Regression Subset Selection in R

For linear regression: lm() from stats package (built-in) For logistic regression: glm() from stats package For lasso and ridge regression: glmnet() from glmnet package

Load packages

```
library(glmnet)
library(QuantPsyc) # for standardized regression coefficients
library(subselect)
#library(lars)
library(tabuSearch)
```

Additionally

```
library(lavaan) # for HolzingerSwineford1939 dataset
HS <- HolzingerSwineford1939

library(elasticnet) # regularized PCA
#library(fanc) # regularized FA
#library(FAiR) # semi-exploratory factor analysis; only works on Windows
library(GA) # genetic algorithm for subset selection</pre>
```

http://www.jstatsoft.org/v53/i04/paper

You can also embed plots, for example:

```
data(diabetes)
X <- diabetes$x
Y <- diabetes$y</pre>
```

```
lm(Y ~ X)
# note: equivalent to
lm(y ~ x,data=diabetes)
# which is equivalent to
lm(diabetes$y ~ diabetes$x)
```

Note, in this dataset, x is essentially a matrix within a dataframe. This is a little unusual, where the typical format would be:

```
diabetes2 <- data.frame(cbind(Y,X))
head(diabetes2)</pre>
```

```
## 1 151 0.038075906 0.05068012 0.06169621 0.021872355 -0.044223498
## 2 75 -0.001882017 -0.04464164 -0.05147406 -0.026327835 -0.008448724
## 3 141 0.085298906 0.05068012 0.04445121 -0.005670611 -0.045599451
## 4 206 -0.089062939 -0.04464164 -0.01159501 -0.036656447 0.012190569
## 5 135 0.005383060 -0.04464164 -0.03638469 0.021872355 0.003934852
## 6 97 -0.092695478 -0.04464164 -0.04069594 -0.019442093 -0.068990650
```

```
##
                          hdl
                                       tch
                                                    ltg
## 1 -0.03482076 -0.043400846 -0.002592262 0.019908421 -0.017646125
## 2 -0.01916334 0.074411564 -0.039493383 -0.068329744 -0.092204050
## 3 -0.03419447 -0.032355932 -0.002592262 0.002863771 -0.025930339
## 4 0.02499059 -0.036037570 0.034308859 0.022692023 -0.009361911
## 5 0.01559614 0.008142084 -0.002592262 -0.031991445 -0.046640874
## 6 -0.07928784 0.041276824 -0.076394504 -0.041180385 -0.096346157
lm(Y ~ ., data=diabetes2)
##
## Call:
## lm(formula = Y ~ ., data = diabetes2)
## Coefficients:
## (Intercept)
                        age
                                     sex
                                                  bmi
                                                               map
##
       152.13
                     -10.01
                                 -239.82
                                               519.84
                                                            324.39
##
                        ldl
                                     hdl
                                                  tch
                                                               ltg
            tc
       -792.18
##
                     476.75
                                  101.04
                                               177.06
                                                            751.28
##
           glu
##
         67.63
```

Using the "." means we want to use all variables that aren't the outcome as predictors Fun Fact: Can do the same thing with a SEM package

```
library(lavaan)
lm.mod <-'
Y ~ age + sex + bmi + map + tc + ldl + hdl + tch + ltg + glu
Y ~ 1 # intercept
'
lm.sem <- sem(lm.mod,diabetes2)
#summary(lm.sem)
#parameterEstimates(lm.sem)
coef(lm.sem)</pre>
```

```
##
      Y~age
               Y~sex
                        Y~bmi
                                 Y~map
                                           Y~tc
                                                   Y~ldl
                                                            Y~hdl
                                                                     Y~tch
##
   -10.012 -239.819
                     519.840
                               324.390 -792.184 476.746 101.045 177.064
##
      Y~ltg
               Y~glu
                          Y~1
   751.279
              67.625 152.133 2859.690
```

Exact same answer.

```
lm.out <- lm(y ~ x,data=diabetes)
#summary(lm.out)

# check assumptions
#plot(lm.out)

# get standardized coefficients
lm.beta(lm.out) # from QuantPsyc</pre>
```

```
##
                                      xbmi
                                                   xmap
                                                                  xtc
           xage
                        xsex
## -0.006178065 -0.147981279
                              0.320769113
                                            0.200166344 -0.488820243
                                                   xltg
##
           xldl
                        xhdl
                                      xtch
                                                                 xglu
   0.294177828
                0.062349936
                              0.109258122
                                            0.463579756
                                                         0.041728501
##
```

So we are doing pretty good, R^2 of 0.51, with only four significant predictors. So the question we are going to answer today is whether we can get rid of a few predictors and still do a good job of predicting the outcome. Now, there are two + reasons to do this:

- 1. In future studies, maybe time is of the essence, or each additional question costs a certain amount of money. By reducing the number of questions we have to ask participants, both money and time can be saved. The question is what is the tradeoff, can we reduce the number of scales/items/questionnaires, and still answer the questions we want?
- 2. Remember when using R^2 as a criterion, by using more variables as predictors, these can only improve are within sample predictive power. But when we become concerned with generalizability, then in some cases, a reduced number of predictors, only important ones, can generalize better than a larger set of X's. This was somewhat demonstrated in the "preprocessing" lab.

Let's try #2 on the diabetes dataset

```
ids <- sample(1:nrow(diabetes2), .5*nrow(diabetes2),replace=FALSE)
diab.train <- diabetes2[ids,]
diab.test <- diabetes2[-ids,]

lm.trainFull <- lm(Y ~ ., data= diab.train)
summary(lm.trainFull)$r.squared

## [1] 0.4973194

lm.trainSub <- lm(Y ~ sex + bmi + map + ltg, data= diab.train)
summary(lm.trainSub)$r.squared

## [1] 0.4575152

pred.full <- predict(lm.trainFull,diab.test)
pred.sub <- predict(lm.trainSub,diab.test)
cor(pred.full,diab.test$Y)**2

## [1] 0.5233413</pre>
```

```
## [1] 0.5166219
```

cor(pred.sub,diab.test\$Y)**2

Not in this case, but let's try some different methods specifically designed for subset selection.

Subset Selection

First off, why don't we just try out all combination of predictors – entering them all separately into lm()? Problems:

- 1. How do we choose. R^2 can only go up with added predictors (RSS can only go down).
- 2. This is usually computationally infeasible, as there are 2^p possible models, where p is the number of predictors. In our case $2^{10} = 1024$, which is a lot but not too many.

Stepwise Selection

Forward

Efficient, but not guaranteed to find best overall model.

```
library(MASS)
lmOut <- lm(Y ~ ., data=diab.train)
stepFor <- stepAIC(lmOut,direction="forward")</pre>
```

stepFor\$anova

```
## Stepwise Model Path
## Analysis of Deviance Table
##
## Initial Model:
## Y ~ age + sex + bmi + map + tc + ldl + hdl + tch + ltg + glu
##
## Final Model:
## Y ~ age + sex + bmi + map + tc + ldl + hdl + tch + ltg + glu
##
## Step Df Deviance Resid. Df Resid. Dev AIC
## 1 210 646261.9 1785.756
```

```
pred.for<- predict(stepFor,diab.test)
cor(pred.for,diab.test$Y)**2</pre>
```

```
## [1] 0.5233413
```

AIC (Akaike Information Criterion) induces a penalty for complexity – meaning that it will try and choose a model that balances predictive accuracy with simplicity (less predictors).

In this example, forward stepwise doesn't suggest getting rid of any predictors

Backward

```
library(MASS)
lmOut <- lm(Y ~ ., data=diab.train)
stepBack <- stepAIC(lmOut,direction="backward")</pre>
```

stepBack\$anova

```
## Stepwise Model Path
## Analysis of Deviance Table
##
## Initial Model:
## Y \sim age + sex + bmi + map + tc + ldl + hdl + tch + ltg + glu
##
## Final Model:
## Y ~ sex + bmi + map + tc + ldl + ltg
##
##
      Step Df Deviance Resid. Df Resid. Dev
## 1
                                     646261.9 1785.756
                               210
## 2 - tch 1 98.53511
                                     646360.4 1783.790
                               211
## 3 - glu 1 217.09857
                                     646577.5 1781.864
                               212
## 4 - hdl 1 663.58536
                               213
                                     647241.1 1780.091
## 5 - age 1 682.91551
                               214
                                     647924.0 1778.324
pred.back<- predict(stepBack,diab.test)</pre>
cor(pred.back,diab.test$Y)**2
```

```
## [1] 0.5275474
```

Here, backwards suggests getting rid of 4 predictors.

Ridge and Lasso Regression

• Including a penalty on the β parameters, and by varying the penalty we can shrink some of the $\beta's$ to zero, doing a form of "automatic" subset selection.

Althought there a number of packages to do this, maybe the best is glmnet

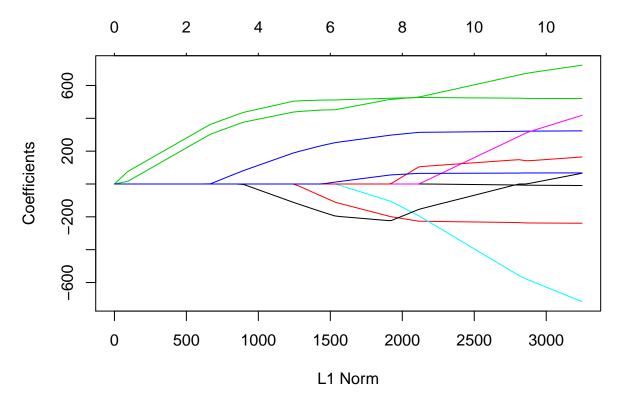
Note, for glmnet, your data has to be set up in two separate matrices. Doing this can be accomplished by:

```
YY <- as.matrix(diabetes2$Y)
XX <- as.matrix(diabetes2[,2:11])
# or
XX <- as.matrix(diabetes2[,c("age","sex","bmi","map","tc","ldl","hdl","tch","ltg","glu")])</pre>
```

Two things to note: 1. Because we are doing regression with a continuous outcome, we specify the family(distribution) as "gaussian" 2. Shrinkage in lasso and ridge is sensitive to the scale of the variables, therefore, it is best to standardize the predictors before entering. glmnet does this by default (look at ?glmnet).

Lasso

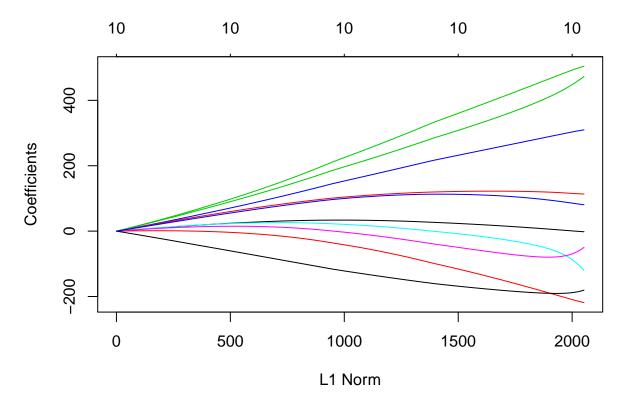
```
?glmnet
lasso.out <- glmnet(XX,YY,family="gaussian",alpha=1)
plot(lasso.out)</pre>
```



#gaussian for continuous outcomes, "binomial" for categorical
alpha=1 is lasso, alpha=0 is ridge

Ridge

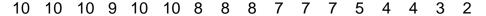
```
ridge.out <- glmnet(XX,YY,family="gaussian",alpha=0)
#plot(ridge.out,type.coef="2norm")
plot(ridge.out)</pre>
```

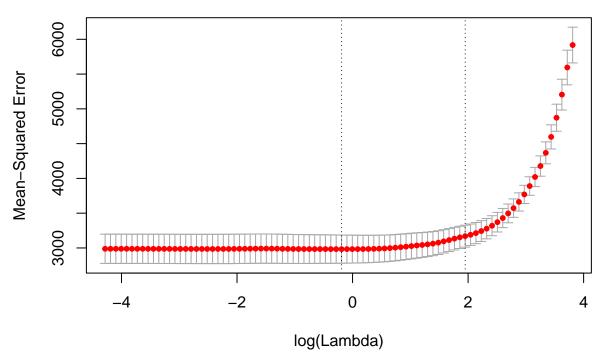


Since ridge regression does not shrink the β coefficients to 0 with increase penalization, it does not do an "automatic" form of subset selection

The problem now becomes, which value of λ (amount of shrinkage) do we choose? Using cross-validation is one of the better ways, and is implemented the glmnet package

```
cv.lasso <- cv.glmnet(XX,YY,family="gaussian",alpha=1)
plot(cv.lasso)</pre>
```





Two-strategies for selecting λ : either pick the lowest CV error, or the best solution within 1 standard error. I don't think that there is a clear best choice. The one advantage of using the 1SE rule is that you need fewer predictors. In our example 4 instead of 7.

```
#str(cv.lasso)
(lmin <- cv.lasso$lambda.min)

## [1] 0.826762

(lminSE <- cv.lasso$lambda.1se)

## [1] 7.025438

lasso.out2 = glmnet(XX,YY,family="gaussian",alpha=1,lambda=lminSE)
lasso.out2

## ## Call: glmnet(x = XX, y = YY, family = "gaussian", alpha = 1, lambda = lminSE)

## ## [1,] 4 0.4753 7.025</pre>
Note that Df correspond to the number of non-zero β's
So how are we doing?
```

```
## [,1]
## s0 0.4891983
```

So with only 4 predictors entered into the model, we only lose 2-3% of our predicted variance (R^2). With the lasso, there are two recommended strategies for using the results. 1. Taking the predictors with non-zero $\beta's$, and just using that subset in linear regression. 2. Or, bypass this all together and use least angle regression.

"One approach for reducing this bias is to run the lasso to identify the set of non-zero coefficients, and then fit an un-restricted linear model to the selected set of features." p. 91 Hastie et al., 2009

In our case, we will take the predictors with non-zero $\beta's$ and use them with lm() to get our final model. This will probably be our most realistic estimate of R^2 when caring about generalization, as we are using the test dataset to derive the estimate.

```
coef(lasso.out2)
```

```
## 11 x 1 sparse Matrix of class "dgCMatrix"
##
## (Intercept) 152.1335
## age
## sex
## bmi
                 498.9887
                 180.6668
## map
## tc
## ldl
## hdl
                -103.2937
## tch
                 433.5503
## ltg
## glu
lm.lasso <- lm(Y ~ bmi + map + hdl + ltg,diab.train)</pre>
lmLas.pred <- predict(lm.lasso,diab.test)</pre>
```

```
## [1] 0.5127864
```

Try Elastic Net - from caret

cor(lmLas.pred,diab.test\$Y)**2

This optimizes both the λ and mixing percentage

```
library(caret)
XX <- as.matrix(diab.train[,-1])
YY <- diab.train$Y # important to change class of variable
enet.out <- train(XX,YY,method="glmnet",tuneLength=8)

row.result <- best(enet.out$results,"Rsquared",maximize=T)
enet.out$results[row.result,]</pre>
```

Stochastic Search

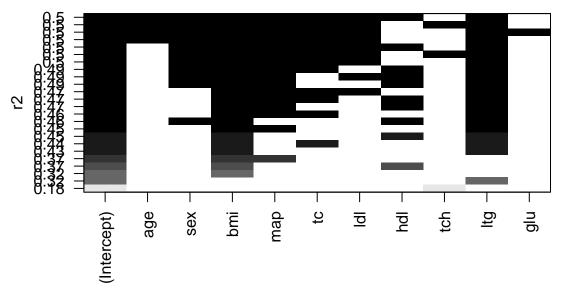
Use 3 packages: "tabuSearch" "leaps" "GA" (genetic algorithm, note there is also "genalg")

```
library(leaps)
```

```
##
## Attaching package: 'leaps'
##
## The following object is masked from 'package:subselect':
##
## leaps

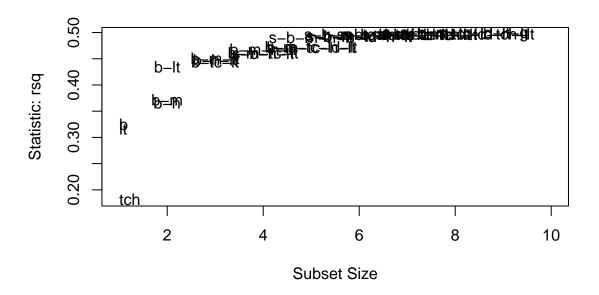
# leaps

# leaps and bounds
leaps <- regsubsets(Y ~.,,data=diab.train,nbest=3)
#summary(leaps)
# plot a table of models showing variables in each model.
# models are ordered by the selection statistic.
plot(leaps,scale="r2")</pre>
```



plot statistic by subset size library(car)

```
##
## Attaching package: 'car'
##
## The following object is masked from 'package:boot':
##
## logit
subsets(leaps, statistic="rsq",legend=F)
```



```
Abbreviation
##
## age
                    a
## sex
                    s
## bmi
                    b
## map
## tc
                   tc
## ldl
                  ld
## hdl
                   h
## tch
                  tch
## ltg
                  lt
## glu
                    g
```

have to press ESC to exit

Based on this, looks like a subset size of 5 might be best, as we get pretty close to an R^2 of 0.5

Maybe R^2 isn't the best, as this doesn't penalize for complexity and will probably not generalize well. In regsubsets() we can use BIC which may help.

summary(leaps)\$bic

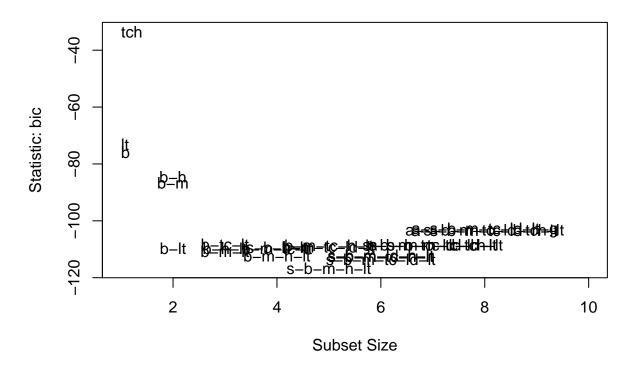
```
## [1] -75.96156 -73.12543 -33.54266 -109.62248 -86.61304 -84.54964

## [7] -110.67974 -109.71542 -108.31248 -112.38244 -109.63451 -109.39965

## [13] -116.69919 -109.11901 -108.57735 -113.64905 -112.48698 -112.10288

## [19] -108.48394 -108.40795 -108.38271 -103.31248 -103.26582 -103.16310

subsets(leaps, statistic="bic",legend=F)
```



```
##
       Abbreviation
## age
## sex
                    s
                    b
## map
                    m
                   tc
## ldl
                   ld
## hdl
                    h
## tch
                  tch
## ltg
                   lt
## glu
                    g
```

Looks like we get a similar answer, but seem to also have a "clearer" best model The

Genetic Algorithm

An example using the "GA" package to do this: http://www.jstatsoft.org/v53/i04/paper But there is an easier way:

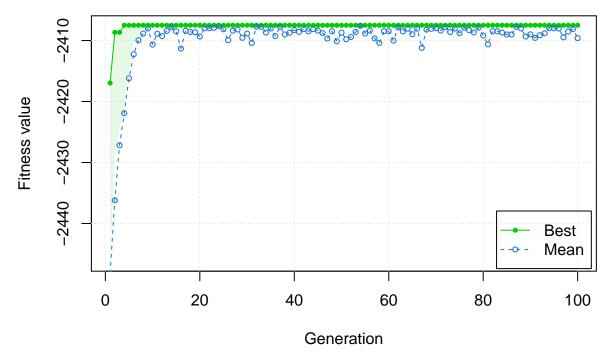
```
library(glmulti)

## Loading required package: rJava

Using "GA"

mod <- lm(Y ~ ., diab.train)

x <- model.matrix(mod)[, -1]
y <- model.response(model.frame(mod))</pre>
```



summary(GA)

```
Genetic Algorithm
##
## GA settings:
## Type
                           binary
## Population size
                     = 50
## Number of generations = 100
## Elitism
## Crossover probability = 0.8
## Mutation probability = 0.1
##
## GA results:
## Iterations
                         = 100
## Fitness function value = -2407.495
##
       age sex bmi map tc ldl hdl tch ltg glu
```

```
summary(GA)$solution
```

```
## age sex bmi map tc ldl hdl tch ltg glu
## [1,] 0 1 1 1 1 1 0 0 1 0
```

Tabu Search

An example: http://www.r-bloggers.com/finding-the-best-subset-of-a-gam-using-tabu-search-and-visualizing-it-in-r/

```
library(tabuSearch)

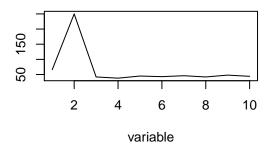
mod <- lm(Y ~ ., diab.train)

x <- model.matrix(mod)[, -1]
y <- model.response(model.frame(mod))

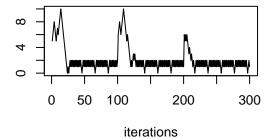
fitness2 <- function(string) {
  inc <- which(string == 1)
  X <- cbind(1, x[,inc])
  mod <- lm.fit(X, y)
  class(mod) <- "lm"
  -AIC(mod) + 100000 # won't take negative
}

result <- tabuSearch(size = 10, iters = 100,objFunc = fitness2)
plot(result) #fit margins too large</pre>
```

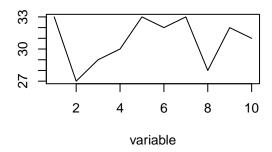
No of times selected



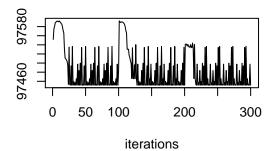
Sum of included variables



Most frequent moves



Objective Function



```
summary(result,verbose=T) # 6 predictors
```

```
## Tabu Settings
                                             = binary configuration
##
    Type
##
    No of algorithm repeats
##
    No of iterations at each prelim search
                                             = 100
    Total no of iterations
                                             = 300
##
    No of unique best configurations
                                             = 53
    Tabu list size
                                             = 9
##
    Configuration length
                                             = 10
    No of neighbours visited at each iteration = 10
##
## Results:
    Highest value of objective fn = 97592.50529
    Occurs # of times
                                   = 2
##
   Optimum number of variables = c(6, 6)
##
## Optimum configuration:
       [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
             1
                 1 1
                          1
                                 1
                                    0
## [2,]
       0
            1 1
                     1
                            1
                                 1
                                      0
                                           0
```

glmulti

Looks for interactions as well

Now we can take the output and test it out in lm()

eq = summary(multi.out)\$bestmodel
lm.multi = lm(eq,data=diab.train)

summary(lm.multi)

```
library(glmulti)
\# method = "g" for genetic algorithm
# default fitfunction = "glm"
multi.out = glmulti(Y ~., data=diab.train,method="g",plotty=F,
                    report=F,fitfunction="lm",crit="aic")
## TASK: Genetic algorithm in the candidate set.
## Initialization...
## Algorithm started...
## Improvements in best and average IC have bebingo en below the specified goals.
## Algorithm is declared to have converged.
## Completed.
#summary(multi.out)
summary(multi.out)$bestmodel
## [1] "Y ~ 1 + sex + bmi + map + tc + ldl + hdl + ltg + map:age + map:bmi + "
## [2] "
          tc:bmi + tc:map + hdl:map + tch:sex + tch:map + ltg:hdl + "
## [3] "
           glu:ldl + glu:hdl + glu:tch"
```

```
##
## Call:
## lm(formula = eq, data = diab.train)
##
## Residuals:
##
        Min
                       Median
                                     3Q
                  1Q
                                             Max
## -115.651 -35.666
                       -0.265
                                31.718
                                        133.029
##
## Coefficients:
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                  140.605
                               4.629
                                       30.372 < 2e-16 ***
                              84.639
## sex
                 -211.729
                                      -2.502 0.013159 *
                  410.735
                              99.186
                                       4.141 5.08e-05 ***
## bmi
## map
                  258.410
                              90.414
                                       2.858 0.004709 **
                             704.476
## tc
                -2261.529
                                      -3.210 0.001543 **
## ldl
                 1948.791
                             609.747
                                        3.196 0.001617 **
                                        1.841 0.067153 .
## hdl
                  507.116
                             275.523
                 1216.043
                             269.027
                                        4.520 1.05e-05 ***
## ltg
                 3134.578
                            1855.303
                                       1.690 0.092662 .
## map:age
## bmi:map
                 5120.912
                            1846.306
                                       2.774 0.006063 **
## bmi:tc
                -3667.190
                            2055.736
                                      -1.784 0.075944 .
                12725.555
                            3612.883
                                       3.522 0.000529 ***
## map:tc
## map:hdl
               -10510.047
                            4107.781
                                      -2.559 0.011243 *
## sex:tch
                -2946.263
                            1687.626
                                      -1.746 0.082365
## map:tch
               -14902.962
                            5002.341
                                      -2.979 0.003244 **
## hdl:ltg
                -3985.408
                            2361.781
                                      -1.687 0.093059
                -7539.661
                                      -2.221 0.027466 *
## ldl:glu
                            3394.820
## hdl:glu
                10460.555
                            3976.401
                                       2.631 0.009179 **
                            4724.852
                                       2.988 0.003152 **
## tch:glu
                14119.843
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 51.88 on 202 degrees of freedom
## Multiple R-squared: 0.5772, Adjusted R-squared:
## F-statistic: 15.32 on 18 and 202 DF, p-value: < 2.2e-16
```

The addition of interactions increases our R^2 even though our criterion for glmulti was AIC.

simulated annealing

http://topepo.github.io/caret/SA.html

part of this, other options including GA available: http://topepo.github.io/caret/featureselection.html To do, have to install most current version of caret from github. CRAN version doesn't include functions The great thing about this function is that we can use it for all of the methods in caret (100+).

```
library(devtools)
devtools::install_github("cran/caret")
library(caret)

ctrl <- safsControl(functions = caretSA)</pre>
```

Use with genetic algorithm: http://topepo.github.io/caret/GA.html

Pretty slow

Classification

All of the methods used previously will also work in the classification context in using forms of logistic regression.

Logistic Regression

```
Ybin <- ifelse(diab.train$Y > mean(diab.train$Y),1,0)
diab.train2 <- diab.train
diab.train2$Y <- Ybin

# logistic
glm.out <- glm(Y ~ ., diab.train2,family="binomial")
#summary(glm.out)</pre>
```

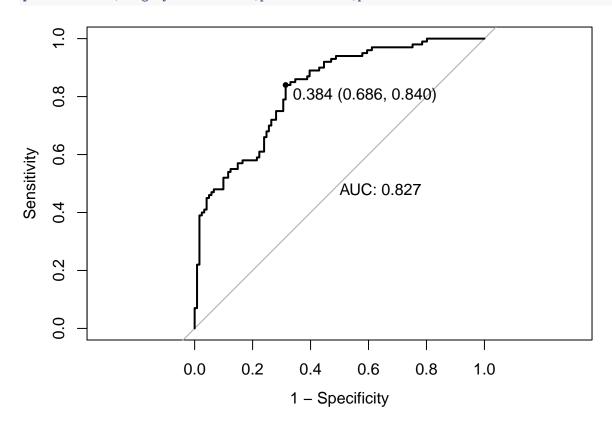
So how well did we do? I like using receive operating characteristic (ROC) curves and the area under the curve (AUC) to evaluate results in classification.

For binary outcomes, my favorite way to assess how well I did is using the confusionMatrix() function from caret

```
sensitivity = true positive – with event AND predicted to have event / having the event people who respondend AND people predicted to respond / people who respondend specificity = samples w/o event AND predicted as non-event / samples w/o event actual non-response AND predicted non-response/ actual non-response false-positive = 1-specificity
```

```
library(pROC)
library(caret)
glm.probs=predict(glm.out,type="response")
glm.pred=ifelse(glm.probs>0.5,1,0)
table(diab.train2$Y,glm.pred)
##
      glm.pred
##
        0 1
##
     0 89 32
##
     1 30 70
confusionMatrix(diab.train2$Y,glm.pred,positive="1") # from caret package
## Confusion Matrix and Statistics
##
             Reference
## Prediction 0 1
##
            0 89 32
            1 30 70
##
##
                  Accuracy: 0.7195
##
##
                    95% CI : (0.6553, 0.7776)
       No Information Rate : 0.5385
##
##
       P-Value [Acc > NIR] : 2.664e-08
##
##
                     Kappa: 0.4348
   Mcnemar's Test P-Value: 0.8989
##
##
##
               Sensitivity: 0.6863
##
               Specificity: 0.7479
            Pos Pred Value : 0.7000
##
##
            Neg Pred Value: 0.7355
##
                Prevalence: 0.4615
##
            Detection Rate: 0.3167
##
      Detection Prevalence : 0.4525
##
         Balanced Accuracy: 0.7171
##
          'Positive' Class : 1
##
rocCurve <- roc(diab.train2$Y,glm.probs)</pre>
auc(rocCurve)
## Area under the curve: 0.8269
ci.roc(rocCurve)
## 95% CI: 0.7739-0.8798 (DeLong)
```

```
plot(rocCurve, legacy.axes = TRUE,print.thres=T,print.auc=T)
```

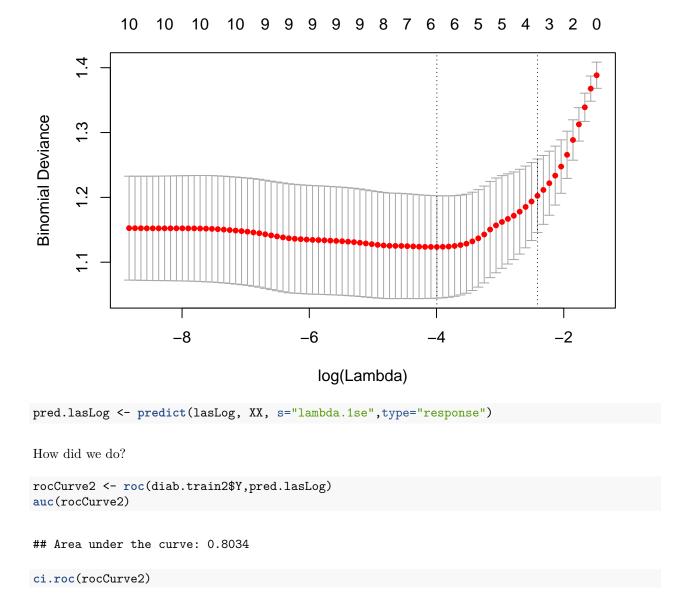


```
##
## Call:
## roc.default(response = diab.train2$Y, predictor = glm.probs)
##
## Data: glm.probs in 121 controls (diab.train2$Y 0) < 100 cases (diab.train2$Y 1).
## Area under the curve: 0.8269</pre>
```

Try also with elastic net

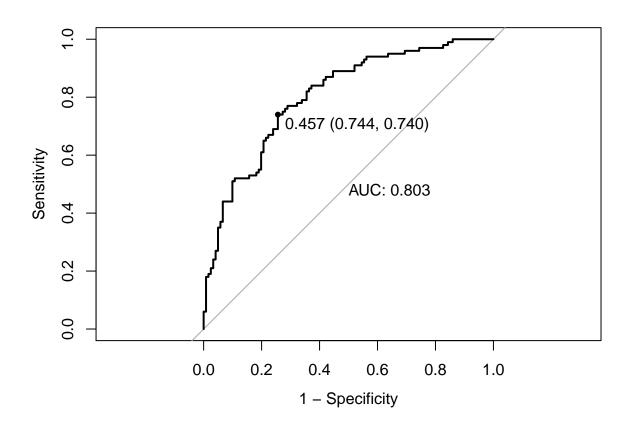
Regularization in caret package: http://topepo.github.io/caret/L1_Regularization.html

```
XX <- as.matrix(diab.train2[,-1])
YY <- diab.train2$Y
lasLog <- cv.glmnet(XX,YY,family="binomial")
plot(lasLog)</pre>
```



95% CI: 0.7461-0.8606 (DeLong)

plot(rocCurve2, legacy.axes = TRUE,print.thres=T,print.auc=T)



```
##
## Call:
## roc.default(response = diab.train2$Y, predictor = pred.lasLog)
##
## Data: pred.lasLog in 121 controls (diab.train2$Y 0) < 100 cases (diab.train2$Y 1).
## Area under the curve: 0.8034</pre>
```

We got rid of 6 predictors and only lost 0.01 in the AUC