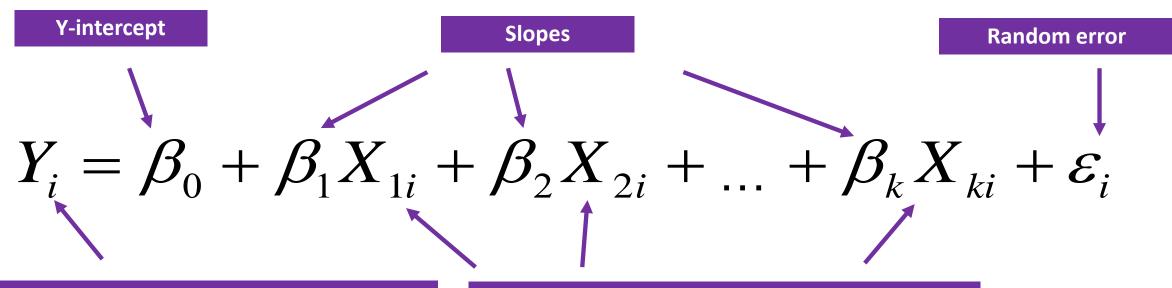
# More Linear Regression Models

Subset Selection
Ridge Regression
Lasso

Principal Components Regression Partial Least Squares Regression

# The Multiple Regression Model

The relationship between one dependent and two or more independent variables can be modeled using a linear function



**Dependent (Response) variable** 

**Independent (Explanatory) variables** 

## Why multiple regression is tricky

Interactions (high correlations) among variables can mask true relationships (Multicollinearity)

We need a higher *n* to better estimate many coefficients

Slopes are estimates with high errors when multicollinear!

MANY organismal measurements are significantly correlated with each other!

#### **Example:**

Does it help to use tibia length and femur length in multiple regression to predict stature? NOT USING OLS REGRESSION!

## **OLS - Ordinary Least Squares Regression**

#### Advantages

- Simpler models, even when multiple regression
- Low bias (if p < n) (number of predictors < sample size)
- Fit can be acceptable even if less than ideal
- Predictive accuracy can be acceptable even if less than ideal

But there are other ways of fitting a straight line to data

- necessary if p > n (OLS impossible) or p "near n (OLS has high variance)

- we can constrain or shrink coefficients to reduce variance (with some bias)

# Other ways of fitting a linear model Advantages

Some predictors are not useful, so should be attenuated in model

- makes models easier to interpret
- in effect, feature selection/variable selection

#### Subset selection

Fit a model using the most valuable predictors

- similar to stepwise selection in classification

## **Best Subset Selection**

## Ideally, fit every combination of predictors

#### Algorithm 6.1 Best subset selection

- 1. Let  $\mathcal{M}_0$  denote the *null model*, which contains no predictors. This model simply predicts the sample mean for each observation.
- 2. For  $k = 1, 2, \dots p$ :
  - (a) Fit all  $\binom{p}{k}$  models that contain exactly k predictors.

**Problem:** Roughly  $2^p$  models Could be > 100,000 models!

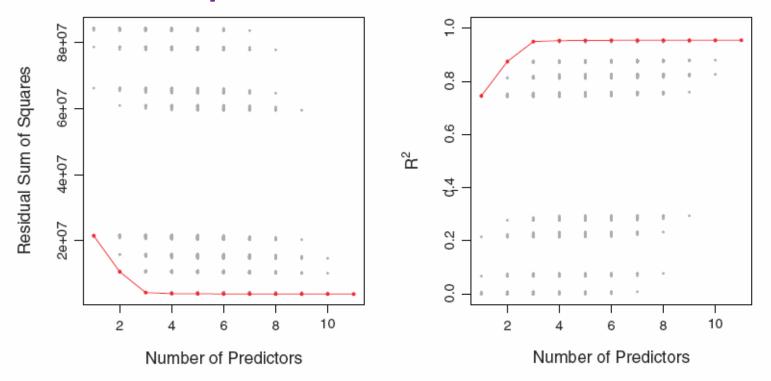
training (b) Pick the best among these  $\binom{p}{k}$  models, and call it  $\mathcal{M}_k$ . Here best is defined as having the smallest RSS, or equivalently largest  $R^2$ .

**Problem**: RSS decreases, R<sup>2</sup> increases with more predictors

3. Select a single best model from among  $\mathcal{M}_0, \dots, \mathcal{M}_p$  using cross-validated prediction error,  $C_p$  (AIC), BIC, or adjusted  $R^2$ .

**Solution:** test samples

# The problems of RSS (MSE) and R<sup>2</sup>: ML provides a solution



**FIGURE 6.1.** For each possible model containing a subset of the ten predictors in the Credit data set, the RSS and  $R^2$  are displayed. The red frontier tracks the best model for a given number of predictors, according to RSS and  $R^2$ . Though the data set contains only ten predictors, the x-axis ranges from 1 to 11, since one of the variables is categorical and takes on three values, leading to the creation of two dummy variables.

# Which predictors estimate best? **Stepwise Methods**

#### All possible subsets

find the best combination of p predictors that maximizes AIC/BIC/adusted R<sup>2</sup>

8 of 15: 6,435 5 of 20: 15,504 10 of 20: 184,756

#### **Forward Selection**

- add the best predictor one at a time (Maximum 240 models for 15 predictors)

#### **Backward Elimination**

get rid of the worst predictors one at a time (smallest effect on RSS) IFF n > p

Hybrid Stepwise (Combination of Forward and Backward)

# **Stepwise Selection**

#### Results can be very similar

- forward stepwise is ALWAYS doable and is ALWAYS faster

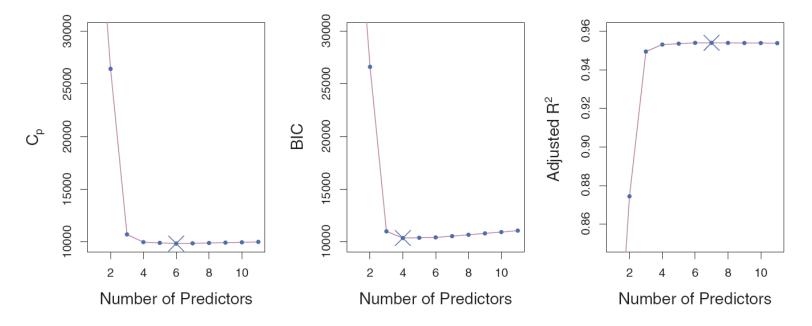
# Variables	Best subset	Forward stepwise
One	rating	rating
Two	rating, income	rating, income
Three	rating, income, student	rating, income, student
Four	cards, income,	rating, income,
	student, limit	student, limit

**TABLE 6.1.** The first four selected models for best subset selection and forward stepwise selection on the Credit data set. The first three models are identical but the fourth models differ.

We can use the training set to assess fit using C<sub>p</sub>, AIC, BIC, or adjusted R<sup>2</sup>

$$C_p = \frac{1}{n} \left( \text{RSS} + 2d\hat{\sigma}^2 \right)$$

where d = number of predictors and  $\hat{\sigma}^2$  is the variance of the error estimate



**FIGURE 6.2.**  $C_p$ , BIC, and adjusted  $R^2$  are shown for the best models of each size for the Credit data set (the lower frontier in Figure 6.1).  $C_p$  and BIC are estimates of test MSE. In the middle plot we see that the BIC estimate of test error shows an increase after four variables are selected. The other two plots are rather flat after four variables are included.

We must use a test set or cross-validation to estimate MSE/RSS

(not training C<sub>p</sub>, AIC, BIC, or adjusted R<sup>2</sup>)

#### We can use training-test samples of 0.75, 0.25 or 10-fold cross-validation

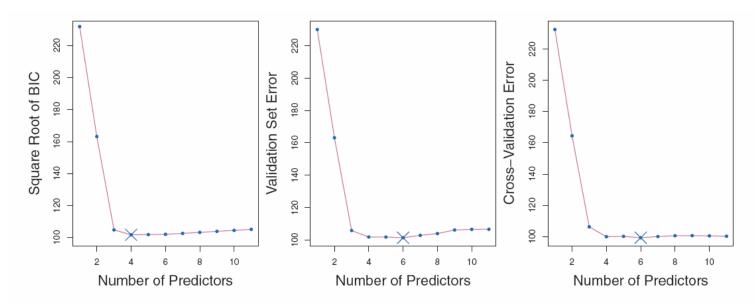


FIGURE 6.3. For the Credit data set, three quantities are displayed for the best model containing d predictors, for d ranging from 1 to 11. The overall best model, based on each of these quantities, is shown as a blue cross. Left: Square root of BIC. Center: Validation set errors. Right: Cross-validation errors.



## Models with 3 to 11 predictors look pretty flat!

- if we ran again, best number of predictors could change

#### How to choose?

Calculate the standard error of the MSE for each number of predictors

Choose the smallest number of predictors within 1 s.e. of smallest value

(Occams' razor - simpler models are better!)

# Other ways of fitting a linear model

## **Shrinkage**

- fit a model using all predictors, but shrink (regularize) all coefficients toward 0.
- if exactly zero, they have been removed
- reduces the variance (regularized) and adds small bias
- tradeoff is worth it!

Be sure to standardize the predictors!

# **Shrinkage**

The OLS model minimizes:

RSS = 
$$\sum_{i=1}^{n} \left( y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^{-1}$$

The shrinkage model minimizes

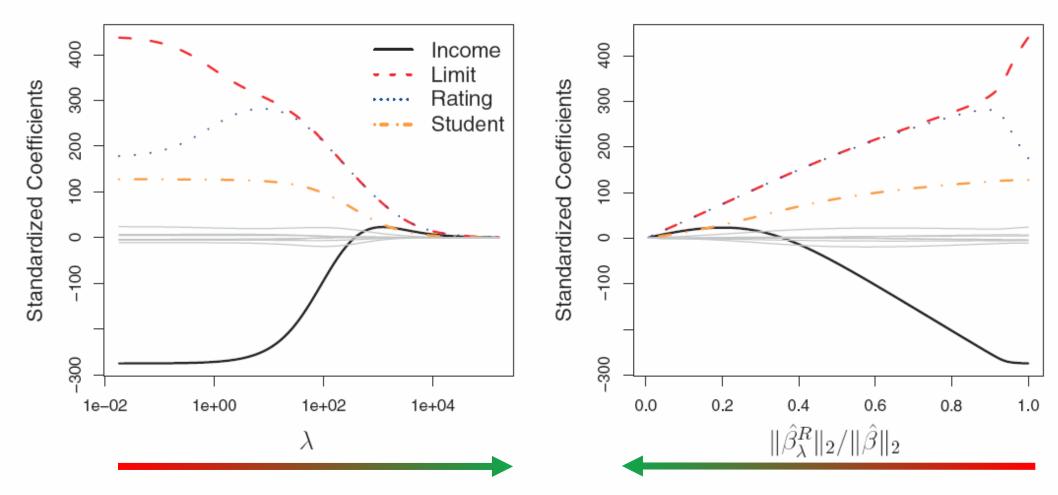
$$RSS + \lambda \sum_{j=1}^{P} \beta_j^2$$

The tuning parameter = lambda > 0

shrinkage penalty (sum of squared coefficients)

# **Shrinkage**

## **Coefficients with shrinkage**

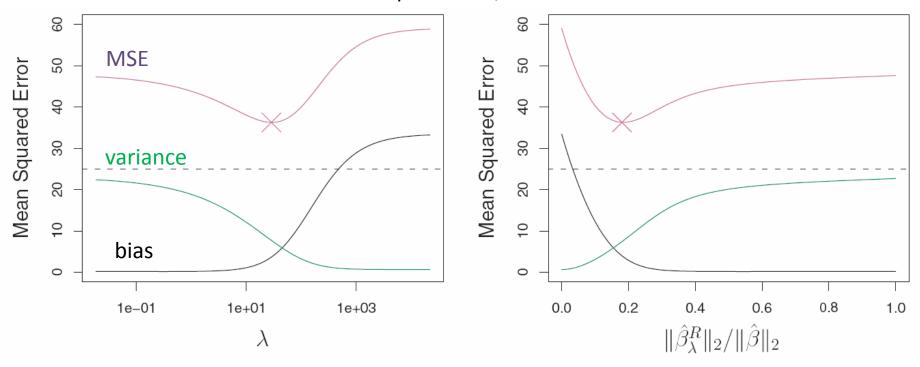


**FIGURE 6.4.** The standardized ridge regression coefficients are displayed for the Credit data set, as a function of  $\lambda$  and  $\|\hat{\beta}_{\lambda}^{R}\|_{2}/\|\hat{\beta}\|_{2}$ .

# **Shrinkage**

## The sweet spot in the bias-variance tradeoff

45 predictors, n = 50



**FIGURE 6.5.** Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of  $\lambda$  and  $\|\hat{\beta}_{\lambda}^{R}\|_{2}/\|\hat{\beta}\|_{2}$ . The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.

Shrinkage uses all predictors, so understanding the model can be difficult

- some are not completely removed

The Lasso actually removes some predictors

- so it performs variable selection

The Lasso produces sparse models - with fewer predictors

- uses a tuning parameter  $\lambda$ , and we can use cross-validation to choose  $\lambda$
- can also use a budget (constraint, s) on how many  $\beta_{\lambda}^{R} > 0$  (Lasso coefficients)
- so we can perform selection on many more predictors

## The shrinkage model minimizes

$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

The tuning parameter = lambda > 0

shrinkage penalty (sum of squared coefficients)

#### The Lasso model minimizes

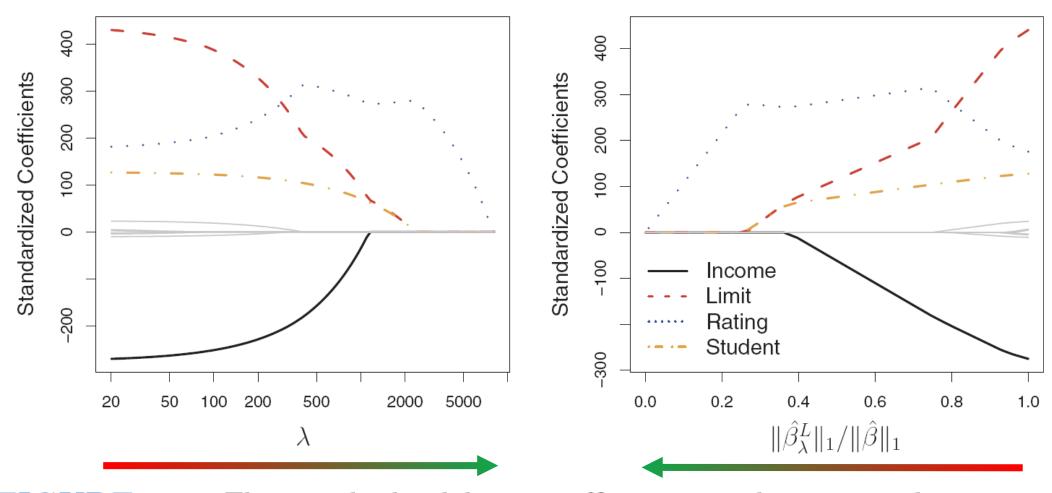
$$RSS + \lambda \sum_{j=1}^{P} |\beta_j|$$

The tuning parameter = lambda > 0

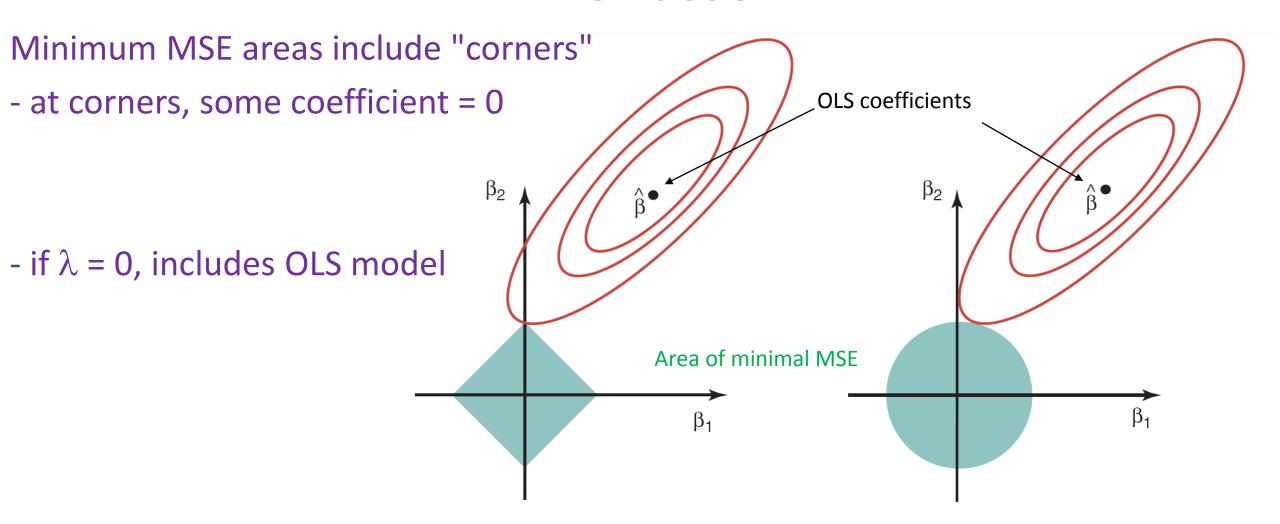
With high  $\lambda$ , some coefficients will be zero

shrinkage penalty (sum of absolute values of coefficients)

#### Coefficients with the lasso: some = 0 before others



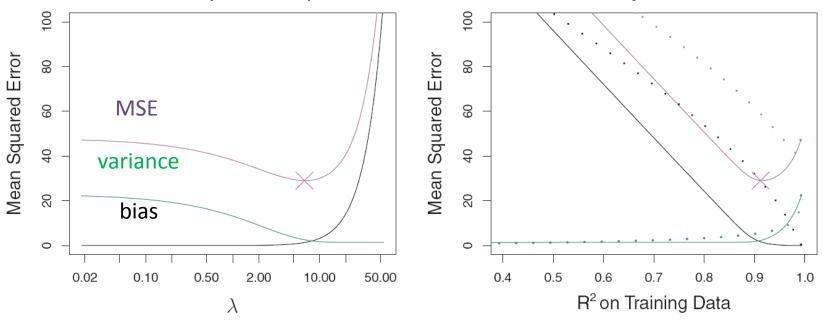
**FIGURE 6.6.** The standardized lasso coefficients on the Credit data set are shown as a function of  $\lambda$  and  $\|\hat{\beta}_{\lambda}^{L}\|_{1}/\|\hat{\beta}\|_{1}$ .



**FIGURE 6.7.** Contours of the error and constraint functions for the lasso (left) and ridge regression (right). The solid blue areas are the constraint regions,  $|\beta_1| + |\beta_2| \le s$  and  $\beta_1^2 + \beta_2^2 \le s$ , while the red ellipses are the contours of the RSS.

## The "sweet spot" using the lasso

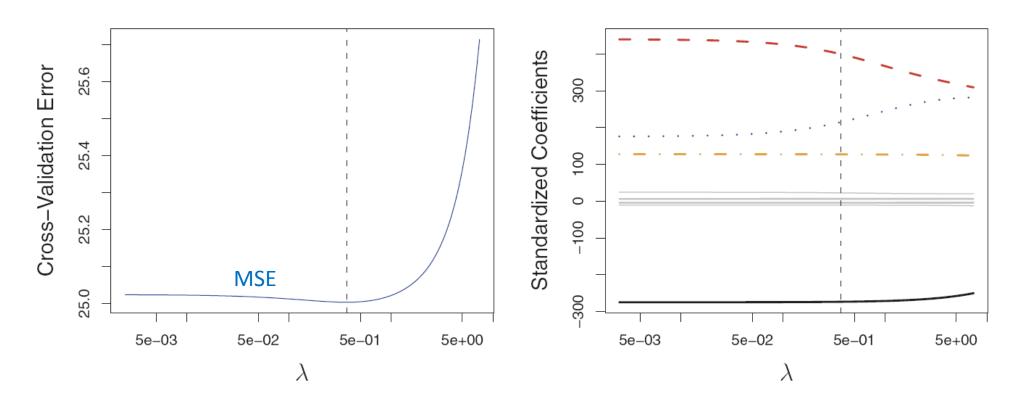




**FIGURE 6.9.** Left: Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso. The simulated data is similar to that in Figure 6.8, except that now only two predictors are related to the response. Right: Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dotted). Both are plotted against their  $R^2$  on the training data, as a common form of indexing. The crosses in both plots indicate the lasso model for which the MSE is smallest.

# **Tuning**

## The "sweet spot" for $\lambda$ using ridge regression



**FIGURE 6.12.** Left: Cross-validation errors that result from applying ridge regression to the Credit data set with various value of  $\lambda$ . Right: The coefficient estimates as a function of  $\lambda$ . The vertical dashed lines indicate the value of  $\lambda$  selected by cross-validation.

# **Tuning**

## The "sweet spot" for $\lambda$ using the lasso

Uses only 2 of 45 predictors correlated with response, n = 50

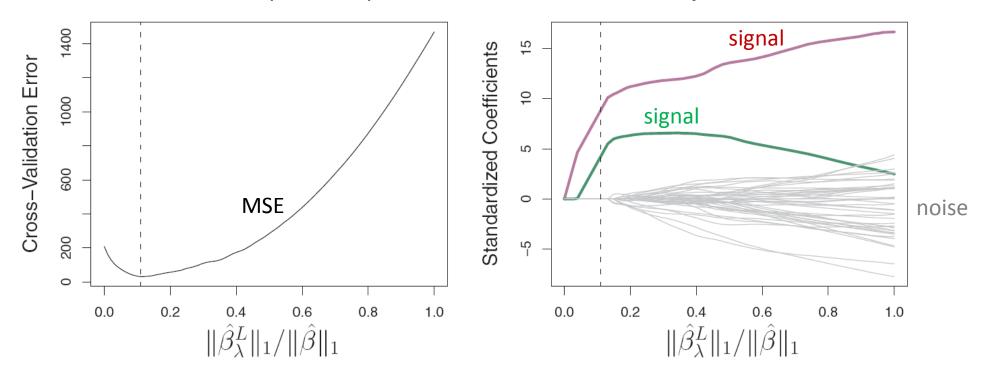


FIGURE 6.13. Left: Ten-fold cross-validation MSE for the lasso, applied to the sparse simulated data set from Figure 6.9. Right: The corresponding lasso coefficient estimates are displayed. The vertical dashed lines indicate the lasso fit for which the cross-validation error is smallest.

# Ridge Regression and the Lasso

**Ridge Regression** will perform better when the outcome is a function of many predictors with roughly equal coefficients

The Lasso will perform better when the outcome is a function of a small number of predictors and the rest are very small or zero

We do not know these things in advance!

So we use cross-validation to see which is best for the data at hand

Use the lasso for interpretations using simpler models

We will use cross-validation to select values for  $\lambda$  and s

# R, Lasso, Ridge Regression

```
# install.packages("glmnet")
library(glmnet) # lasso and ridge regression
#install.packages("ISLR")
library(ISLR)
#library(caret) #tune hyper-parameters
library(leaps) # subset selection

Hitters <- na.omit(Hitters)</pre>
```

#### str(Hitters) # in ISLR 'data.frame': 322 obs. of 20 variables: 293 315 479 496 321 594 185 298 323 401 ... \$ AtBat : num \$ Hits 66 81 130 141 87 169 37 73 81 92 ... : num \$ HmRun : num 18 20 10 4 1 0 6 17 ... Runs 30 24 66 65 39 74 23 24 26 49 ... : num 29 38 72 78 42 51 8 24 32 66 ... \$ RBI : num \$ Walks 14 39 76 37 30 35 21 7 8 65 ... : num 1 14 3 11 2 11 2 3 2 13 ... \$ Years : num 293 3449 1624 5628 396 ... \$ CAtBat : num 66 835 457 1575 101 ... \$ CHits : num \$ CHmRun 1 69 63 225 12 19 1 0 6 253 ... : num \$ CRuns 30 321 224 828 48 501 30 41 32 784 ... : num 29 414 266 838 46 336 9 37 34 890 ... \$ CRBI : num \$ CWalks 14 375 263 354 33 194 24 12 8 866 ... : num \$ League : Factor w/ 2 levels "A", "N": 1 2 1 2 2 1 2 1 2 1 ... \$ Division : Factor w/ 2 levels "E", "W": 1 2 2 1 1 2 1 2 2 1 ... 446 632 880 200 805 282 76 121 143 0 ... \$ PutOuts : num \$ Assists : num 33 43 82 11 40 421 127 283 290 0 ... \$ Errors 20 10 14 3 4 25 7 9 19 0 ... : num NA 475 480 500 91.5 750 70 100 75 1100 ... \$ Salary : num

\$ NewLeague: Factor w/ 2 levels "A", "N": 1 2 1 2 2 1 1 1 2 1 ...

#### **Hitters**

A data frame with 322 observations of major league players on the following 20 variables.

AtBat Number of times at bat in 1986

Hits Number of hits in 1986

HmRun Number of home runs in 1986

Runs Number of runs in 1986

RBI Number of runs batted in in 1986

Walks Number of walks in 1986

Years Number of years in the major leagues

CAtBat Number of times at bat during his career

CHits Number of hits during his career

CHmRun Number of home runs during his career

CRuns Number of runs during his career

CRBI Number of runs batted in during his career

CWalks Number of walks during his career

League A factor with levels A and N indicating player's league at the end of 1986

Division A factor with levels E and W indicating player's division at the end of 1986

PutOuts Number of put outs in 1986

Assists Number of assists in 1986

Errors Number of errors in 1986

Salary 1987 annual salary on opening day in thousands of dollars

NewLeague A factor with levels A and N indicating player's league at the beginning of 1987

```
# We want to predict salary using ALL SUBSETS through regsubsets
reg.ss <- regsubsets(Salary~., Hitters)</pre>
summary (reg.ss)
Subset selection object
Call: regsubsets.formula(Salary ~ ., Hitters)
19 Variables (and intercept)
           Forced in Forced out
AtBat
               FALSE
                           FALSE
Hits
               FALSE
                           FALSE
HmRun
               FALSE
                           FALSE
Runs
               FALSE
                           FALSE
. . .
CWalks
               FALSE
                           FALSE
LeagueN
               FALSE
                           FALSE
DivisionW
               FALSE
                           FALSE
PutOuts
               FALSE
                           FALSE
Assists
                           FALSE
               FALSE
Errors
               FALSE
                           FALSE
NewLeagueN
               FALSE
                           FALSE
1 subsets of each size up to 8
Selection Algorithm: exhaustive
         AtBat Hits HmRun Runs RBI Walks Years CAtBat CHits CHmRun CRuns CRBI CWalks LeagueN DivisionW PutOuts Assists Errors NewLeagueN
                                                                                                           11 11
   (1)"
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   (1)"*"
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                                                              . .
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                                                                                                           11 🛠 11
   (1)""
                                                        11 * 11
                                                              11 🛠 11
                                                                                                11 * 11
                                                                                                           II * II
```

II \* II

II \* II

. .

**Subset Selection** # We want ALL 19 vars reg.ss <- regsubsets(Salary~., Hitters, nvmax =19)</pre> res.reg.ss <- summary(reg.ss)</pre> Subset selection object Call: regsubsets.formula(Salary ~ ., Hitters, nvmax = 19) 19 Variables (and intercept) Forced in Forced out **FALSE AtBat** FALSE NewLeagueN FALSE FALSE 1 subsets of each size up to 19 Selection Algorithm: exhaustive AtBat Hits HmRun Runs RBI Walks Years CAtBat CHits CHmRun CRuns CRBI CWalks LeagueN DivisionW PutOuts Assists Errors NewLeagueN . . (1) (1) . . . . 11 🛠 11 (1)

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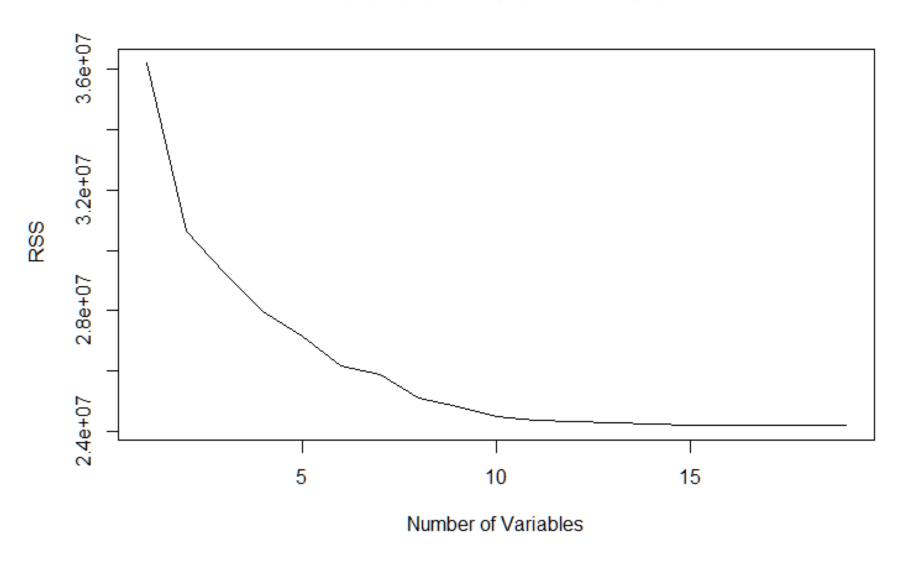
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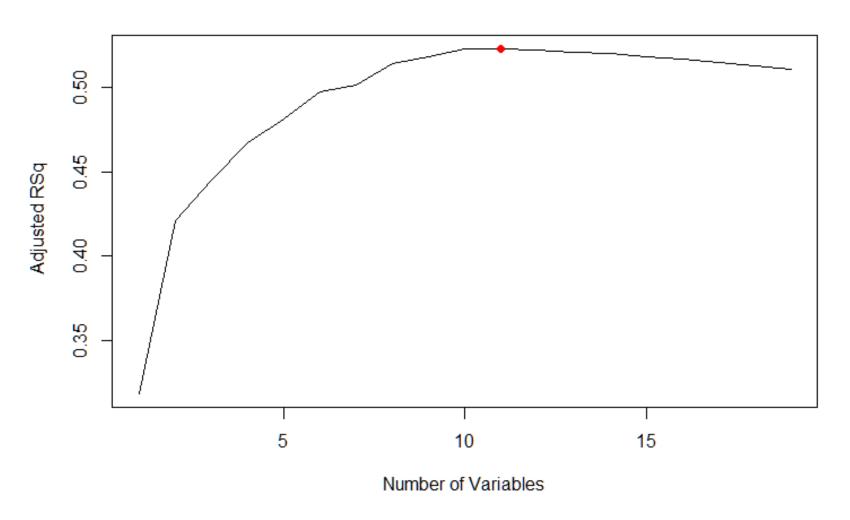
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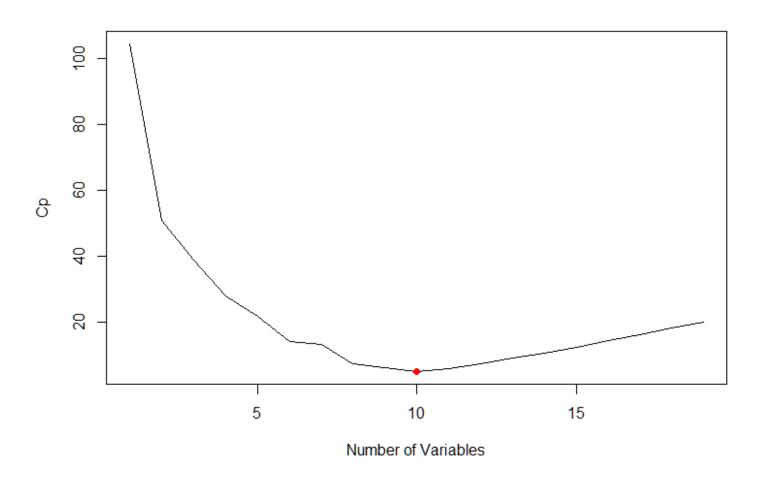
```
# We want information on each model
res.reg.ss$rsq
 [1] 0.3214501 0.4252237 0.4514294 0.4754067 0.4908036 0.5087146 0.5141227 0.5285569 0.5346124 0.5404950
[11] 0.5426153 0.5436302 0.5444570 0.5452164 0.5454692 0.5457656 0.5459518 0.5460945 0.5461159
# let's plot some results
\#par(mfrow = c(2,2))
plot(res.reg.ss$rss ,xlab=" Number of Variables ",ylab=" RSS", type = 'l')
plot(res.req.ss$adjr2 ,xlab = "Number of Variables ", ylab= Adjusted RSq",type = 'l')
bestset <- which.max(res.reg.ss$adjr2)</pre>
bestset
points (bestset, res.reg.ss$adjr2[bestset], col = "red",cex = 1.5, pch = 20)
plot(res.reg.ss$cp ,xlab =" Number of Variables ", ylab = "Cp", type = 'l')
cpmin <- which.min (res.reg.ss$cp )</pre>
cpmin
points (cpmin, res.req.ss$cp [cpmin], col = "red", cex = 1.5, pch = 20)
bicmin <- which.min(res.reg.ss$bic)</pre>
bicmin
plot(res.reg.ss$bic ,xlab=" Number of Variables ", ylab = " BIC",type = 'l')
points (bicmin, res.reg.ss$bic [6], col = red, cex = 2, pch = 20)
par(mfrow = c(1,1))
```



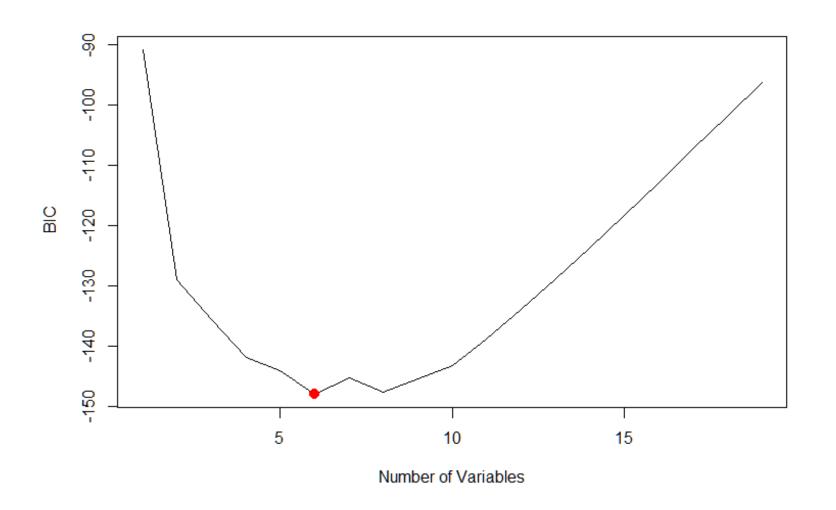
plot(res.reg.ss\$rss ,xlab=" Number of Variables ",ylab=" RSS", type = 'l')



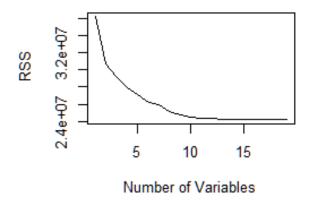
plot(res.reg.ss\$adjr2 ,xlab =" Number of Variables ", ylab=" Adjusted RSq",type = 'l')
bestset <- which.max(res.reg.ss\$adjr2)
points (bestset, res.reg.ss\$adjr2[bestset], col = "red",cex = 1.5, pch = 20)</pre>

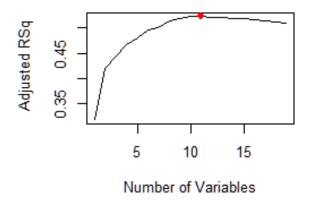


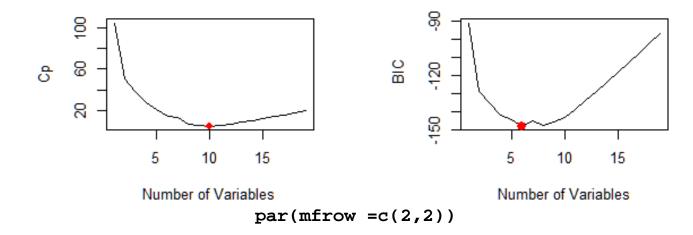
plot(res.reg.ss\$cp ,xlab =" Number of Variables ", ylab = "Cp", type = 'l')
cpmin <- which.min (res.reg.ss\$cp )
points (cpmin, res.reg.ss\$cp [cpmin], col ="red",cex = 1.5, pch = 20)</pre>



bicmin <- which.min(res.reg.ss\$bic) # bicmin = 6
plot(res.reg.ss\$bic ,xlab=" Number of Variables ", ylab = " BIC",type = 'l')
points (bicmin, res.reg.ss\$bic [6], col =" red", cex = 2, pch = 20)</pre>





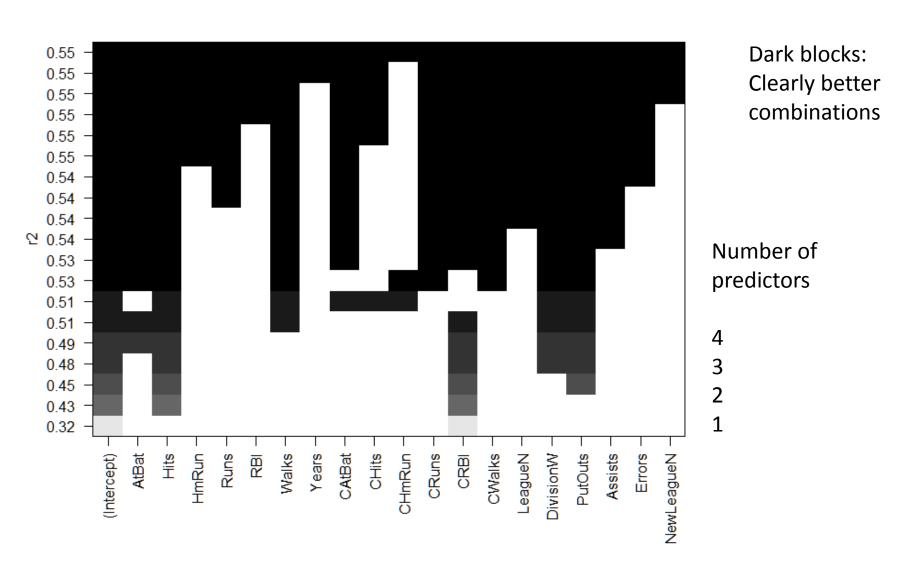


## We can also do other diagnostic graphs related to variable importance

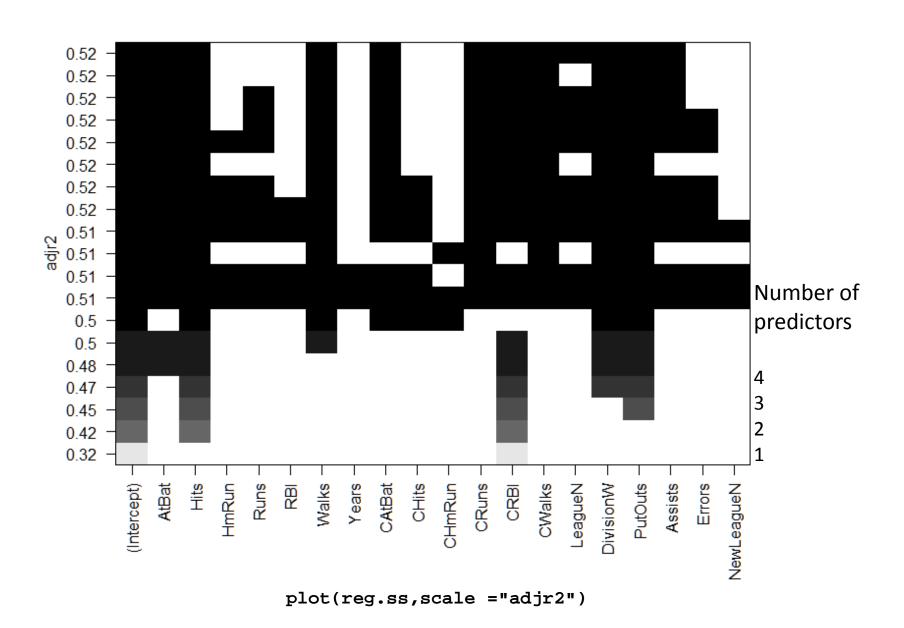
```
plot(reg.ss,scale = "r2")
plot(reg.ss,scale = "adjr2")
plot(reg.ss,scale = "Cp")
plot(reg.ss,scale = "bic")
```

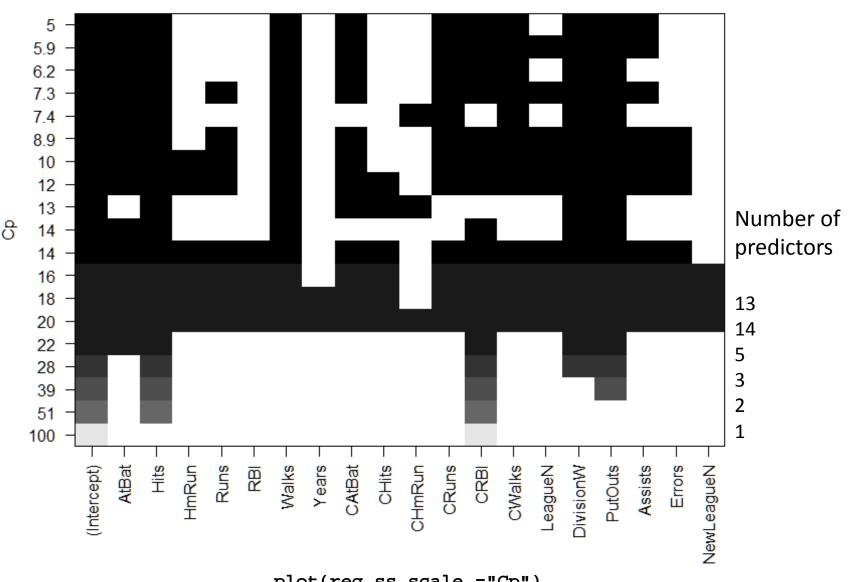
#### bicmin

[1] 6

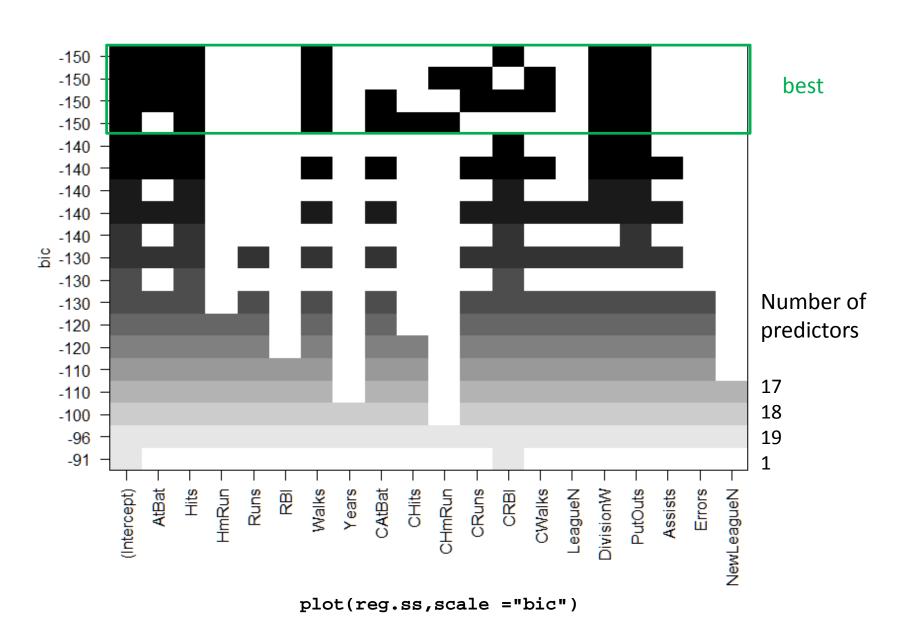


plot(reg.ss,scale ="r2")





plot(reg.ss,scale ="Cp")



### Look at the coefficients for the best-fit model using BIC

#### bicmin

```
[1] 6
```

#### coef(reg.ss, bicmin)

(Intercept)	AtBat	Hits	Walks	CRBI	DivisionW	PutOuts
91.5117981	-1.8685892	7.6043976	3.6976468	0.6430169	-122.9515338	0.2643076

These are the OLS coefficients and can be used directly to calculate salary

We can also use forward stepwise selection of predictors using regsubsets and forward

```
reg.fwd <- regsubsets (Salary~., data= Hitters ,nvmax = 19, method = "forward")
```

### **Forward Selection**

#### summary(reg.fwd)

```
Subset selection object
Call: regsubsets.formula(Salary ~ ., data = Hitters, nvmax = 19, method = "forward")
19 Variables (and intercept)
                                                                                  which.min(summary(reg.fwd)$bic)
           Forced in Forced out
                                                                                  [1] 6
At.Bat.
                FALSE
                            FALSE
                                                                                  which.min(summary(reg.fwd)$adjr2)
Hits
                FALSE
                            FALSE
                                                                                  which.min(summary(reg.fwd)$cp)
NewLeagueN
                FALSE
                            FALSE
                                                                                  [1] 10
1 subsets of each size up to 19
Selection Algorithm: forward
          AtBat Hits HmRun Runs RBI Walks Years CAtBat CHits CHmRun CRuns CRBI CWalks LeagueN DivisionW PutOuts Assists Errors NewLeagueN
   (1)
                                                                                                               11 * 11
   (1)
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                                                                                                                                 11 * 11
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                                                                                                                        11 * 11
                                                                                                                                        11 🛠 11
```

### Let's compare best-subsets and forward-stepwise models

```
# best subsets using bicmin (6)
coef(req.ss, 6)
 (Intercept)
                  AtBat
                                Hits
                                           Walks
                                                         CRBI
                                                                 DivisionW
                                                                               PutOuts
 91.5117981 -1.8685892
                           7.6043976
                                      3.6976468
                                                    0.6430169 - 122.9515338
                                                                             0.2643076
# best 6 using forward stepwise
coef(req.fwd, 6)
 (Intercept)
                  AtBat
                                Hits
                                           Walks
                                                         CRBI
                                                                 DivisionW
                                                                               PutOuts
 91.5117981 -1.8685892
                           7.6043976
                                        3.6976468
                                                    0.6430169 - 122.9515338
                                                                             0.2643076
# best subsets with 7
coef(reg.ss, 7)
 (Intercept)
                   Hits
                               Walks
                                          CAtBat
                                                        CHits
                                                                    CHmRun
                                                                             DivisionW
                                                                                           PutOuts
                           3.2274264
 79.4509472
            1.2833513
                                       -0.3752350
                                                  1.4957073
                                                                 1.4420538 -129.9866432
                                                                                          0.2366813
# best forward with 7
coef(reg.fwd, 7)
(Intercept)
                                Hits
                                           Walks
                                                         CRBI
                                                                    CWalks
                                                                             DivisionW
                  AtBat
                                                                                           PutOuts
109.7873062 -1.9588851
                           7.4498772
                                        4.9131401
                                                    0.8537622
                                                                -0.3053070 -127.1223928
                                                                                          0.2533404
```

## Choosing the best prediction models

Model-fitting (number of predictors) will be done using training set Test error will be estimated using test set

```
set.seed (7)
# not "stratified" but does not make sense here, simply random 50/50, T/F for every record
train <- sample(c(TRUE ,FALSE), nrow(Hitters),rep = TRUE)
test <- (!train)

# use best subset selection on training set
regfit.ss = regsubsets(Salary~., data = Hitters[train,], nvmax =19)
# set up "x" model matrix
test.mat <- model.matrix(Salary~., data = Hitters[test,])</pre>
```

## Choosing the best prediction models

# The "x" model matrix

test.mat

	(Intercept)	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	CHits	CHmRun	CRuns	CRBI	CWalks	LeagueN	DivisionW	PutOuts	Assists	Errors	NewLeagueN
-Alan Ashby	1	315	81	7	24	38	39	14	3449	835	69	321	414	375	1	1	632	43	10	1
-Alvin Davis	1	479	130	18	66	72	76	3	1624	457	63	224	266	263	0	1	880	82	14	0
-Andre Dawson	1	496	141	20	65	78	37	11	5628	1575	225	828	838	354	1	0	200	11	3	1
-Andres Galarraga	1	321	87	10	39	42	30	2	396	101	12	48	46	33	1	0	805	40	4	1
-Alfredo Griffin	1	594	169	4	74	51	35	11	4408	1133	19	501	336	194	0	1	282	421	25	0
-Al Newman	1	185	37	1	23	8	21	2	214	42	1	30	9	24	1	0	76	127	7	0
-Argenis Salazar	1	298	73	0	24	24	7	3	509	108	0	41	37	12	0	1	121	283	9	0
-Andres Thomas	1	323	81	6	26	32	8	2	341	86	6	32	34	8	1	1	143	290	19	1
-Andre Thornton	1	401	92	17	49	66	65	13	5206	1332	253	784	890	866	0	0	0	0	0	0
-Buddy Bell	1	568	158	20	89	75	73	15	8068	2273	177	1045	993	732	1	1	105	290	10	1
-Barry Bonds	1	413	92	16	72	48	65	1	413	92	16	72	48	65	1	0	280	9	5	1
-Bobby Bonilla	1	426	109	3	55	43	62	1	426	109	3	55	43	62	0	1	361	22	2	1
-Brett Butler	1	587	163	4	92	51	70	6	2695	747	17	442	198	317	0	0	434	9	3	0
-Bob Dernier	1	324	73	4	32	18	22	7	1931	491	13	291	108	180	1	0	222	3	3	1

- and the column names are different League --> LeagueN, reflecting factor levels.
- Alan Ashby is in the National League, (League = 'N', not 'A', so LeagueN = 1)

<sup>^^^</sup> notice that the column values are all 0,1 for factors

```
# get MSE using test data
val.errors =rep(NA ,19)
for(i in 1:19)
  coefi <- coef(regfit.ss, id=i)</pre>
  pred <- test.mat[,names(coefi)]%*% coefi # matrix multiplication</pre>
  val.errors[i] <- mean(( Hitters$Salary[test]-pred)^2)</pre>
val.errors
 [1] 136066.8 143503.4 134202.7 106604.0 111873.1 113970.1 105141.6 109710.0 109247.8 113079.4
[11] 114646.0 113463.2 116690.8 120297.5 119492.7 118188.6 113200.9 112782.0 112333.4
which.min(val.errors) # different from book; different from you?
[1] 7
coef(regfit.ss,7)
 (Intercept)
                  AtBat
                               Hits
                                          Walks
                                                      Years
                                                                  CHits
                                                                          DivisionW
                                                                                        PutOuts
 401.9777394 -2.4522168
                          7.5045989
                                     4.4089801
                                                 -48.2143365
                                                              0.6684161 -125.0446386
                                                                                       0.2259642)
```

```
# That was tedious, so make it into a function we can use later
predict.regsubsets = function(object, newdata, id,...)
  form = as.formula(object$call[[2]]) # extract model ("call")
  mat = model.matrix (form, newdata)
  coefi = coef(object, id=id)
  xvars = names(coefi)
 mat[,xvars] %*% coefi
And now do best subset selection on the FULL dataset, choose the best 7-variable model
regfit.ss = regsubsets(Salary~., data=Hitters, nvmax =19)
# these are different from before
coef(regfit.ss,7)
                             Walks
                                                     CHits
 (Intercept)
                  Hits
                                        CAtBat
                                                                CHmRun
                                                                        DivisionW
                                                                                      PutOuts
 79.4509472
           1.2833513
                         3.2274264
                                    -0.3752350
                                               1.4957073
                                                             1.4420538 -129.9866432
                                                                                    0.2366813
```

So we need to choose a model using some kind of cross-validation or holdout sample!

```
# set up k-fold cross-validation of MSE
# set up k folds
k = 10
set.seed(7)
folds = sample(1:k, nrow(Hitters), replace = TRUE)
# set up cv MSE table
cv.mse = matrix (NA ,k,19, dimnames =list(NULL , paste (1:19) ))
# loop through all folds
for(j in 1:k)
  best.ss = regsubsets (Salary ~., data = Hitters [folds != j,], nvmax =19)
  # compile mean MSE of all folds for each number of predictors
  for(i in 1:19)
    pred = predict(best.ss, Hitters[folds == j,], id=i)
    cv.mse[j,i] = mean((Hitters$Salary[folds == j] - pred)^2)
```

cv.mse # the MSEs for each fold and number of predictors

```
6
                                                                                                       10
[1,] 145608.84 131762.73 140073.23 132248.48 142804.42 128394.39 148369.98 117656.34 138676.15 133762.79
                         43528.06
                                   35784.03 67546.33 81480.04 80170.10
                36320.26
                                                                            79475.24
 [3,] 128478.90 116278.29 141513.75 234357.39 198646.23 185804.96 167033.74 154538.53 151378.01 147499.39
 [4,] 223570.13 236372.82 246601.89 230305.38 223016.63 210604.53 211196.15 202203.66 206103.83 202211.08
 [5,] 172322.29 139474.55 127043.54 110167.90 106235.44 96087.32 100545.39
                                                                             91107.10
 [6,] 116075.54 69920.61
                          71025.79 89086.82 88879.24 64408.89 67426.49
                                                                            51126.83
                                                                                       48231.82
                                                                                                 47502.24
 [7,] 153182.53 131082.43 135296.19 127391.45 139288.29 133766.89 156842.06 150425.78 151271.81 140891.29
 [8,] 160762.16 124524.01 127529.10 121597.00 117507.07 115600.69 125954.18 126804.69 120849.30 109752.49
               85665.74 139480.88 141344.23 127102.27 100684.38 96255.76
 [9,] 139890.39
                                                                             75131.95
                                                                                       76115.17
                                                                                                 88279.40
               93634.05 115987.71 118739.58 115093.18
                                                        88762.29
                                                                   99741.85
                                                                             89276.23
                                                                                                 89500.83
            11
                      12
                                13
                                                     15
                                                               16
                                                                         17
                                                                                   18
                                                                                             19
                                           14
[1,] 144181.75 135771.72 135419.66 135059.83 132586.51 132398.57 131207.58 130975.75 131304.17
                                    89330.13
                                              87220.62
                                                        87009.28
      82677.71
                87478.21
                          87486.59
                                                                  86606.26
                                                                            87889.09
 [3,] 144496.02 148836.88 149032.48 144943.91 144883.43 142465.51 143618.46 147276.90 148109.69
    197894.80 196801.62 196839.07 196803.42 196065.19 196210.47 196024.16 195892.06 196253.71
[5,]
      86572.38
                84791.78
                          87977.59
                                    89495.22
                                              91199.72
                                                        89160.49
                                                                  89072.61
                                                                             88996.76
                53466.71
                          54803.84
                                    53730.70
                                              54001.73
                                                         54011.71
                                                                   53897.82
      50748.42
                                                                             53620.95
 [7,] 142970.72 148645.01 149378.21 147191.63 148025.88 148332.05 148756.35 148362.74 149007.97
[8,] 116903.14 123422.39 122602.59 126075.47 126011.80 126046.54 124923.79 125631.71 125199.61
[9,1
      73492.93
                78449.44
                          85158.42
                                    85040.60
                                              86586.44 91701.31
                                                                   91651.47
                                                                             91514.78
[10.]
      91627.29
                89333.78
                          91634.03
                                    90359.54
                                              89654.58
                                                        89800.63
                                                                   89628.77
                                                                             89511.37
```

```
# get the mean of the means after run
mean.cv.mse = apply(cv.errors, 2, mean)
mean.cv.mse
                                                                                   10
                                                                                            11
140458.8 116503.5 128808.0 134102.2 132611.9 120559.4 125353.6 113774.6 115611.3 113054.0 113156.5
                                           16
114699.8 116033.2 115803.0 115623.6 115713.7 115538.7 115967.2 116237.6
par(mfrow = c(1,1))
plot(mean.cv.errors, type = 'b', xlab = 'Predictors'
                                                    135000
# what about the "NULL" model?
# What IS the NULL model?
```

15

10

Predictors

```
# get the mean of the means after run
mean.cv.mse = apply(cv.errors, 2, mean)
mean.cv.mse
                                                                                   10
                                                                                             11
140458.8 116503.5 128808.0 134102.2 132611.9 120559.4 125353.6 113774.6 115611.3 113054.0 113156.5
                                           16
114699.8 116033.2 115803.0 115623.6 115713.7 115538.7 115967.2 116237.6
par(mfrow = c(1,1))
plot(mean.cv.errors, type = 'b', xlab = 'Predictors'
                                                    35000
# what about the "NULL" model?
# What IS the NULL model?
# Using just the mean!
mean((Hitters$Salary - mean(Hitters$Salary))^2)
[1] 202734.3
                                                                                                   15
                                                                                    10
```

Predictors

# Let's use 10 predictors and get "final" model, we can save time by limiting nvmax reg.final = regsubsets(Salary~., data = Hitters, nvmax = 11)

#### coef(reg.final, 10)

(Intercept)	AtBat	Hits	Walks	CAtBat	CRuns	CRBI	CWalks
162.5354420	-2.1686501	6.9180175	5.7732246	-0.1300798	1.4082490	0.7743122	-0.8308264
DivisionW	PutOuts	Assists					
-112.3800575	0.2973726	0.2831680					

### # 11 produces the same as on page 250-251

#### coef(reg.final, 11)

(Intercept)	AtBat	Hits	Walks	CAtBat	CRuns	CRBI	CWalks
135.7512195	-2.1277482	6.9236994	5.6202755	-0.1389914	1.4553310	0.7852528	-0.8228559
LeagueN	DivisionW	PutOuts	Assists				
43.1116152	-111.1460252	0.2894087	0.2688277				

```
# glmnet uses an x matrix and y, not a model ~ statement
# model.matrix changes factors into numbers
x <- model.matrix (Salary~., Hitters )[,-1]
y <- Hitters$Salary
require(glmnet)
# set up a grid of values for lambda; the higher the lambda, the greater the shrinkage penalty
grid <- 10'seq (10,-2, length =100)
grid
  [1] 1.000000e+10 7.564633e+09 5.722368e+09 4.328761e+09 3.274549e+09 2.477076e+09 1.873817e+09 1.417474e+09
  [9] 1.072267e+09 8.111308e+08 6.135907e+08 4.641589e+08 3.511192e+08 2.656088e+08 2.009233e+08 1.519911e+08
 [17] 1.149757e+08 8.697490e+07 6.579332e+07 4.977024e+07 3.764936e+07 2.848036e+07 2.154435e+07 1.629751e+07
 [25] 1.232847e+07 9.326033e+06 7.054802e+06 5.336699e+06 4.037017e+06 3.053856e+06 2.310130e+06 1.747528e+06
 [33] 1.321941e+06 1.000000e+06 7.564633e+05 5.722368e+05 4.328761e+05 3.274549e+05 2.477076e+05 1.873817e+05
 [41] 1.417474e+05 1.072267e+05 8.111308e+04 6.135907e+04 4.641589e+04 3.511192e+04 2.656088e+04 2.009233e+04
 [49] 1.519911e+04 1.149757e+04 8.697490e+03 6.579332e+03 4.977024e+03 3.764936e+03 2.848036e+03 2.154435e+03
 [57] 1.629751e+03 1.232847e+03 9.326033e+02 7.054802e+02 5.336699e+02 4.037017e+02 3.053856e+02 2.310130e+02
 \lceil 65 \rceil 1.747528e+02 1.321941e+02 1.000000e+02 7.564633e+01 5.722368e+01 4.328761e+01 3.274549e+01 2.477076e+01
 \lceil 73 \rceil 1.873817e+01 1.417474e+01 1.072267e+01 8.111308e+00 6.135907e+00 4.641589e+00 3.511192e+00 2.656088e+00
 [81] 2.009233e+00 1.519911e+00 1.149757e+00 8.697490e-01 6.579332e-01 4.977024e-01 3.764936e-01 2.848036e-01
 [89] 2.154435e-01 1.629751e-01 1.232847e-01 9.326033e-02 7.054802e-02 5.336699e-02 4.037017e-02 3.053856e-02
 [97] 2.310130e-02 1.747528e-02 1.321941e-02 1.000000e-02
```

```
#### glmnet automatically scales predictors #### (unless: ,standardize = F)
# if alpha = 0, perform ridge regression
ridge.mod <- glmnet(x, y, alpha = 0, lambda = grid)</pre>
coef(ridge.mod) # 20 predictors, 100 lambdas
20 x 100 sparse Matrix of class "dqCMatrix"
        [[ suppressing 81 column names 's0', 's1', 's2' ... ]]
                suppressing 81 column names 's0', 's1', 's2' ... ]]
(Intercept) \ 5.359257e + 02 \ 5.359256e + 02 \ 5.359256e + 02 \ 5.359256e + 02 \ 5.359254e + 02 \ 5.359253e + 02 \ 5.359251e + 02 \ 5.359249e + 02 \ 5.359246e + 02 \ 5.359246e + 02 \ 5.359236e + 02 \ 5.359236e + 02 \ 5.359236e + 02 \ 5.359254e + 02 \ 5.359254e + 02 \ 5.359254e + 02 \ 5.359256e + 02 \ 5.35925
                     5.443467e-08 7.195940e-08 9.512609e-08 1.257511e-07 1.662355e-07 2.197535e-07 2.905011e-07 3.840251e-07 5.076583e-07 6.710939e-07 8.871458e-07 1.172753e-06
AtBat
Hits
                     1.974589e-07 2.610289e-07 3.450649e-07 4.561554e-07 6.030105e-07 7.971441e-07 1.053777e-06 1.393031e-06 1.841504e-06 2.434358e-06 3.218075e-06 4.254101e-06
HmRun
                     7.956523e-07 1.051805e-06 1.390424e-06 1.838059e-06 2.429805e-06 3.212059e-06 4.246151e-06 5.613159e-06 7.420260e-06 9.809139e-06 1.296709e-05 1.714170e-05
                     3.339178e-07 4.414196e-07 5.835307e-07 7.713931e-07 1.019736e-06 1.348031e-06 1.782017e-06 2.355720e-06 3.114121e-06 4.116682e-06 5.442006e-06 7.194001e-06
Runs
RBI
                     3.527222e-07 4.662778e-07 6.163918e-07 8.148335e-07 1.077162e-06 1.423944e-06 1.882370e-06 2.488380e-06 3.289490e-06 4.348509e-06 5.748467e-06 7.599123e-06
ridge.mod$lambda [50]
[1] 11497.57
coef(ridge.mod)[,50]
coef(ridge.mod)[,50]
    (Intercept)
                                             AtBat
                                                                            Hits
                                                                                                       HmRun
                                                                                                                                                                     RBI
                                                                                                                                                                                              Walks
                                                                                                                                                                                                                                                      CAtBat
                                                                                                                                                                                                                                                                                     CHits
                                                                                                                                      Runs
                                                                                                                                                                                                                           Years
407.356050200
                                 0.036957182
                                                              0.138180344
                                                                                           0.524629976
                                                                                                                        0.230701523
                                                                                                                                                    0.239841459
                                                                                                                                                                                  0.289618741
                                                                                                                                                                                                              1.107702929
                                                                                                                                                                                                                                           0.003131815
                                                                                                                                                                                                                                                                        0.011653637
              CHmRun
                                             CRuns
                                                                            CRBI
                                                                                                     CWalks
                                                                                                                                LeaqueN
                                                                                                                                                        DivisionW
                                                                                                                                                                                          PutOuts
                                                                                                                                                                                                                      Assists
                                                                                                                                                                                                                                                                          NewLeagueN
                                                                                                                                                                                                                                                      Errors
    0.087545670
                                0.023379882
                                                              0.024138320
                                                                                           0.025015421
                                                                                                                       0.085028114
                                                                                                                                                -6.215440973
                                                                                                                                                                                 0.016482577
                                                                                                                                                                                                              0.002612988
                                                                                                                                                                                                                                         -0.020502690
                                                                                                                                                                                                                                                                        0.301433531
```

ridge.mod\$lambda [50] # a "large" value, should shrink coefficients

[1] 11497.57

#### coef(ridge.mod)[,50]

CHits	CAtBat	Years	Walks	RBI	Runs	HmRun	Hits	AtBat	(Intercept)
0.011653637	0.003131815	1.107702929	0.289618741	0.239841459	0.230701523	0.524629976	0.138180344	0.036957182	407.356050200
NewLeagueN	Errors	Assists	PutOuts	DivisionW	LeagueN	CWalks	CRBI	CRuns	CHmRun
0.301433531	-0.020502690	0.002612988	0.016482577	-6.215440973	0.085028114	0.025015421	0.024138320	0.023379882	0.087545670

#### ridge.mod\$lambda [60] # a smaller value, shrinks coefficients less

[1] 705.4802

#### coef(ridge.mod)[,60]

CHits	CAtBat	Years	Walks	RBI	Runs	HmRun	Hits	AtBat	(Intercept)
0.04674557	0.01083413	2.59640425	1.31987948	0.84718546	0.93769713	1.17980910	0.65622409	0.11211115	54.32519950
NewLeagueN	Errors	Assists	PutOuts	DivisionW	LeagueN	CWalks	CRBI	CRuns	CHmRun
8.61181213	-0.70358655	0.01606037	0.11852289	-54.65877750	13.68370191	0.07189612	0.09780402	0.09355528	0.33777318

### # We can get coefficients for a specific lambda(s) - round for looking at

round(predict(ridge.mod, s=50, type = "coefficients")[1:20,],3)

(Intercept)	AtBat	Hits	HmRun	Runs	RBI	Walks	Years	CAtBat	CHits
48.766	-0.358	1.969	-1.278	1.146	0.804	2.716	-6.218	0.005	0.106
CHmRun	CRuns	CRBI	CWalks	LeagueN	DivisionW	PutOuts	Assists	Errors	NewLeagueN
0.624	0.221	0.219	-0.150	45.926	-118.201	0.250	0.122	-3.279	-9.497

```
# let's get the mean MSE in a test sample
set.seed(7)
train <- sample(1:nrow(x), nrow(x)/2)
test <- (-train )</pre>
y.test <- y[test]
# use the grid again
ridge.mod <- glmnet(x[train,], y[train], alpha =0, lambda =grid, thresh = 1e-12)</pre>
# predict using glmnet : note the use of newx
ridge.pred <- predict(ridge.mod, s = 4, newx = x[test ,])
mean((ridge.pred - y.test)^2)
# [1] 142668
                                                         # NULL model
ridge.pred
                                                         mean((mean(y[train]) - y.test)^2)
                                                         [1] 257648.4
-Alan Ashby
                   379.96271
                                                         # hmmmm
-Andres Galarraga 443.53309
                                                         ridge.pred <- predict(ridge.mod, s=1e10, newx=x[test,])</pre>
-Alfredo Griffin
                   542.27969
                                                         mean((ridge.pred - y.test)^2)
-Al Newman
                   271.22654
                                                         [1] 257648.4
-Andres Thomas
                   105.28723
-Alan Trammell
                   788.37334
-Alex Trevino
                   221.63960
```

-Andy VanSlyke

406.59938

```
# test linear regression (set lambda = 0)
ridge.pred <- predict(ridge.mod, s = 0, newx = x[test,])
mean((ridge.pred - y.test)^2)
[1] 141620.5
lm(y~x, subset =train)
Call:
lm(formula = y \sim x, subset = train)
Coefficients:
                               xHits
                                                                                 xWalks
                                                                                                                       xCHits
(Intercept)
                 xAtBat
                                           xHmRun
                                                        xRuns
                                                                      xRBI
                                                                                              xYears
                                                                                                         xCAtBat
                             6.92120
                                         -2.29256
                                                                                             5.85338
                                                                                                         -0.16762
                                                                                                                      0.50393
   90.46667
               -1.93630
                                                      0.75298
                                                                   0.74394
                                                                                3.33849
   xCHmRun
                 xCRuns
                               xCRBI
                                         xCWalks
                                                     xLeaqueN
                                                                xDivisionW
                                                                               xPutOuts
                                                                                            xAssists
                                                                                                         xErrors
                                                                                                                  xNewLeaqueN
                0.72515
                                         -0.73113
   2.41127
                             0.01203
                                                    191.15886
                                                                 -67.36335
                                                                                0.21135
                                                                                             0.47537
                                                                                                         -7.03317
                                                                                                                   -147.83212
round(predict(ridge.mod, s = 0,type = "coefficients") [1:20,],5)
(Intercept)
                 AtBat
                              Hits
                                         HmRun
                                                     Runs
                                                                  RBI
                                                                            Walks
                                                                                        Years
                                                                                                   CAtBat
                                                                                                               CHits
```

0.73435

DivisionW

-67.36116

3.34119

PutOuts

0.21138

5.76525

Assists

0.47427

-0.16494

Errors

0.49189

NewLeagueN

-7.02181 -147.73255

0.74132

LeagueN

191.09147

90.38494

CHmRun

2.38881

-1.93801

0.72991

CRuns

6.93392

0.01959

CRBI

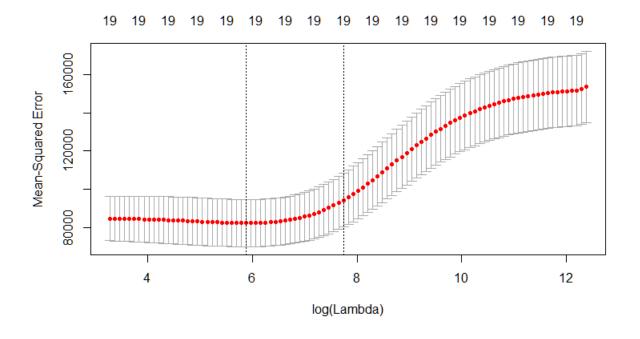
-2.26032

-0.73233

CWalks

# RR: Choosing the best $\lambda$ using CV

```
Naturally, we will use cross-validation
# We can use the built-in cv.glmnet() function that will test many values of lambda
set.seed (7)
cv.out <- cv.glmnet(x[train,], y[train], alpha = 0)
plot(cv.out)
bestlam <- cv.out$lambda.min
bestlam
[1] 357.2905</pre>
```



# RR: Choosing the best $\lambda$ using CV

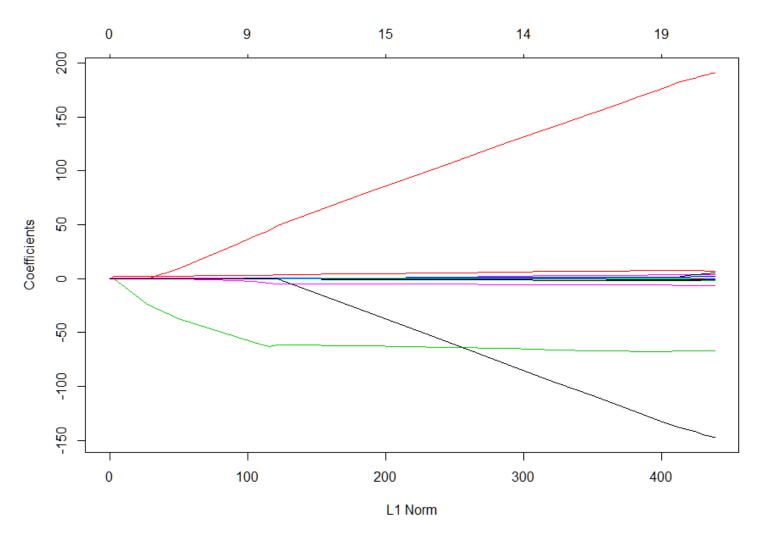
```
# What improvement in the MSE? What are the coefficients?
ridge.pred <- predict(ridge.mod, s = bestlam, newx = x[test,])</pre>
mean((ridge.pred - y.test)^2)
[1] 158571.7
# in this case, it got worse, in contrast to chapter results!
# ridge again
rreg2 <- glmnet(x, y, alpha = 0)</pre>
predict(rreg2, type = "coefficients", s = bestlam)[1:20,]
 (Intercept)
                                 Hits
                                                                                                                          CHits
                   AtBat
                                             HmRun
                                                           Runs
                                                                         RBI
                                                                                   Walks
                                                                                                Years
                                                                                                            CAtBat
17.98653140
              0.08411834
                           0.83177568
                                        0.68925817
                                                     1.05138274
                                                                  0.87894452
                                                                              1.58791179
                                                                                           1.56259857
                                                                                                        0.01134104
                                                                                                                     0.05604141
                                            CWalks
                                                        LeaqueN
                                                                   DivisionW
                                                                                              Assists
                                                                                                                     NewLeagueN
      CHmRun
                   CRuns
                                 CRBI
                                                                                  PutOuts
                                                                                                            Errors
  0.39785795
              0.11183616
                           0.11813278
                                        0.05673971 21.05095331 -76.20171988
                                                                              0.16058669
                                                                                           0.02721512
                                                                                                       -1.27171087
                                                                                                                     9.30936778
# from chapter:
                                                                                   Walks
                                                                                                                         CHits
(Intercept)
                    AtBat
                                Hits
                                            HmRun
                                                                       RBI
                                                                                                           CAtBat
                                                          Runs
                                                                                                Years
                   0.0314
     9.8849
                              1.0088
                                           0.1393
                                                       1.1132
                                                                    0.8732
                                                                                  1.8041
                                                                                               0.1307
                                                                                                           0.0111
                                                                                                                        0.0649
   CHmRun
                               CRBI
                                         CWalks
                                                                  DivisionW
                                                                                           Assists
                   CRuns
                                                   LeaqueN
                                                                                PutOuts
                                                                                                           Errors
                                                                                                                    NewLeagueN
   0.4516
                   0.129
                                         0.0291
                                                   27.1823
                                                                   -91.6341
                                                                                             0.0425
                                                                                                                        7.2121
                             0.1374
                                                                                0.1915
                                                                                                           -1.8124
```

# RR: REALLY Choosing the best $\lambda$ using CV

```
DRAFT CODE - to be improved
# set up k-fold cross-validation of MSE
# set up k folds
k = 10
# set.seed(7)
# set up cv MSE table
cv.mse = matrix (NA ,k,length(grid), dimnames =list(NULL , paste (1:100) ))
# loop through all folds
  # compile mean MSE of all folds for each number of predictors
for(i in 1:length(grid))
   for(j in 1:k)
   folds = sample(1:k, nrow(Hitters), replace = TRUE)
   ridge.mod = cv.glmnet(x[train,], y[train], alpha = 0)
   ridge.pred <- predict(ridge.mod, s=grid[i], newx=x[test,])</pre>
   cv.mse[j,i] = mean((Hitters$Salary[folds == j] - ridge.pred)^2)
```

### The Lasso

```
#### glmnet automatically scales predictors #### (unless: ,standardize = F)
# if alpha = 1, perform the Lasso
lasso.mod <- glmnet(x[train,], y[train], alpha = 1, lambda = grid)
plot(lasso.mod)</pre>
```



### The Lasso

```
#Let's cross-validate to get the best lambda
set.seed(7)
cv.out <- cv.glmnet(x[train,], y[train], alpha = 1)</pre>
plot(cv.out)
bestlam <- cv.out$lambda.min</pre>
lasso.pred <- predict(lasso.mod, s = bestlam, newx=x[test,])</pre>
mean((lasso.pred - y.test)^2)
                                                                      19 17 14 14 14 15 15 13 10 9 8
[1] 152424.1
bestlam
[1] 13.45176
                                                           140000
log(bestlam)
                                                        Mean-Squared Error
[1] 2.59911
                                                           120000
                                                           100000
                                                           80000
```

log(Lambda)

### The Lasso

```
#Let's use a lambda of 2.8
lasso.pred <- predict(lasso.mod, s = 2.8, newx=x[test,])
mean((lasso.pred - y.test)^2) # before was 152424.1
[1] 142898.3

#Let's use a lambda of 2.4
lasso.pred <- predict(lasso.mod, s = 2.4, newx=x[test,])
mean((lasso.pred - y.test)^2) # before was 152424.1
[1] 142391.8</pre>
```

So we will need to sample multiple times and/or average our models!