
                                                      11 - 11
careaWest Ridge latitude longitude
```

Stepwise Selection

- 1 Forward Stepwise Selection
 - Start with no predictors
 - ► Test all models with 1 predictor. Choose the one with smallest prediction error using cross validation
 - Add 1 predictor at a time, without taking away.
 - ▶ Of the p+1 models, choose the one with smallest prediction error using cross validation
- 2 Backward Stepwise Selection
 - Same idea but start with a complete model and go backwards, taking one at a time.

```
forward <- train(price ~ ., data = matchdata,</pre>
                method = "leapForward",
                trControl = trainControl(method = "cv", number = 10))
forward
## Linear Regression with Forward Selection
## 3204 samples
    17 predictor
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 2884, 2884, 2884, 2883, 2883, 2883, ...
## Resampling results across tuning parameters:
##
    nymax RMSE
               Rsquared MAE
      84219.28 0.6768962 55184.58
   3 79212.49 0.7147519 51009.82
##
          78595.00 0.7193113 50631.17
## RMSE was used to select the optimal model using the smallest value.
```

The final value used for the model was nvmax = 4.

summary(forward\$finalModel)

```
## Subset selection object
## 26 Variables (and intercept)
                       Forced in Forced out
## 1 subsets of each size up to 4
## Selection Algorithm: forward
            year2005 lnland lnbldg rooms bedrooms bathrooms centair fireplace
            brick garage1 garage2 dcbd rr yrbuilt careaEdgewater careaEdison Park
            careaForest Glen careaJefferson Park careaLincoln Square
            careaNorth Park careaNorwood Park careaRogers Park careaUptown
            careaWest Ridge latitude longitude
```

```
backwards <- train(price ~ ., data = matchdata,
                method = "leapBackward",
                trControl = trainControl(method = "cv", number = 10))
backwards
## Linear Regression with Backwards Selection
## 3204 samples
    17 predictor
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 2884, 2882, 2884, 2885, 2883, 2884, ...
## Resampling results across tuning parameters:
##
    nymax RMSE
               Rsquared MAE
      84353.39 0.6769755 55217.19
  3 79280.53 0.7153318 51000.22
##
          78137 63 0 7235894 49820 72
## RMSE was used to select the optimal model using the smallest value.
```

The final value used for the model was nymax = 4.

summary(backwards\$finalModel)

```
## Subset selection object
## 26 Variables (and intercept)
## Selection Algorithm: backward
            year2005 lnland lnbldg rooms bedrooms bathrooms centair fireplace
            brick garage1 garage2 dcbd rr yrbuilt careaEdgewater careaEdison Park
            careaForest Glen careaJefferson Park careaLincoln Square
            careaNorth Park careaNorwood Park careaRogers Park careaUptown
            careaWest Ridge latitude longitude
```

Regularization

- ► Isn't it worth starting with the general model (p-variables) and crossing out the non-significant coefficients?
- ▶ Or we could go the following path:
 - Run model, get coefficients and p-values
 - Take out those with p-values bellow a certain α (we can adjust for FDR)
 - ▶ Why is this a bad idea?
- Backward selection approximates that idea (not exactly) and does a better job that the previous point

Regularization

- ► The key of moder statistics is regularization
- ► The strategy involves penalizing complexity so as to depart from optimality and stabilize the system
- 'Crossing out' variables / coefficients is an extreme way to 'shrink' them.
- Lasso: a formal and algorithmic way of accomplishing this task.

Lasso

For $\lambda \ge 0$ given, consider minimizing the following objective function

$$min_{\beta}L(\beta) = \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda \sum_{s=2}^{p} |\beta_s|$$
 (2)

- ► Note:
 - First coef. constant
 - $\lambda = 0$?
 - $\lambda = \infty$?

Lasso

$$min_{\beta}L(\beta) = \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda \sum_{s=2}^{p} |\beta_s|$$
 (3)

- ► LASSO magic: it automatically choses which variables go in $(\beta_s \neq 0)$ and which are out $(\beta_s = 0)$
- ▶ Why? Coefficients that don't go in are corner solutions
- $ightharpoonup L(\beta)$ in non differentiable



► Lasso Intuition

$$min_{\beta}L(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda|\beta|$$
 (4)

- ▶ Only one predictor, i.e., one coefficient.
- ► Standardize predictor $\sum x_i^2 = 1$ so

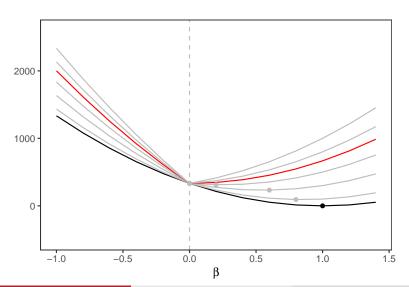
$$\hat{\beta}_{OLS} = \frac{\sum_{i} x_i y_i}{\sum_{i} x_i^2} \tag{5}$$

$$min_{\beta}L(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda|\beta|$$
 (6)

$$L(\beta) = \sum_{i=1}^{n} (y_i - x_i \beta)^2 + \lambda |\beta| = \begin{cases} \sum_{i=1}^{n} (y_i - x_i \beta)^2 + \lambda \beta & \text{if } \beta \ge 0\\ \sum_{i=1}^{n} (y_i - x_i \beta)^2 - \lambda \beta & \text{if } \beta \le 0 \end{cases}$$
(7)

- Non differentiable at $\beta = 0$
- ▶ Differentiable otherwise $\beta \neq 0$





$$\frac{dL(\beta)^{+}}{d\beta} = -2\sum y_{i}x_{i} + 2\beta\sum x_{i}^{2} + \lambda$$

$$= -2\sum y_{i}x_{i} + \beta + \lambda$$
(8)

$$\frac{dL(0)^+}{d\beta} = -2\sum y_i x_i + \lambda$$

then, if

$$\lambda \ge 2\sum y_i x_i \tag{9}$$

we have $\hat{\beta}_{lasso} = 0$



if $\lambda < 2 \sum y_i x_i$ we have an interior solution

$$-2\sum y_i x_i + \hat{\beta}_{lasso} + \lambda = 0 \tag{10}$$

$$\hat{\beta}_{lasso} = \sum y_i x_i - \frac{\lambda}{2} \tag{11}$$

$$\hat{\beta}_{lasso} = \hat{\beta}_{OLS} - \frac{\lambda}{2} \tag{12}$$

Ridge

For $\lambda \ge 0$ given, consider minimizing the following objective function

$$min_{\beta}R(\beta) = \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda \sum_{s=2}^{p} (\beta_s)^2$$
 (13)

- ► Note:
 - Intuition is similar to Lasso, however the problem is completely different

Ridge

$$min_{\beta}R(\beta) = \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda(\beta_s)^2$$
(14)

FOC

$$-2\sum_{i=1}^{n} y_i x_i + 2\beta + 2\lambda \beta_s = 0$$
 (15)

$$\hat{\beta}_{ridge} = \frac{\sum_{i=1}^{n} y_i x_i}{(1+\lambda)}$$

$$= \frac{\beta_{OLS}}{(1+\lambda)}$$
(16)

- Solution is always interior (unlike Lasso)
- Solutions is "shrunken"



Lasso and Ridge Intuition

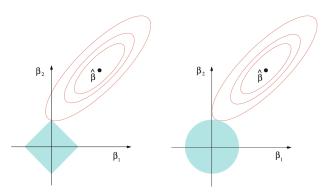


FIGURE 3.11. Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions $|\beta_1| + |\beta_2| \le t$ and $\beta_1^2 + \beta_2^2 \le t^2$, respectively, while the red ellipses are the contours of the least squares error function.

Technical comments

- We showed that Ridge is biased, but for certain λ $MSE(\beta_{ridge}) < MSE(\beta_{OLS})$
- ► Not possible to derive an exact result for Lasso, but ridge approximates to lasso
- Lasso shrinks everything towards zero, Ridge not quite so
- ► Application wise:
 - Standardize the data
 - ▶ Selection of λ ?

Technical comments: λ Selection

- \triangleright Selection of λ ?
- ▶ Use CV
- ► Choose a grid of λ values, and compute the CV error for each value
- ► Select the λ^* that minimizes the prediction error
- Estimate using all the observations and the selected λ^*

Extension

► Family of penalized regressions

$$min_{\beta}R(\beta) = \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda \sum_{s=2}^{p} |\beta_s|^p$$
 (17)



FIGURE 3.12. Contours of constant value of $\sum_{j} |\beta_{j}|^{q}$ for given values of q.

Combination? Elastic Net

$$min_{\beta}EL(\beta) = \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda_1 \sum_{s=2}^{p} |\beta_s| + \lambda_2 \sum_{s=2}^{p} \beta_s^2$$

$$= \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda \sum_{s=2}^{p} ((1 - \alpha)\beta_s^2 + \alpha|\beta_s|)$$
(18)

lambda $<-10^seq(-2, 3, length = 10)$

```
lasso <- train(
 price ".. data = matchdata, method = "glmnet",
 trControl = trainControl("cv", number = 10),
 tuneGrid = expand.grid(alpha = 1.
 lambda=lambda), preProcess = c("center", "scale")
lasso
## 3204 samples
    17 predictor
##
##
## Pre-processing: centered (26), scaled (26)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 2884, 2885, 2882, 2883, 2885, 2883, ...
## Resampling results across tuning parameters:
##
                  RMSE
                            Rsquared
##
     lambda
                                       MAE
    1.000000e-02 74410.32 0.7487304
                                       48120.44
##
    3.593814e-02 74410.32 0.7487304 48120.44
    1.291550e-01 74410.32 0.7487304 48120.44
##
    4.641589e-01 74410.32 0.7487304 48120.44
##
    1.668101e+00 74410.32 0.7487304 48120.44
##
    5.994843e+00 74410.32 0.7487304 48120.44
##
    2.154435e+01 74410.32 0.7487304 48120.44
    7.742637e+01 74411.91 0.7487131 48102.41
##
##
     2.782559e+02 74485.72 0.7481557 48011.74
##
     1.000000e+03 74702.02 0.7467291 47865.45
##
## Tuning parameter 'alpha' was held constant at a value of 1
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were alpha = 1 and lambda = 21.54435.
```

Lecture 16

```
ridge <- train(
 price ".. data = matchdata, method = "glmnet",
 trControl = trainControl("cv", number = 10),
 tuneGrid = expand.grid(alpha = 0,lambda=lambda), preProcess = c("center", "scale")
ridge
## 3204 samples
    17 predictor
##
## Pre-processing: centered (26), scaled (26)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 2884, 2883, 2883, 2884, 2884, 2883, ...
## Resampling results across tuning parameters:
##
                        Rsquared
##
    lambda
                  RMSE
                                       MAE
    1.000000e-02 75133.92 0.7479252 47361.73
##
##
    3.593814e-02 75133.92 0.7479252 47361.73
    1.291550e-01 75133.92 0.7479252 47361.73
##
##
     4.641589e-01 75133.92 0.7479252 47361.73
    1.668101e+00 75133.92 0.7479252 47361.73
##
    5.994843e+00 75133.92 0.7479252 47361.73
##
    2.154435e+01 75133.92 0.7479252 47361.73
##
    7.742637e+01 75133.92 0.7479252 47361.73
##
    2.782559e+02 75133.92 0.7479252 47361.73
##
     1.000000e+03 75133.92 0.7479252 47361.73
##
## Tuning parameter 'alpha' was held constant at a value of 0
```

RMSE was used to select the optimal model using the smallest value.
The final values used for the model were alpha = 0 and lambda = 1000.

```
el <- train(
 price ~., data = matchdata, method = "glmnet",
 trControl = trainControl("cv", number = 10), preProcess = c("center", "scale")
e1
## glmnet
##
## 3204 samples
    17 predictor
##
## Pre-processing: centered (26), scaled (26)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 2885, 2885, 2883, 2884, 2883, 2884, ...
## Resampling results across tuning parameters:
##
##
                       RMSE
    alpha lambda
                                Rsquared
                                           MAE
    0.10
             230.7569
                      74163.82 0.7525328
                                           48112.63
    0.10 2307.5689 74241.34 0.7518849 47772.50
##
    0.10 23075.6893 76941.03 0.7489116 48065.77
    0.55
           230.7569 74161.27 0.7524710 48056.67
##
##
    0.55 2307.5689 74420.59 0.7505525 47656.06
    0.55
           23075.6893 82931.37 0.7161268 52413.46
##
##
   1.00 230.7569 74189.84 0.7522040 48029.77
##
   1.00
            2307.5689 74622.97 0.7493269 47527.50
##
    1.00
           23075.6893 88016.04 0.6846917 57561.95
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were alpha = 0.55 and lambda = 230.7569.
```

```
models <- list(ridge = ridge, lasso = lasso, elastic = el)</pre>
resamples(models) %>% summary( metric = "RMSE")
##
## Call:
## summary.resamples(object = ., metric = "RMSE")
##
```

Mean 3rd Qu.

Models: ridge, lasso, elastic ## Number of resamples: 10

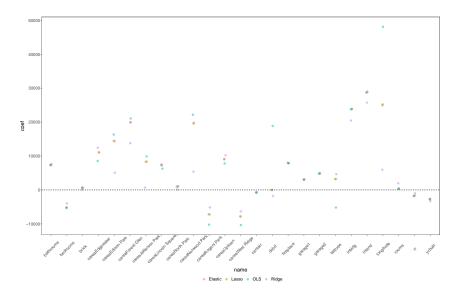
Min. 1st Qu. Median

ridge 64485.44 70582.29 74874.23 75133.92 77717.74 89880.65

66245.34 71294.79 74792.57 74410.32 78080.16 80946.67 ## elastic 59004.20 69395.53 71960.20 74161.27 78485.49 88578.06

RMSE

lasso



Further Readings

- ▶ Friedman, J., Hastie, T., & Tibshirani, R. (2001). The elements of statistical learning (Vol. 1, No. 10). New York: Springer series in statistics.
- ▶ James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). An introduction to statistical learning (Vol. 112, p. 18). New York: springer.
- ► Kuhn, M. (2012). The caret package. R Foundation for Statistical Computing, Vienna, Austria. https://topepo.github.io/caret/index.html
- ► Taddy, M. (2019). Business data science: Combining machine learning and economics to optimize, automate, and accelerate business decisions. McGraw Hill Professional.