Subset Selection, Ridge Regression and LASSO

Here we apply the best subset selection approach to the Hitters data. We wish to predict a baseball player's Salary on the basis of various statistics associated with performance in the previous year.

First of all, we note that the Salary variable is missing for some of the players. The is.na() function can be used to identify the missing observations. It returns a vector of the same length as the input vector, with a TRUE for any elements that are missing, and a FALSE for non-missing elements. The sum() function can then be used to count all of the missing elements.

```
library(ISLR2)
names(Hitters)
```

##	[1]	"AtBat"	"Hits"	"HmRun"	"Runs"	"RBI"	"Walks"	
##	[7]	"Years"	"CAtBat"	"CHits"	"CHmRun"	"CRuns"	"CRBI"	
##	[13]	"CWalks"	"League"	"Division"	"PutOuts"	"Assists"	"Errors"	
##	[19]	"Salary"	"NewLeague"					
dim(Hitters)								

[1] 322 20
sum(is.na(Hitters\$Salary))

[1] 59

The na.omit() function removes all of the rows that have missing values in any variable.

```
Hitters <- na.omit(Hitters)
dim(Hitters)
```

[1] 263 20

sum(is.na(Hitters))

[1] 0

Best subset selection and stepwise selection

The **regsubsets()** function (part of the **leaps** library) performs best subset selection by identifying the best model that contains a given number of predictors, where best is quantified using RSS. An asterisk indicates that a given variable is included in the corresponding model. For instance, this output indicates that the best two-variable model contains only **Hits** and **CRBI**.

```
library(leaps)
regfit.full <- regsubsets(Salary ~ ., data = Hitters)
summary(regfit.full)
## Subset selection object
## Call: regsubsets.formula(Salary ~ ., data = Hitters)
## 19 Variables (and intercept)
## Forced in Forced out
## AtBat FALSE FALSE
## Hits FALSE FALSE
## Hits FALSE FALSE</pre>
```

```
## HmRun
                  FALSE
                              FALSE
                  FALSE
                              FALSE
## Runs
## 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
                  FALSE
                              FALSE
## PutOuts
## Assists
                  FALSE
                              FALSE
## Errors
                  FALSE
                              FALSE
## NewLeagueN
                  FALSE
                              FALSE
## 1 subsets of each size up to 8
## Selection Algorithm: exhaustive
##
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## 3
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## 4
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## 4
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                                                       ...
## 5
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     (1)""
                   н н
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                            "*"
## 6
     (1)""
                   н н
                            "*"
                                      "*"
                                               . .
                                                       ## 7
                                               н н
                            "*"
                                      "*"
## 8 (1) "*"
```

By default, regsubsets() only reports results up to the best eight-variable model. But the nvmax option can be used in order to return as many variables as are desired. Here we fit up to a 19-variable model.

The summary() function also returns R^2 , RSS, adjusted R^2 , C_p , and BIC. We can examine these to try to select the best overall model.

names(reg.summary)

[1] "which" "rsq" "rss" "adjr2" "cp" "bic" "outmat" "obj"

The \mathbb{R}^2 statistic increases monotonically as more variables are included:

reg.summary\$rsq

[1] 0.3214501 0.4252237 0.4514294 0.4754067 0.4908036 0.5087146 0.5141227

[8] 0.5285569 0.5346124 0.5404950 0.5426153 0.5436302 0.5444570 0.5452164
[15] 0.5454692 0.5457656 0.5459518 0.5460945 0.5461159

The C_p statistics:

reg.summary\$cp

[1] 104.281319 50.723090 38.693127 27.856220 21.613011 14.023870
[7] 13.128474 7.400719 6.158685 5.009317 5.874113 7.330766
[13] 8.888112 10.481576 12.346193 14.187546 16.087831 18.011425
[19] 20.000000

which.min(reg.summary\$cp)

[1] 10

The BIC:

reg.summary\$bic

[1] -90.84637 -128.92622 -135.62693 -141.80892 -144.07143 -147.91690
[7] -145.25594 -147.61525 -145.44316 -143.21651 -138.86077 -133.87283
[13] -128.77759 -123.64420 -118.21832 -112.81768 -107.35339 -101.86391
[19] -96.30412

which.min(reg.summary\$bic)

[1] 6

We can also use the regsubsets() function to perform forward stepwise or backward stepwise selection, using the argument method = "forward" or method = "backward".

```
regfit.fwd <- regsubsets(Salary ~ ., data = Hitters, nvmax = 19, method = "forward")
summary(regfit.fwd)</pre>
```

```
## 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
```

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(1)	"*"	"*"	",	k"		"*"	"*"	"*"	"	"		
(1)	"*"	"*"	",	k"		"*"	"*"	"*"	"			
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(1)	"*"	"*"	",	k"		"*"	"*"	"*"	"*			
(1)	"*"	"*"	",	k"		"*"	"*"	"*"	"*			
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##	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	-								
##	Selection Alg									
##		at Hits HmRu								CRBI
##	1 (1) ""								"*"	
##	2 (1) ""	-1-							"*"	
##	3 (1) ""	4.							"*"	
##	4 (1) "*"								"*"	
##	5 (1) "*"			-1-					"*"	
##	6 (1) "*"			-1-					"*"	
##	7 (1) "*"			-1-					"*"	
##	8 (1) "*"			-1-					"*"	"*"
##	9 (1) "*"	"*" " "		"*"		"*"			"*"	"*"
##	10 (1)"*"			-1-		"*"			"*"	"*"
##	11 (1) "*"					"*"			"*"	"*"
##	12 (1)"*"	"*" " "	"*" " "	"*"		"*"			"*"	"*"
##	13 (1) "*"	"*" " "	"*" " "	"*"		"*"			"*"	"*"
##	14 (1)"*"	"*" "*"	"*" " "	"*"	11 11	"*"			"*"	"*"
##	15 (1)"*"	"*" "*"	"*" " "		11 11	"*"	"*"		"*"	"*"
##	16 (1)"*"	"*" "*"	"*" "*"	"*"	11 11	"*"	"*"		"*"	"*"
##	17 (1)"*"	"*" "*"		"*"	11 11	"*"	"*"		"*"	"*"
##	18 (1)"*"	"*" "*"		"*"	"*"	"*"	"*"	" "	"*"	"*"
##	19 (1) "*"	"*" "*"	"*" "*"	"*"	"*"	"*"	"*"	"*"	"*"	"*"
##	CWa	lks LeagueN	DivisionW	PutOuts	s Assis	ts Erro	rs Nev	League	1	
##	1 (1) ""				" "			1		
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##	9 (1) "*"		"*"	"*"				ı		
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	14 (1) "*"	"*"	"*"	"*"	"*"	"*"		ı		
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19 (1) "*" "*" "*" "*" "*" "*"

For this data, the best one-variable through six-variable models are each identical for best subset and forward selection. However, the best seven-variable models identified by forward stepwise selection, backward stepwise selection, and best subset selection are different.

```
coef(regfit.full, 7)
                                                                                 CHmRun
##
    (Intercept)
                          Hits
                                       Walks
                                                    CAtBat
                                                                    CHits
##
     79.4509472
                    1.2833513
                                   3.2274264
                                                -0.3752350
                                                               1.4957073
                                                                             1.4420538
##
      DivisionW
                       PutOuts
## -129.9866432
                    0.2366813
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
```

We just saw that it is possible to choose among a set of models of different sizes using C_p , BIC, and adjusted R^2 . We will now consider how to do this using the validation set and cross-validation approaches.

In order to use the validation set approach, we begin by splitting the observations into a training set and a test set.

```
set.seed(1)
train <- sample(c(TRUE, FALSE), nrow(Hitters), replace = TRUE)
test <- (!train)</pre>
```

We apply regsubsets() to the training set in order to perform best subset selection.

regfit.best <- regsubsets(Salary ~ ., data = Hitters[train,], nvmax = 19)</pre>

We now compute the validation set error for the best model of each model size. We first make a model matrix from the test data. The model.matrix() function is used in many regression packages for building an "X' matrix from data.

test.mat <- model.matrix(Salary ~ ., data = Hitters[test,])</pre>

Now we run a loop, and for each size i, we extract the coefficients from regfit.best for the best model of that size, multiply them into the appropriate columns of the test model matrix to form the predictions, and compute the test MSE.

```
val.errors <- rep(NA, 19)
for (i in 1:19) {
    coefi <- coef(regfit.best, id = i)
    pred <- test.mat[, names(coefi)] %*% coefi
    val.errors[i] <- mean((Hitters$Salary[test] - pred)^2)
}</pre>
```

We find that the best model is the one that contains seven variables.

```
val.errors
```

##

##

67.1085369

DivisionW

[1] 164377.3 144405.5 152175.7 145198.4 137902.1 139175.7 126849.0 136191.4
[9] 132889.6 135434.9 136963.3 140694.9 140690.9 141951.2 141508.2 142164.4
[17] 141767.4 142339.6 142238.2
which.min(val.errors)
[1] 7
coef(regfit.best, 7)
(Intercept) AtBat Hits Walks CRuns CWalks

-118.4364998 0.2526925
Finally, we perform best subset selection on the full data set, and select the best seven-variable model. Note that we perform best subset selection on the full data set and select the best seven-variable model, rather than simply using the variables that were obtained from the training set, because the best seven-variable

8.0716640

1.2425113

-0.8337844

```
model on the full data set may differ from the corresponding model on the training set.
regfit.best <- regsubsets(Salary ~ ., data = Hitters, nvmax = 19)
coef(regfit.best, 7)</pre>
```

7.0149547

##	(Intercept)	Hits	Walks	CAtBat	CHits	CHmRun
##	79.4509472	1.2833513	3.2274264	-0.3752350	1.4957073	1.4420538
##	DivisionW	PutOuts				
##	-129.9866432	0.2366813				

We write a function for the predict() method for regsubsets().

-2.1462987

PutOuts

```
predict.regsubsets <- function(object, newdata, id, ...) {
  form <- as.formula(object$call[[2]])
  mat <- model.matrix(form, newdata)
  coefi <- coef(object, id = id)
  xvars <- names(coefi)
  mat[, xvars] %*% coefi
}</pre>
```

We now try to choose among the models of different sizes using cross-validation. We must perform best subset selection within each of the k training sets. First, we create a vector that allocates each observation to one of k = 10 folds, and we create a matrix in which we will store the results.

```
k <- 10
n <- nrow(Hitters)
set.seed(1)
folds <- sample(rep(1:k, length = n))
cv.errors <- matrix(NA, k, 19,)</pre>
```

In the *j*th fold, the elements of **folds** that equal **j** are in the test set, and the remainder are in the training set. We make our predictions for each model size, compute the test errors on the appropriate subset, and store them in the matrix **cv.errors**. This has given us a 10×19 matrix, of which the (j, i)th element corresponds to the test MSE for the *j*th cross-validation fold for the best *i*-variable model.

```
for (j in 1:k) {
   best.fit <- regsubsets(Salary ~ ., data = Hitters[folds != j, ], nvmax = 19)
   for (i in 1:19) {
    pred <- predict(best.fit, Hitters[folds == j, ], id = i)</pre>
```

```
cv.errors[j, i] <- mean((Hitters$Salary[folds == j] - pred)^2)
}</pre>
```

We use the apply() function to average over the columns of this matrix in order to obtain a vector for which the *i*th element is the cross-validation error for the *i*-variable model. We see that cross-validation selects a 10-variable model.

```
mean.cv.errors <- apply(cv.errors, 2, mean)
mean.cv.errors
## [1] 143439.8 126817.0 134214.2 131782.9 130765.6 120382.9 121443.1 114363.7
## [9] 115163.1 109366.0 112738.5 113616.5 115557.6 115853.3 115630.6 116050.0
## [17] 116117.0 116419.3 116299.1</pre>
```

We now perform best subset selection on the full data set in order to obtain the 10-variable model.

```
reg.best <- regsubsets(Salary ~ ., data = Hitters, nvmax = 19)
coef(reg.best, 10)</pre>
```

##	(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	

Ridge regression and the LASSO

We will use the function glmnet() in the glmnet package. We will now perform ridge regression and the lasso in order to predict Salary on the Hitters data. The model.matrix() function is useful for creating x; not only does it produce a matrix corresponding to the 19 predictors but it also automatically transforms any qualitative variables into dummy variables. glmnet() can only take numerical, quantitative inputs. [, -1] removes the intercept.

```
x <- model.matrix(Salary ~ ., Hitters)[, -1]
y <- Hitters$Salary</pre>
```

The glmnet() function has an alpha argument that determines what type of model is fit. If alpha=0 then a ridge regression model is fit, and if alpha=1 then a LASSO model is fit. We implement the function over a grid: $\lambda = 10^{10}$ to $\lambda = 10^{-2}$, covering the null model containing only the intercept, to the least squares fit. By default, the glmnet() function standardizes the variables so that they are on the same scale.

library(glmnet)

```
## Matrix
## Loaded glmnet 4.1-2
grid <- 10^seq(10, -2, length = 100)
ridge.mod <- glmnet(x, y, alpha = 0, lambda = grid)</pre>
```

Associated with each value of λ is a vector of ridge regression coefficients, stored in a matrix that can be accessed by **coef()**. In this case, it is a 20 × 100 matrix, with 20 rows (one for each predictor, plus an intercept) and 100 columns (one for each value of λ).

dim(coef(ridge.mod))

[1] 20 100

We can use the predict() function for a number of purposes. For instance, we can obtain the ridge regression coefficients for a new value of λ , say 50:

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

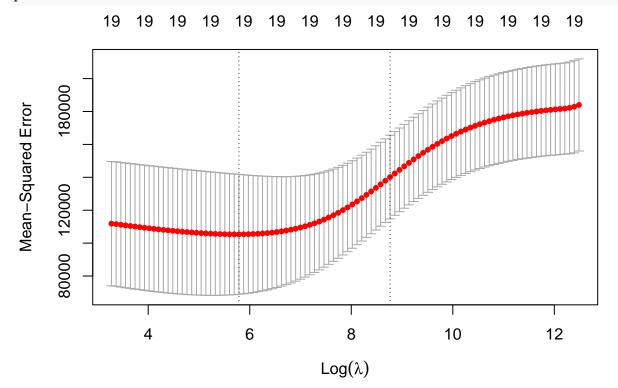
##	(Intercept)	AtBat	Hits	HmRun	Runs
##	4.876610e+01	-3.580999e-01	1.969359e+00	-1.278248e+00	1.145892e+00
##	RBI	Walks	Years	CAtBat	CHits
##	8.038292e-01	2.716186e+00	-6.218319e+00	5.447837e-03	1.064895e-01
##	CHmRun	CRuns	CRBI	CWalks	LeagueN
##	6.244860e-01	2.214985e-01	2.186914e-01	-1.500245e-01	4.592589e+01
##	DivisionW	PutOuts	Assists	Errors	NewLeagueN
##	-1.182011e+02	2.502322e-01	1.215665e-01	-3.278600e+00	-9.496680e+00

We now split the samples into a training set and a test set in order to estimate the test error of ridge regression and the LASSO We randomly choose a subset of numbers between 1 and n as the indices for the training observations.

```
set.seed(1)
train <- sample(1:nrow(x), nrow(x) / 2)
test <- (-train)
y.test <- y[test]
ridge.mod <- glmnet(x[train, ], y[train], alpha = 0, lambda = grid)</pre>
```

We use cross-validation to choose the tuning parameter λ . We can do this using the built-in cross-validation function, cv.glmnet(). By default, the function performs ten-fold cross-validation, though this can be changed using the argument nfolds.

```
set.seed(1)
cv.out <- cv.glmnet(x[train, ], y[train], alpha = 0)
plot(cv.out)</pre>
```



bestlam <- cv.out\$lambda.min
bestlam</pre>

[1] 326.0828

The test MSE associated with this value of λ :

```
ridge.pred <- predict(ridge.mod, s = bestlam, newx = x[test, ])
mean((ridge.pred - y.test)^2)</pre>
```

[1] 139833.6

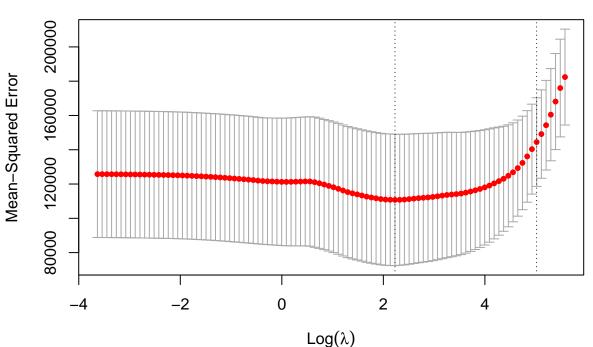
We examine the coefficient estimates. None of the coefficients are zero: ridge regression does not perform variable selection.

```
out <- glmnet(x, y, alpha = 0)
predict(out, type = "coefficients", s = bestlam)[1:20, ]</pre>
```

##	(Intercept)	AtBat	Hits	HmRun	Runs	RBI
##	15.44383135	0.07715547	0.85911581	0.60103107	1.06369007	0.87936105
##	Walks	Years	CAtBat	CHits	CHmRun	CRuns
##	1.62444616	1.35254780	0.01134999	0.05746654	0.40680157	0.11456224
##	CRBI	CWalks	LeagueN	DivisionW	PutOuts	Assists
##	0.12116504	0.05299202	22.09143189	-79.04032637	0.16619903	0.02941950
##	Errors	NewLeagueN				
##	-1.36092945	9.12487767				

In order to fit a LASSO model, we once again use the glmnet() function with alpha=1. We perform cross-validation and compute the associated test error.

```
lasso.mod <- glmnet(x[train, ], y[train], alpha = 1, lambda = grid)
set.seed(1)
cv.out <- cv.glmnet(x[train, ], y[train], alpha = 1)
plot(cv.out)</pre>
```



19 19 19 19 17 17 15 14 12 10 10 8 8 4 3 2

[1] 143673.6

However, the lasso has a substantial advantage over ridge regression in that the resulting coefficient estimates are sparse.

```
out <- glmnet(x, y, alpha = 1, lambda = grid)
lasso.coef <- predict(out, type = "coefficients", s = bestlam)[1:20, ]
lasso.coef</pre>
```

##	(Intercept)	AtBat	Hits	HmRun	Runs
##	1.27479059	-0.05497143	2.18034583	0.0000000	0.0000000
##	RBI	Walks	Years	CAtBat	CHits
##	0.0000000	2.29192406	-0.33806109	0.0000000	0.0000000
##	CHmRun	CRuns	CRBI	CWalks	LeagueN
##	0.02825013	0.21628385	0.41712537	0.0000000	20.28615023
##	DivisionW	PutOuts	Assists	Errors	NewLeagueN
##	-116.16755870	0.23752385	0.0000000	-0.85629148	0.0000000