Regression in R

Ross Jacobucci April 30, 2015

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
```

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>
```

```
## Y age sex bmi map tc
## 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
## 6 97 -0.092695478 -0.04464164 -0.04069594 -0.019442093 -0.068990650
##
                       hdl
           ldl
                                   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)
                                  sex
                                              bmi
                     age
                                                          map
##
       152.13
                   -10.01
                              -239.82
                                           519.84
                                                       324.39
                     ldl
##
          tc
                                 hdl
                                              tch
                                                          ltg
      -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~bmi
                                Y~map
                                          Y~tc
                                                  Y~ldl
                                                           Y~hdl
                                                                    Y~tch
              Y~sex
  -10.012 -239.819
                     519.840
                              324.390 -792.184 476.746 101.045 177.064
##
     Y~ltg
              Y~glu
                         Y~1
                                 Y~~Y
  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] 0.5760298

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

## [1] 0.5422063

pred.full <- predict(lm.trainFull,diab.test)
pred.sub <- predict(lm.trainSub,diab.test)

cor(pred.full,diab.test$Y)**2</pre>
```

```
## [1] 0.4114991
```

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

```
## [1] 0.4102339
```

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 599776.7 1769.259
```

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

```
## [1] 0.4114991
```

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 ~ age + bmi + map + tc + ltg + glu
##
##
      Step Df Deviance Resid. Df Resid. Dev
                                                   AIC
## 1
                              210
                                    599776.7 1769.259
## 2 - tch 1 3189.725
                              211
                                    602966.5 1768.431
## 3 - hdl 1 1239.994
                              212
                                    604206.5 1766.885
## 4 - sex 1 3706.779
                              213
                                    607913.2 1766.237
## 5 - ldl 1 2482.020
                              214
                                    610395.3 1765.138
pred.back<- predict(stepBack,diab.test)</pre>
cor(pred.back,diab.test$Y)**2
```

```
## [1] 0.391118
```

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

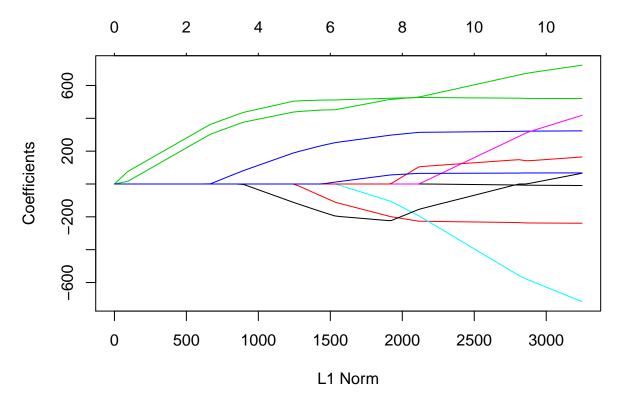
Note, for glmnet, your data has to be set up in two separate matrices. Doing this can be accomplished by:

```
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

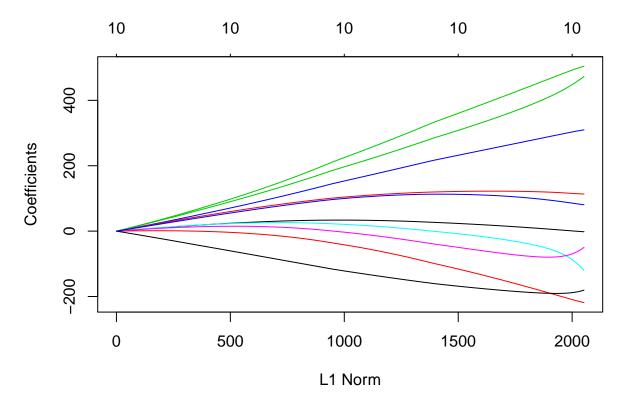
```
?glmnet
lasso.out <- glmnet(XX,YY,family="gaussian",alpha=1)
plot(lasso.out)</pre>
```



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

Ridge

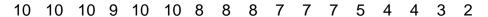
```
ridge.out <- glmnet(XX,YY,family="gaussian",alpha=0)
#plot(ridge.out,type.coef="2norm")
plot(ridge.out)</pre>
```

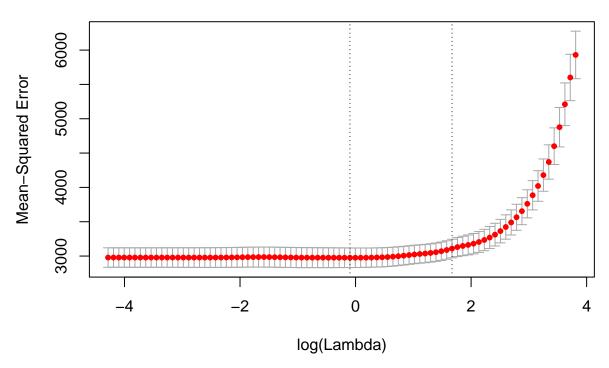


Since ridge regression does not shrink the β coefficients to 0 with increase penalization, it does not do an "automatic" form of subset selection

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] 0.9073702

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

## [1] 5.314486

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,] 5 0.4867 5.314

Note that Df correspond to the number of non-zero β's
So how are we doing?</pre>
```

```
## [,1]
## s0 0.4954284
```

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) 152.13348
## age
                -33.36204
## sex
## bmi
                508.20584
                210.39166
## map
## tc
## ldl
## hdl
               -138.88864
## tch
                 444.52684
## ltg
## glu
lm.lasso <- lm(Y ~ bmi + map + hdl + ltg,diab.train)</pre>
lmLas.pred <- predict(lm.lasso,diab.test)</pre>
```

```
lmLas.pred <- predict(lm.lasso,diab.test)

cor(lmLas.pred,diab.test$Y)**2</pre>
```

```
## [1] 0.4175754
```

Try Elastic Net - from caret

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>
```

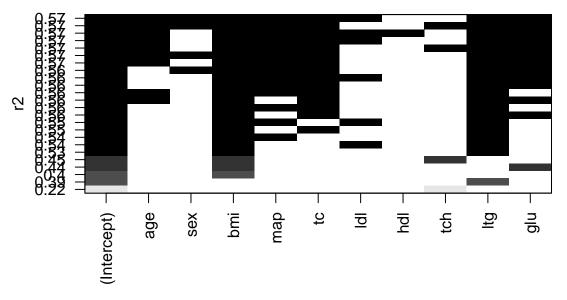
Stochastic Search

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

```
library(leaps)
```

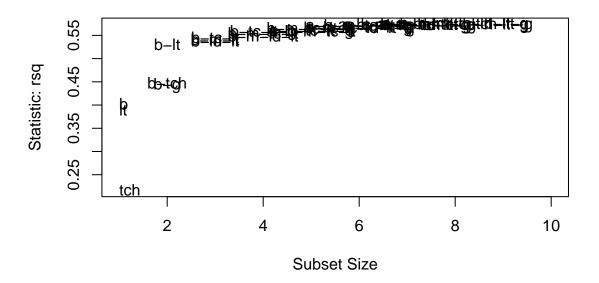
```
##
## Attaching package: 'leaps'
##
## The following object is masked from 'package:subselect':
##
## leaps

# leaps
# leaps <- 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
## sex
                   S
                   b
## bmi
## map
                   m
## 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

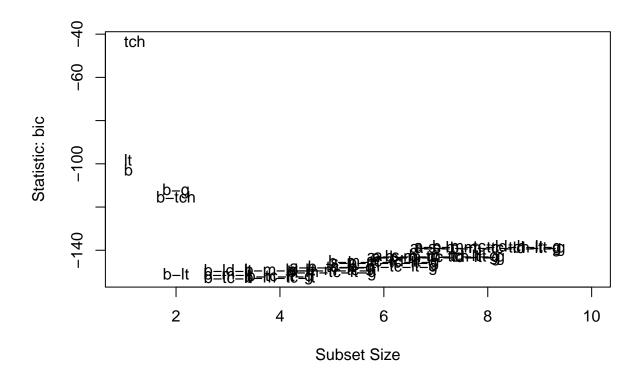
```
## [1] -102.86578 -98.21292 -43.25037 -150.94917 -115.21667 -112.54437

## [7] -152.66275 -150.83658 -149.05093 -152.35805 -152.28095 -148.81092

## [13] -150.44265 -148.92727 -148.14226 -147.97283 -146.12627 -145.69830

## [19] -143.47514 -143.27669 -143.18626 -139.42866 -139.12444 -138.73903

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



##		${\tt Abbreviation}$
##	age	a
##	sex	s
##	bmi	b
##	\mathtt{map}	m
##	tc	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

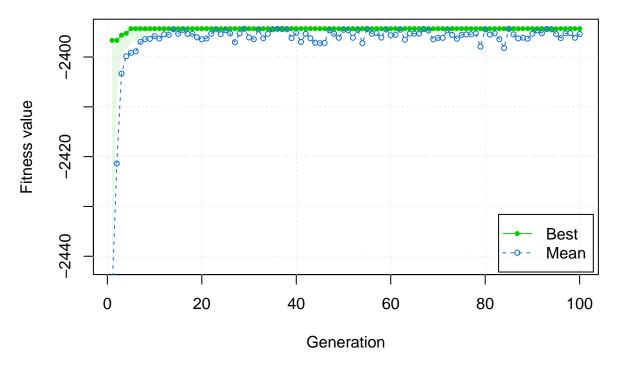
An example using the "GA" package to do this: $http://www.jstatsoft.org/v53/i04/paper \\ But there is an easier way:$

```
library(glmulti)
```

```
## Loading required package: rJava
```

Using "GA"

```
mod <- lm(Y ~ ., diab.train)
x <- model.matrix(mod)[, -1]</pre>
```



summary(GA)

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)

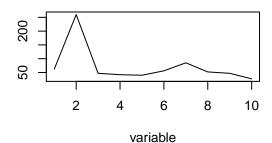
mod <- lm(Y ~ ., diab.train)

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

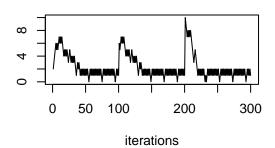
fitness2 <- function(string) {
  inc <- which(string == 1)
  X <- cbind(1, x[,inc])
  mod <- lm.fit(X, y)
  class(mod) <- "lm"
  -AIC(mod) + 100000 # won't take negative
}

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

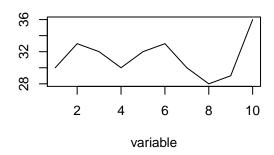
No of times selected



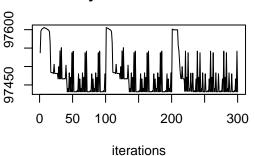
Sum of included variables



Most frequent moves



Objective Function



summary(result,verbose=T) # 6 predictors

```
## Tabu Settings
##
     Type
                                                 = binary configuration
##
     No of algorithm repeats
                                                   1
                                                 = 100
##
     No of iterations at each prelim search
##
     Total no of iterations
                                                 = 300
     No of unique best configurations
                                                 = 60
##
     Tabu list size
                                                   9
##
     Configuration length
                                                 = 10
##
##
     No of neighbours visited at each iteration = 10
## Results:
##
     Highest value of objective fn
                                       = 97605.69163
     Occurs # of times
##
     Optimum number of variables
                                       = c(6, 6)
## Optimum configuration:
        [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
## [1,]
                     1
                          1
                                1
                                     0
                                          0
## [2,]
                     1
                                     0
           1
                0
                          1
                                1
                                          0
                                               0
```

glmulti

Looks for interactions as well

```
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)$bestmodel
## [1] "Y ~ 1 + age + sex + bmi + map + ldl + tch + ltg + glu + sex:age + "
## [2] "
           tc:age + ldl:age + hdl:tc + hdl:ldl + tch:tc + tch:ldl + "
## [3] "
           ltg:sex + ltg:ldl + glu:sex + glu:bmi"
Now we can take the output and test it out in lm()
eq = summary(multi.out)$bestmodel
lm.multi = lm(eq,data=diab.train)
summary(lm.multi)
##
## Call:
## lm(formula = eq, data = diab.train)
##
## Residuals:
##
       Min
                 1Q Median
                                  3Q
## -136.136 -31.757 -1.431
                              25.732 126.821
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
                144.348 4.833 29.866 < 2e-16 ***
## (Intercept)
                -115.115
                            80.588 -1.428 0.154720
## age
                           79.534 -1.488 0.138199
## sex
               -118.383
## bmi
                548.274
                           94.927 5.776 2.88e-08 ***
                           84.204
                                    3.052 0.002581 **
## map
                256.982
                         106.987 -3.140 0.001946 **
## ldl
               -335.907
## tch
                ## ltg
                609.321
                         112.282 5.427 1.64e-07 ***
## glu
                197.569
                           88.933
                                     2.222 0.027429 *
## age:sex
               6918.375
                         1732.975
                                   3.992 9.17e-05 ***
## age:tc
              11724.785 3975.316
                                     2.949 0.003561 **
              -14275.438 4147.325 -3.442 0.000702 ***
## age:ldl
## tc:hdl
               -7730.393
                          3658.401 -2.113 0.035830 *
                                   2.271 0.024206 *
## ldl:hdl
               9335.140 4110.571
## tch:tc
             -20572.114 5356.244 -3.841 0.000164 ***
## ldl:tch
             17171.070 4980.873 3.447 0.000689 ***
## sex:ltg
               -3711.197
                          1698.937 -2.184 0.030088 *
## ldl:ltg
              6327.308
                          2454.247 2.578 0.010649 *
```

```
## sex:glu 3193.858 1798.158 1.776 0.077216 .
## bmi:glu 3816.172 1648.036 2.316 0.021590 *
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 49.55 on 201 degrees of freedom
## Multiple R-squared: 0.6512, Adjusted R-squared: 0.6183
## F-statistic: 19.75 on 19 and 201 DF, p-value: < 2.2e-16</pre>
```

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+).

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
## 0 111 17
## 1 27 66
```

```
confusionMatrix(diab.train2$Y,glm.pred,positive="1") # from caret package
```

```
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
               0
##
            0 111 17
##
            1 27
##
##
                  Accuracy : 0.8009
                    95% CI: (0.7421, 0.8515)
##
##
       No Information Rate: 0.6244
##
       P-Value [Acc > NIR] : 1.111e-08
##
```

```
Kappa : 0.5855
##
    Mcnemar's Test P-Value: 0.1748
##
##
##
               Sensitivity: 0.7952
               Specificity: 0.8043
##
##
            Pos Pred Value: 0.7097
##
            Neg Pred Value : 0.8672
                Prevalence: 0.3756
##
##
            Detection Rate: 0.2986
##
      Detection Prevalence : 0.4208
##
         Balanced Accuracy: 0.7998
##
##
          'Positive' Class : 1
##
```

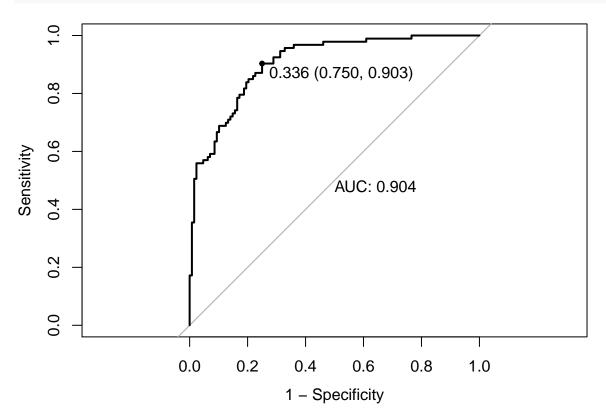
```
rocCurve <- roc(diab.train2$Y,glm.probs)
auc(rocCurve)</pre>
```

Area under the curve: 0.9043

```
ci.roc(rocCurve)
```

95% CI: 0.8659-0.9427 (DeLong)





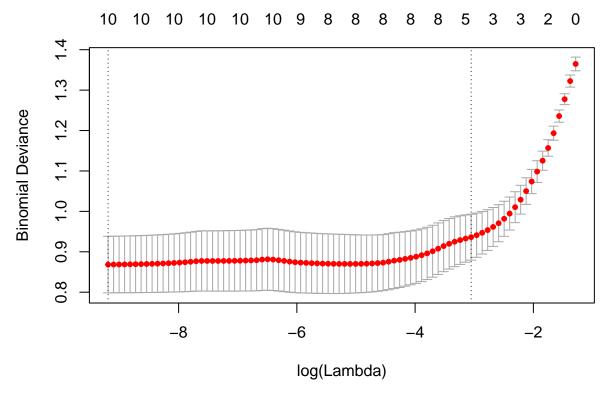
##

```
## Call:
## roc.default(response = diab.train2$Y, predictor = glm.probs)
##
## Data: glm.probs in 128 controls (diab.train2$Y 0) < 93 cases (diab.train2$Y 1).
## Area under the curve: 0.9043</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>
```



```
pred.lasLog <- predict(lasLog, XX, s="lambda.1se",type="response")</pre>
```

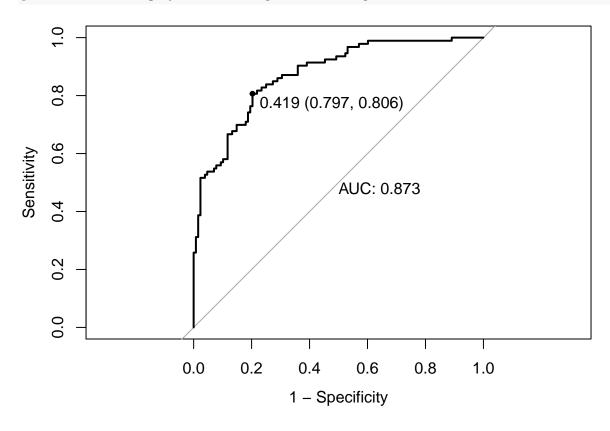
How did we do?

```
rocCurve2 <- roc(diab.train2$Y,pred.lasLog)
auc(rocCurve2)</pre>
```

Area under the curve: 0.8731

```
ci.roc(rocCurve2)
```

95% CI: 0.8275-0.9186 (DeLong)



```
##
## Call:
## roc.default(response = diab.train2$Y, predictor = pred.lasLog)
##
## Data: pred.lasLog in 128 controls (diab.train2$Y 0) < 93 cases (diab.train2$Y 1).
## Area under the curve: 0.8731</pre>
```

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