PENALIZED REGRESSION

Ridge and The LASSO

Note: The example contained herein was copied from the lab exercise in Chapter 6 of Introduction to Statistical Learning by .

For this exercise, we'll use some baseball data from 1986-1987. The Hitters dataset contains information about 322 baseball players and 20 attributes as follows:

1. AtBat: Number of times at bat in 1986
2. Hits: Number of hits in 1986
3. HmRun: Number of home runs in 1986
4. Runs: Number of runs in 1986
5. RBI: Number of runs batted in in 1986
6. Walks: Number of walks in 1986
7. Years: Number of years in the major leagues
8. CAtBat: Number of times at bat during his career
9. CHits: Number of hits during his career
10. CHmRun: Number of home runs during his career
11. CRuns: Number of runs during his career
12. CRBI: Number of runs batted in during his career
13. CWalks: Number of walks during his career
14. League: A factor with levels A and N indicating player's league at the end of 1986
15. Division: A factor with levels E and W indicating player's division at the end of 1986
16. PutOuts: Number of put outs in 1986
17. Assists: Number of assists in 1986

18. Errors: Number of errors in 1986
19. Salary: 1987 annual salary on opening day in thousands of dollars
20. NewLeague: A factor with levels A and N indicating player's league at the beginning of 1987

This dataset is available in the ISLR library. The target variable of interest here is the players' salaries. The target variable is missing for 59 of the players, thus we must omit those players from our analysis.

```
> load("Hitters.Rdata")
> Hitters = na.omit(Hitters)
```

Stepwise Selection Methods

We'll start by looking at forward backward selection using the leaps library and the regsubsets command.

```
> library(leaps)
> regfit.fwd = regsubsets(Salary ~ ., data=Hitters, nvmax=19, method="forward")
> regfit.bwd = regsubsets(Salary ~ ., data=Hitters, nvmax=19, method="backward")
> summary(regfit.fwd)
```

```
Subset selection object
Call: regsubsets.formula(Salary ~ ., data = Hitters, nvmax = 19, method = "forward")
19 Variables  (and intercept)
           Forced in Forced out
AtBat          FALSE      FALSE
Hits           FALSE      FALSE
HmRun          FALSE      FALSE
Runs           FALSE      FALSE
RBI            FALSE      FALSE
Walks          FALSE      FALSE
Years          FALSE      FALSE
CAtBat         FALSE      FALSE
CHits          FALSE      FALSE
CHmRun         FALSE      FALSE
CRuns          FALSE      FALSE
CRBI           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 19
Selection Algorithm: forward
          AtBat Hits HmRun Runs RBI Walks Years CAtBat CHits CHmRun CRuns CRBI
1  ( 1 )  " "   " "  " "   " "  " " " "   " "   " "    " "   " "    " "   "*"
2  ( 1 )  " "   "*"  " "   " "  " " " "   " "   " "    " "   " "    " "   "*"
3  ( 1 )  " "   "*"  " "   " "  " " " "   " "   " "    " "   " "    " "   "*"
4  ( 1 )  " "   "*"  " "   " "  " " " "   " "   " "    " "   " "    " "   "*"
5  ( 1 )  "*"   "*"  " "   " "  " " " "   " "   " "    " "   " "    " "   "*"
6  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   " "    " "   " "    " "   "*"
7  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   " "    " "   " "    " "   "*"
8  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   " "    " "   " "    "*"   "*"
9  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   "*"    " "   " "    "*"   "*"
```

```
10  ( 1 ) "*"   "*"  " "   " "  " " "*"   " "   "*"    " "   " "    "*"   "*"
11  ( 1 ) "*"   "*"  " "   " "  " " "*"   " "   "*"    " "   " "    "*"   "*"
12  ( 1 ) "*"   "*"  " "   "*"  " " "*"   " "   "*"    " "   " "    "*"   "*"
13  ( 1 ) "*"   "*"  " "   "*"  " " "*"   " "   "*"    " "   " "    "*"   "*"
14  ( 1 ) "*"   "*"  "*"   "*"  " " "*"   " "   "*"    " "   " "    "*"   "*"
15  ( 1 ) "*"   "*"  "*"   "*"  " " "*"   " "   "*"    "*"   " "    "*"   "*"
16  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   " "   "*"    "*"   " "    "*"   "*"
17  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   " "   "*"    "*"   " "    "*"   "*"
18  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   "*"   "*"    "*"   " "    "*"   "*"
19  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   "*"   "*"    "*"   "*"    "*"   "*"
          CWalks LeagueN DivisionW PutOuts Assists Errors NewLeagueN
1   ( 1 )  " "    " "      " "       " "     " "     " "    " "
2   ( 1 )  " "    " "      " "       " "     " "     " "    " "
3   ( 1 )  " "    " "      " "       "*"     " "     " "    " "
4   ( 1 )  " "    " "      "*"       "*"     " "     " "    " "
5   ( 1 )  " "    " "      "*"       "*"     " "     " "    " "
6   ( 1 )  " "    " "      "*"       "*"     " "     " "    " "
7   ( 1 )  "*"    " "      "*"       "*"     " "     " "    " "
8   ( 1 )  "*"    " "      "*"       "*"     " "     " "    " "
9   ( 1 )  "*"    " "      "*"       "*"     " "     " "    " "
10  ( 1 ) "*"    " "      "*"       "*"     "*"     " "    " "
11  ( 1 ) "*"    "*"      "*"       "*"     "*"     " "    " "
12  ( 1 ) "*"    "*"      "*"       "*"     "*"     " "    " "
13  ( 1 ) "*"    "*"      "*"       "*"     "*"     "*"    " "
14  ( 1 ) "*"    "*"      "*"       "*"     "*"     "*"    " "
15  ( 1 ) "*"    "*"      "*"       "*"     "*"     "*"    " "
16  ( 1 ) "*"    "*"      "*"       "*"     "*"     "*"    " "
17  ( 1 ) "*"    "*"      "*"       "*"     "*"     "*"    "*"
18  ( 1 ) "*"    "*"      "*"       "*"     "*"     "*"    "*"
19  ( 1 ) "*"    "*"      "*"       "*"     "*"     "*"    "*"
```

```
> summary(regfit.bwd)
```

```
Subset selection object
Call: regsubsets.formula(Salary ~ ., data = Hitters, nvmax = 19, method = "backward")
19 Variables  (and intercept)
           Forced in Forced out
AtBat          FALSE      FALSE
Hits           FALSE      FALSE
HmRun          FALSE      FALSE
Runs           FALSE      FALSE
RBI            FALSE      FALSE
Walks          FALSE      FALSE
Years          FALSE      FALSE
CAtBat         FALSE      FALSE
CHits          FALSE      FALSE
CHmRun         FALSE      FALSE
CRuns          FALSE      FALSE
CRBI           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 19
Selection Algorithm: backward
```

```
          AtBat Hits HmRun Runs RBI Walks Years CAtBat CHits CHmRun CRuns CRBI
1  ( 1 )  " "   " "  " "   " "  " " " "   " "   " "    " "   " "    "*"   " "
2  ( 1 )  " "   "*"  " "   " "  " " " "   " "   " "    " "   " "    "*"   " "
3  ( 1 )  " "   "*"  " "   " "  " " " "   " "   " "    " "   " "    "*"   " "
4  ( 1 )  "*"   "*"  " "   " "  " " " "   " "   " "    " "   " "    "*"   " "
5  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   " "    " "   " "    "*"   " "
6  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   " "    " "   " "    "*"   " "
7  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   " "    " "   " "    "*"   " "
8  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   " "    " "   " "    "*"   "*"
9  ( 1 )  "*"   "*"  " "   " "  " " "*"   " "   "*"    " "   " "    "*"   "*"
10  ( 1 ) "*"   "*"  " "   " "  " " "*"   " "   "*"    " "   " "    "*"   "*"
11  ( 1 ) "*"   "*"  " "   " "  " " "*"   " "   "*"    " "   " "    "*"   "*"
12  ( 1 ) "*"   "*"  " "   "*"  " " "*"   " "   "*"    " "   " "    "*"   "*"
13  ( 1 ) "*"   "*"  " "   "*"  " " "*"   " "   "*"    " "   " "    "*"   "*"
14  ( 1 ) "*"   "*"  "*"   "*"  " " "*"   " "   "*"    " "   " "    "*"   "*"
15  ( 1 ) "*"   "*"  "*"   "*"  " " "*"   " "   "*"    "*"   " "    "*"   "*"
16  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   " "   "*"    "*"   " "    "*"   "*"
17  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   " "   "*"    "*"   " "    "*"   "*"
18  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   "*"   "*"    "*"   " "    "*"   "*"
19  ( 1 ) "*"   "*"  "*"   "*"  "*" "*"   "*"   "*"    "*"   "*"    "*"   "*"
          CWalks LeagueN DivisionW PutOuts Assists Errors NewLeagueN
1  ( 1 )  " "    " "     " "       " "     " "     " "    " "
2  ( 1 )  " "    " "     " "       " "     " "     " "    " "
3  ( 1 )  " "    " "     " "       "*"     " "     " "    " "
4  ( 1 )  " "    " "     " "       "*"     " "     " "    " "
5  ( 1 )  " "    " "     " "       "*"     " "     " "    " "
6  ( 1 )  " "    " "     "*"       "*"     " "     " "    " "
7  ( 1 )  "*"    " "     "*"       "*"     " "     " "    " "
8  ( 1 )  "*"    " "     "*"       "*"     " "     " "    " "
9  ( 1 )  "*"    " "     "*"       "*"     " "     " "    " "
10  ( 1 ) "*"    " "     "*"       "*"     "*"     " "    " "
11  ( 1 ) "*"    "*"     "*"       "*"     "*"     " "    " "
12  ( 1 ) "*"    "*"     "*"       "*"     "*"     " "    " "
13  ( 1 ) "*"    "*"     "*"       "*"     "*"     "*"    " "
14  ( 1 ) "*"    "*"     "*"       "*"     "*"     "*"    " "
15  ( 1 ) "*"    "*"     "*"       "*"     "*"     "*"    " "
16  ( 1 ) "*"    "*"     "*"       "*"     "*"     "*"    " "
17  ( 1 ) "*"    "*"     "*"       "*"     "*"     "*"    "*"
18  ( 1 ) "*"    "*"     "*"       "*"     "*"     "*"    "*"
19  ( 1 ) "*"    "*"     "*"       "*"     "*"     "*"    "*"
```

The summaries tell us which variables show up in the best p-variable models where p ranges from 1 input to all 19 inputs. This spacious output can be hard to read, but we can use the *vorder* output vector to tell us in what order the variables the model should contain if we allow p variables into the model. You can easily see that each selection method provided us with different models, no matter what number of variables we choose to allow.

```
> regfit.fwd$vorder
```

```
 [1]  1 13  3 17 16  2  7 14 12  9 18 15  5 19  4 10  6 20  8 11
```

```
> regfit.bwd$vorder
```

```
 [1]  1 12  3 17  2  7 16 14 13  9 18 15  5 19  4 10  6 20  8 11
```

We can get the actual coefficients from the chosen models using the coef() function and specifying the number of variables we want:

```
> coef(regfit.fwd, 7)
```

```
 (Intercept)        AtBat         Hits        Walks         CRBI       CWalks
 109.7873062   -1.9588851    7.4498772    4.9131401    0.8537622   -0.3053070
   DivisionW      PutOuts
-127.1223928    0.2533404
```

```
> coef(regfit.bwd, 7)
```

```
 (Intercept)        AtBat         Hits        Walks        CRuns       CWalks
 105.6487488   -1.9762838    6.7574914    6.0558691    1.1293095   -0.7163346
   DivisionW      PutOuts
-116.1692169    0.3028847
```

Now the task is to pick the *size* of our model. The best way to do this is to use validation or cross-validation. In this next process, we'll have to redo the variable selection process so that only the training data is used to select the best model of a given size. This is a very important point! If all of the data is used to perform the variable selection step, the validation set errors will not be accurate estimates of the test error. For that matter, cross-validation might seem a little confusing in this context. If for every fold we're going to repeat the variable selection process, it is possible that different subsets of variables will be chosen for each fold! This is actually ok, because we are not validating the final model - we are simply choosing the best number of variables that the final model should contain. Once we decide what number of variables works best (say p^* inputs) through cross validation we re-run the variable selection on the whole dataset and use the best model with p^* inputs.

Here, we will keep the computation simpler and just use a single validation dataset. To create the index vectors for the training and test datasets, we'll create a random logical vector which selects true values (for the training set) 60% of the time.

```
> set.seed(7515)
> train=sample(c(T,F), nrow(Hitters), rep=TRUE, p=c(0.6,0.4))
> test=!train
> regfit.fwd = regsubsets(Salary~., data=Hitters[train, ], method="forward", nvmax=19)
> regfit.bwd = regsubsets(Salary~., data=Hitters[train, ], method="backward",nvmax=19)
```

Since the regsubsets function only outputs a set of coefficients for each value of p, we need a model matrix to compute the predictions, $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$, on the test data. The model.matrix command makes this easy for us. Keep in mind that matrix multiplication in R is done using the %*% command, and that we only want to score the test data.

```
> X = model.matrix(Salary~., data=Hitters[test, ])
> fwd.val.MSE=vector()
> bwd.val.MSE=vector()
> for (i in 1:19) {
+   beta.fwd = coef(regfit.fwd, i)
+   beta.bwd = coef(regfit.bwd, i)
+   pred.fwd = X[,names(beta.fwd)] %*% beta.fwd
+   pred.bwd = X[,names(beta.bwd)] %*% beta.bwd
+   fwd.val.MSE[i] = mean((Hitters$Salary[test] - pred.fwd)^2)
+   bwd.val.MSE[i] = mean((Hitters$Salary[test] - pred.bwd)^2)
+ }
> min(fwd.val.MSE)
```

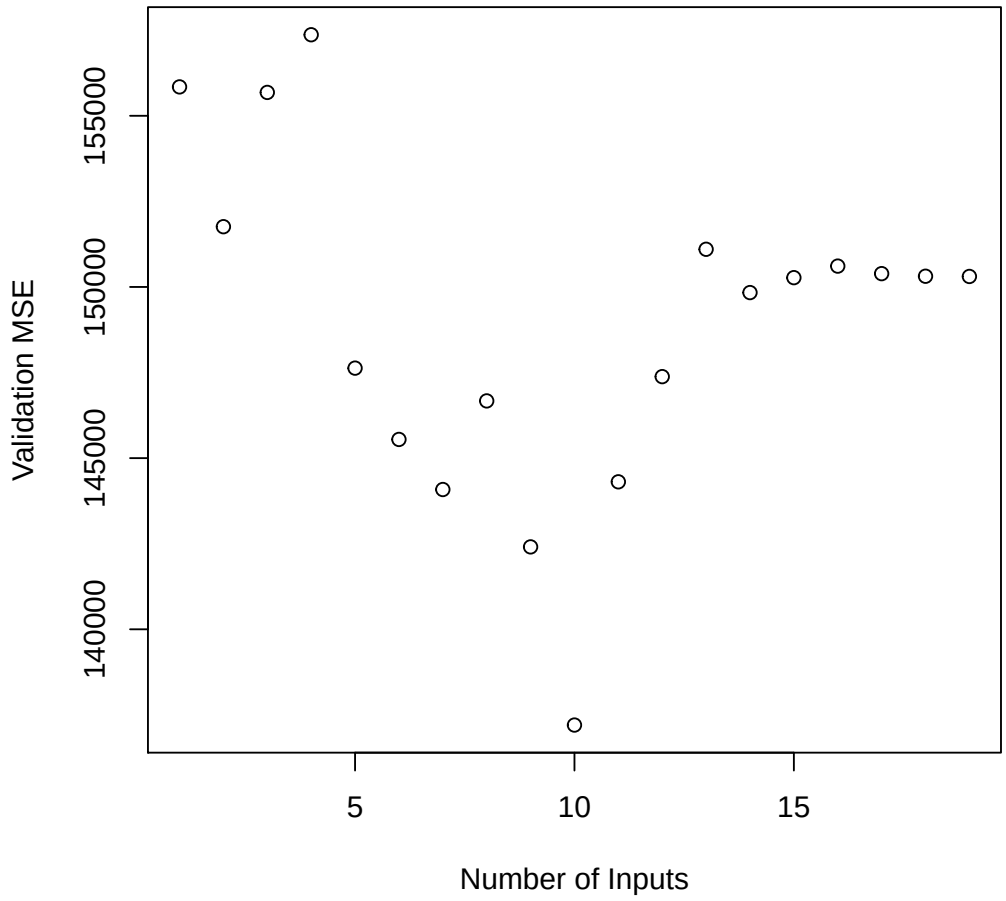
```
[1] 137203.1
```

```
> min(bwd.val.MSE)
```

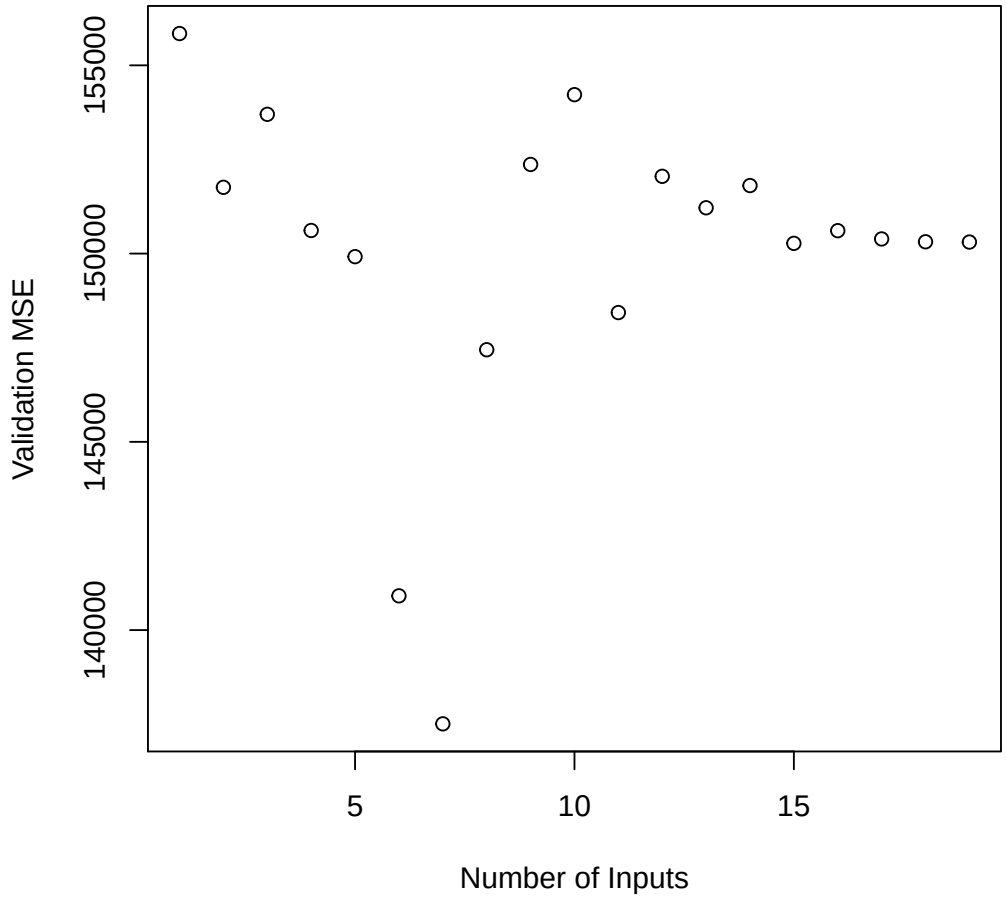
```
[1] 137510.2
```

Now that we have the validation MSE for each number of parameters and each selection technique, we simply choose the number of parameters that minimizes the validation MSE for each selection method.

```
> plot(1:19,fwd.val.MSE, xlab="Number of Inputs", ylab = "Validation MSE")
```




```
> plot(1:19,bwd.val.MSE, xlab="Number of Inputs", ylab = "Validation MSE")
```



The two graphs are quite different. Forward selection chooses a 10 variable model whereas backward selection chooses a 7 variable model.

```
> coef(regfit.fwd,10)
```

```
(Intercept)       AtBat        Hits        Runs       Walks      CAtBat
 93.9840930  -2.5569014  11.1792265  -5.4583086   8.0172922  -0.1594122
     CHmRun       CRuns      CWalks   DivisionW     PutOuts
  0.7415922   2.2277955  -0.8530738 -64.3153622   0.1866306
```

```
> coef(regfit.bwd,7)
```

```
(Intercept)       AtBat        Hits       Walks      CHmRun       CRuns
 17.9102884  -2.8964270   9.9139855   8.4739365   0.8614003   1.0895680
     CWalks     PutOuts
 -0.9142449   0.1631992
```

In order to finalize the coefficients for the chosen models, we'd re-run the variable selection process on the entire dataset using only the chosen number of variables.

```
> regfit.fwd.best = regsubsets(Salary~., data=Hitters, method="forward", nvmax=10)
> regfit.bwd.best = regsubsets(Salary~., data=Hitters, method="backward", nvmax=7)
> coef(regfit.fwd.best,10)
```

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

```
> coef(regfit.bwd.best,7)
```

```
 (Intercept)        AtBat         Hits        Walks        CRuns       CWalks
 105.6487488   -1.9762838    6.7574914    6.0558691    1.1293095   -0.7163346
   DivisionW      PutOuts
-116.1692169    0.3028847
```

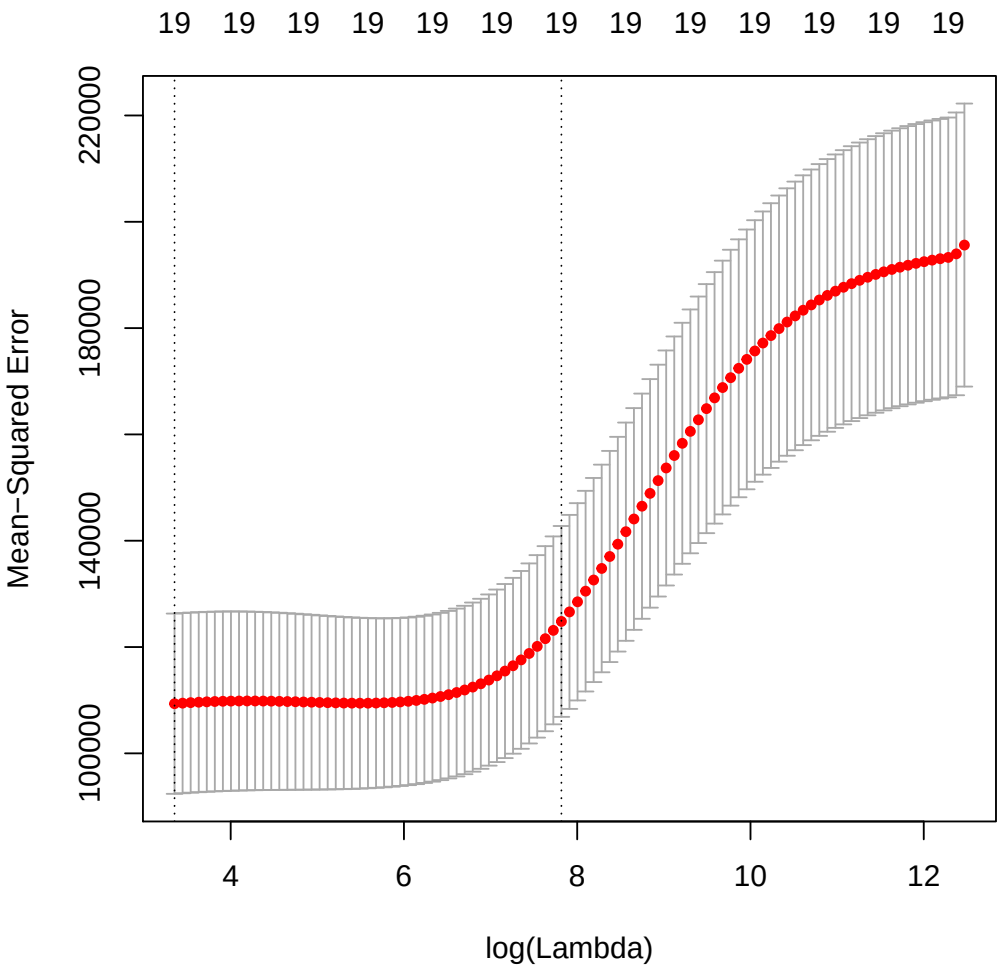
Ridge Regression

For the sake of argument, let's see what type of results Ridge Regression will provide on our validation data. We'll first tune the shrinkage parameter, λ, using cross-validation because this is standard practice. This will be done using the glmnet package and glmnet() function. This package has built in capabilities for doing a cross-validation loop which makes it convenient for our purposes. The glmnet() function wants the user to specify a model matrix $\mathbf{X}$ (design matrix) and a vector containing the target variable $\mathbf{y}$, it does not use the y$\tilde{\text{x}}$ syntax that many other modeling packages use.

```
> X=model.matrix(Salary~. ,data=Hitters)[,-1]
> y = Hitters$Salary
```

We'll now perform cross-validation to determine an optimal value of λ. We'll only use the training data for the cross-validation step. We can then test the ridge regression model with this lambda on our validation dataset from the previous section. The option alpha=0 specifies ridge regression. We will change this to alpha=1 to implement the LASSO.

```
> library(glmnet)
> set.seed(1)
> cv.out = cv.glmnet(X[train,], y[train], alpha=0)
> plot(cv.out)
```



The method will choose the value of λ that has the best performance on cross-validation. We can grab that value from the output, create a ridge model using it and then check the performance of the ridge regression model on our out-of-sample test data used previously.

```
> bestlambda=cv.out$lambda.min
> bestlambda
```

```
[1] 28.55636
```

```
> ridge.mod = glmnet(X[train,], y[train], alpha=0, lambda=bestlambda)
> pred.ridge = predict(ridge.mod, newx=X[test,])
> val.MSE.ridge = mean((pred.ridge - y[test])^2)
> val.MSE.ridge
```

```
[1] 131170.1
```

Notice that the validation MSE for this ridge regression is a dramatic reduction from the MSE of the full model in the original least-squares context. Just take a look at the validation MSE graphs from forward/backward selection when the number of inputs is p>9. This ridge regression model does contain

all 19 predictor variables, but still performs well on out-of-sample data. That's quite a feat! In certain situations, it is not reasonable to keep all of the predictor variables in the model, but when it is feasible, ridge regression is an excellent alternative to classical least-squares.

To get the final parameter estimates for the ridge regression model, we'd use the full data:

```
> out=glmnet(X,y,alpha=0, lambda=bestlambda)
> ridge.coef = predict(out, type="coefficients")
> ridge.coef
```

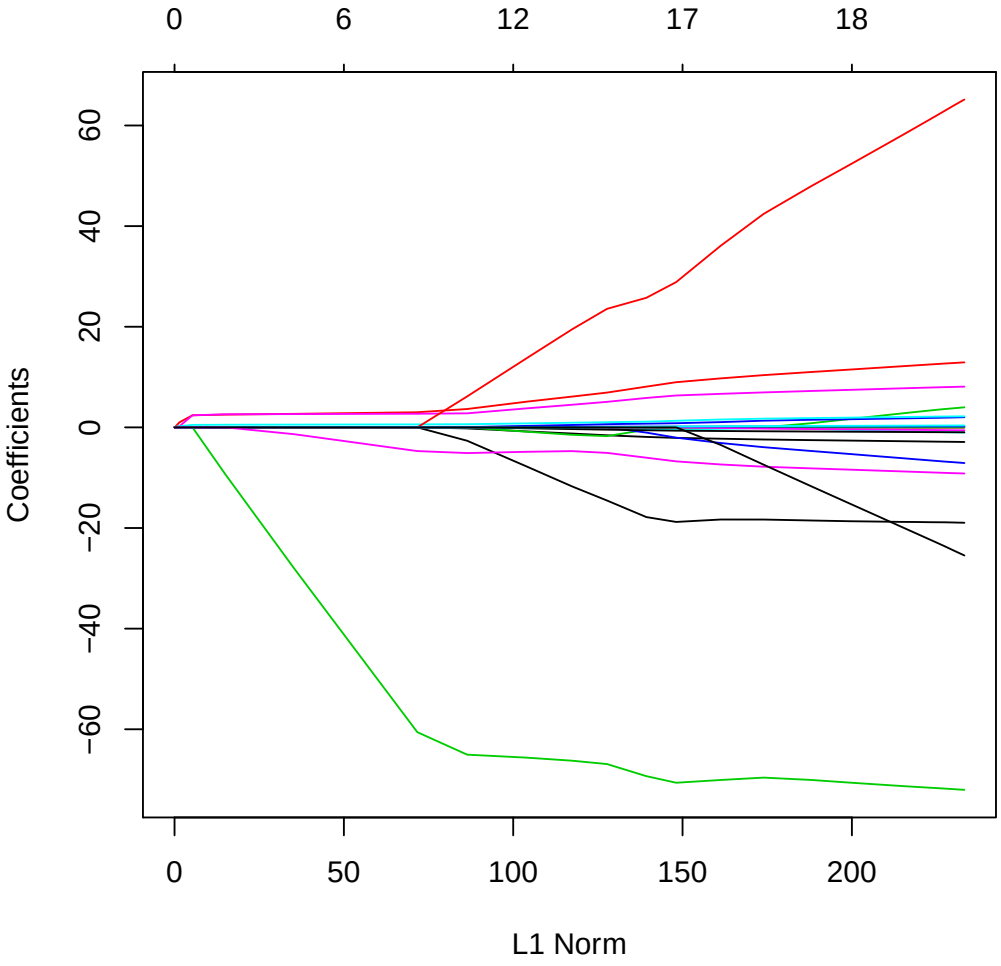
```
20 x 1 sparse Matrix of class "dgCMatrix"
                      s0
(Intercept)  7.470361e+01
AtBat       -6.213053e-01
Hits         2.616265e+00
HmRun       -1.370556e+00
Runs         1.062393e+00
RBI          7.377029e-01
Walks        3.252261e+00
Years       -8.542415e+00
CAtBat       1.052958e-03
CHits        1.296194e-01
CHmRun       6.746749e-01
CRuns        2.741870e-01
CRBI         2.530448e-01
CWalks      -2.527248e-01
LeagueN      5.210903e+01
DivisionW   -1.223474e+02
PutOuts      2.619033e-01
Assists      1.607600e-01
Errors      -3.636362e+00
NewLeagueN  -1.678202e+01
```

The LASSO

If we wanted to use the LASSO in a context similar to forward selection, we'd probably start by looking at the following plot, which shows how the coefficients in the model change as the shrinkage parameter λ declines. When λ is very large, we are prohibited from adding any parameters to the model. We start with the intercept-only null model. As λ gets smaller (moving to the right of the plot) we see that we can start allowing variables to enter the model if they will drive down the sum of squared error. In this way, LASSO acts as a selection technique, with one variable entering the model at a time.

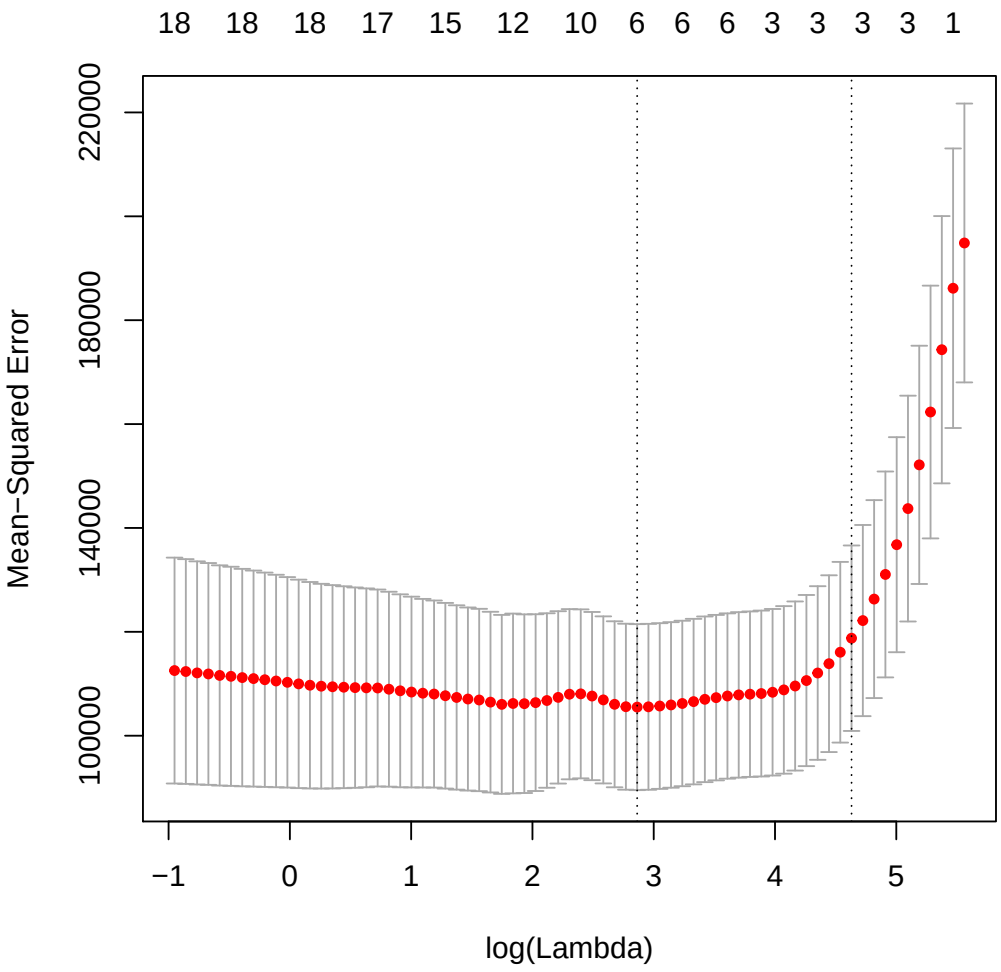
Again, to run LASSO, we use the glmnet() function with the option alpha=1. The lambda=grid option will compute the coefficients for the specified values of $\lambda = 10^k$ where k decreases incrementally 100 times from 10 to -2.

```
> grid = 10^seq(10,-2,length=100)
> lasso.mod = glmnet(X[train,],y[train],alpha=1,lambda=grid)
> plot(lasso.mod)
```



Although this plot is difficult to read, we can see that many of the coefficients remain exactly zero, depending on the choice of the shrinkage parameter λ. We can tune the shrinkage parameter again using cross-validation on the training data, and then compare the resulting model on our validation data.

```
> set.seed(1)
> cv.out=cv.glmnet(X[train,],y[train],alpha=1)
> plot(cv.out)
```



We can then use the information from the output dataset to obtain the best lambda and predict the salaries of hitters from the out-of-sample validation data, computing the MSE as before.

```
> bestlambda=cv.out$lambda.min
> pred.lasso = predict(lasso.mod, s=bestlambda, newx=X[test,])
> val.MSE.lasso = mean((pred.lasso-y[test])^2)
> val.MSE.lasso
```

```
[1] 138231.5
```

The advantage of the LASSO over ridge regression is that the resulting coefficient estimates are sparse. Below we see that 12 of the 19 coefficient estimates are exactly zero. So the LASSO model contains only 7 variables.

```
> out=glmnet(X,y,alpha=1,lambda=bestlambda)
> lasso.coef=predict(out, type="coefficients")
> lasso.coef
```

```
20 x 1 sparse Matrix of class "dgCMatrix"
                      s0
```

```
(Intercept)   22.09921558
AtBat          .
Hits           1.86043600
HmRun          .
Runs           .
RBI            .
Walks          2.21068867
Years          .
CAtBat         .
CHits          .
CHmRun         .
CRuns          0.20689273
CRBI           0.41139580
CWalks         .
LeagueN        0.09429113
DivisionW   -102.17929783
PutOuts        0.21904019
Assists        .
Errors         .
NewLeagueN     .
```

You'll notice if you play with the random seed in the cross validation step, you may get results that look quite different. In fact, they are not as different as they seem - while so many coefficients may not be exactly zero, they are close enough to zero that omitting those variables from the model will not have such a drastic effect on the validation MSE. Once you get the final list of parameters, you may have to make a judgement call on which parameter estimates are large enough to include. An alternative approach is to use bestlambda=lambda.1se. The lambda.1se is the value of lambda that provided the simplest model but which has cross-validation error within 1 standard deviation of the minimum error. This value of lambda tends to provide results that are more stable across validation datasets. In our example, lambda.1se tends to produce models with only 5 variables.