ShatterLine Blog

Honing the Art of Machine Learning with R

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Regularization – Predictive Modeling Beyond Ordinary Least Squares Fit

Posted in Linear Regression at 6:07 pm by Auro Tripathy

Introduction to Linear Functions and Regularization

A simple yet powerful prediction **model** assumes that the function is **linear** in the input even in cases where the input consists of hundreds of variables and the input variables far outstrip the number of observations. Such prediction models, known are linear regression/classification models, can often outperform fancier non-linear models.

The most popular method of estimation of the parameters (used interchangeably with the word, coefficients) is the method of **Ordinary Least Squares** (OLS). The linear model can be written as

$$f(x) = \beta_o + \sum X_j \beta_j$$

where j=1 to p, X is the input vector, and β_js are the unknown coefficients.

We solve for the coefficients β (β_o,β_1,…β_p) that minimize the residual sum of squares (RSS).

$$RSS() = \sum(y_i - \beta_o - \sum X_{ij}\beta_j)^2$$

where i=1 to N observations, j= 1 to p variables

Reasons why OLS estimation is often unsatisfactory are:

1. Large variance in prediction accuracy. A solution to improving the overall accuracy is to **shrink** (or set to zero) some of the coefficients. The overall effect is to prevent or reduce over-fitting.
2. With a large number of input predictors, one would like to determine a smaller subset that would exhibit the strongest effects so we see the big picture.

The process of regularization involves a family of penalty **terms** that can be added to OLS to achieve the shrinkage (in the coefficients).

The **Ridge** penalty term shrinks the regression coefficients by introducing the complexity parameter, **λ**, the greater the value of λ, the greater the amount of shrinkage. By varying λ, the coefficients are shrunk towards zero (and to each other).

$$\lambda \sum \beta_j^2 \text{ where j=1 to p}$$

While the Ridge penalty does a proportional shrinkage, the **LASSO** penalty λ, translates each coefficients by a constant factor stopping at zero. LASSO also does feature-selection; if many features are correlated, LASSO will just pick one.

$$\lambda \sum |\beta j|, \text{ where j=1 to p}$$

Elastic Net penalty is a **combination** of the LASSO and Ridge regression penalty.

$$\lambda\sum(\alpha|\beta_j| + (1 - \alpha)\beta_j^2), \text{ where j=1 to p}$$

The first term encourages a sparse solution in the coefficients and the second term encourages highly correlated features to be averaged. The parameter α determines the mix of penalties and lies in the range of 0 and 1. With α set to 0, we get the Ridge penalty and with α set to 1, we get the LASSO penalty.

Example

We now demonstrate this with a example dataset with 204 binary attributes and 704 observations.

Getting the Data

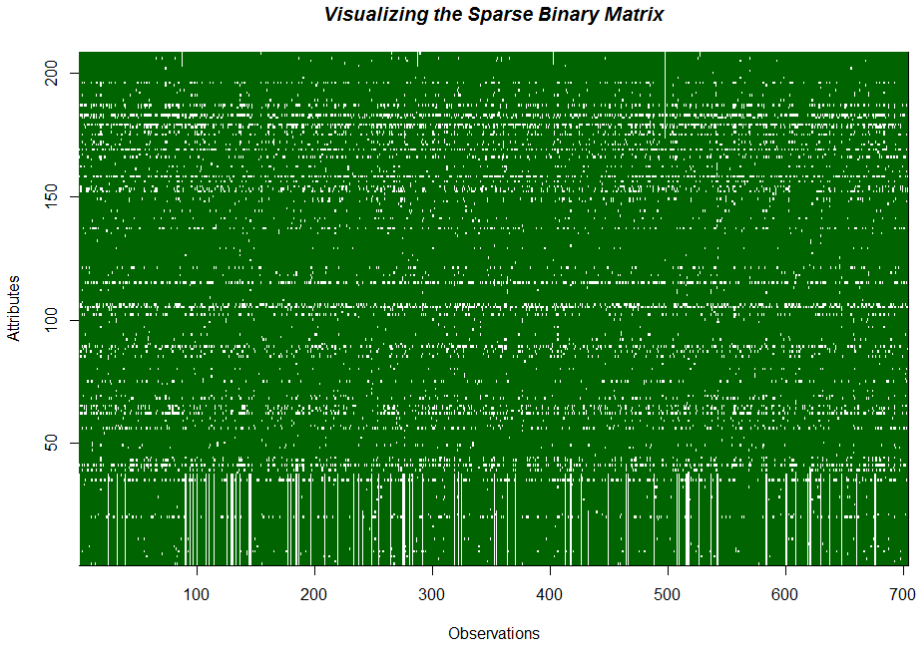
The R snippet below will download the dataset from where it is hosted. The data has been previously saved as an R object in the .rda format. We reload it back in to the R object, hiv.data.

```
download.file("http://www.shatterline.com/MachineLearning/data/hiv.rda","hiv.rda", mode="wb")

load("hiv.rda", verbose=TRUE) #contains hiv.train & hiv.test
```

Visualizing the Data

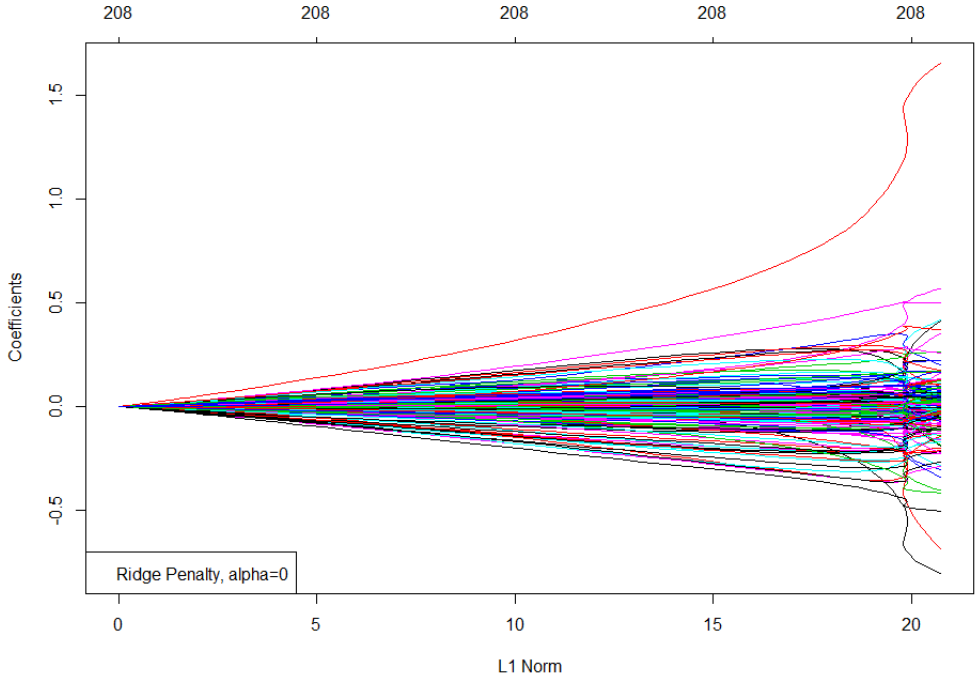
The image function in R helps us visualize the dataset. You can see below the relatively strong correlation between the variables. See the visualize.matrix function below.



Fitting/Plotting Data

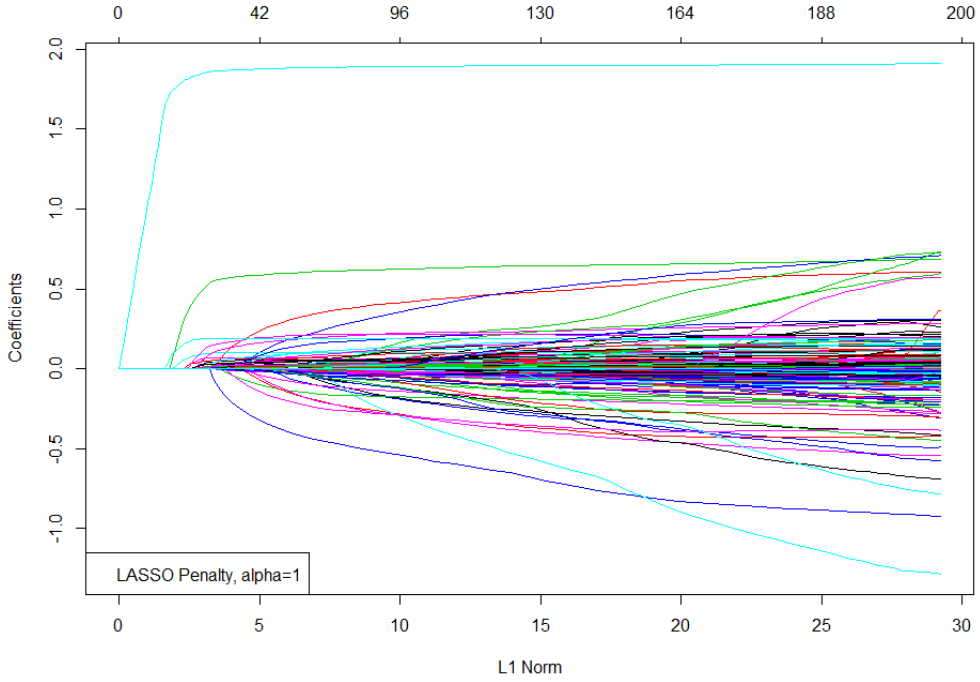
The code snippet below shows the coefficient shrinkage is proportional to λ when we apply the Ridge penalty.

```
fit <- glmnet(hiv.train$x,hiv.train$y, alpha=0) #Ridge penalty
```



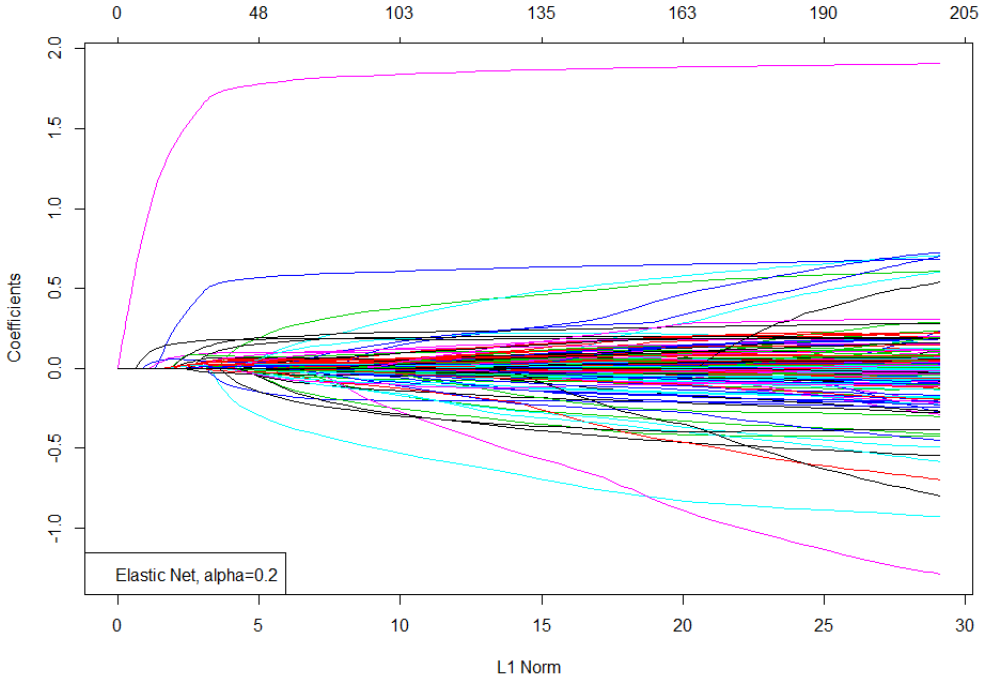
The code snippet below shows that, with the LASSO penalty, the coefficient **hit zero** (unlike Ridge) as λ shrinks**.**

```
fit <- glmnet(hiv.train$x,hiv.train$y, alpha=1) #Lasso penalty
```



The code snippet below shows a mix of the Ridge and LASSO penalties with the Elastic Net penalty for a specific value of α=0.2 (could also be chose with cross-validation).

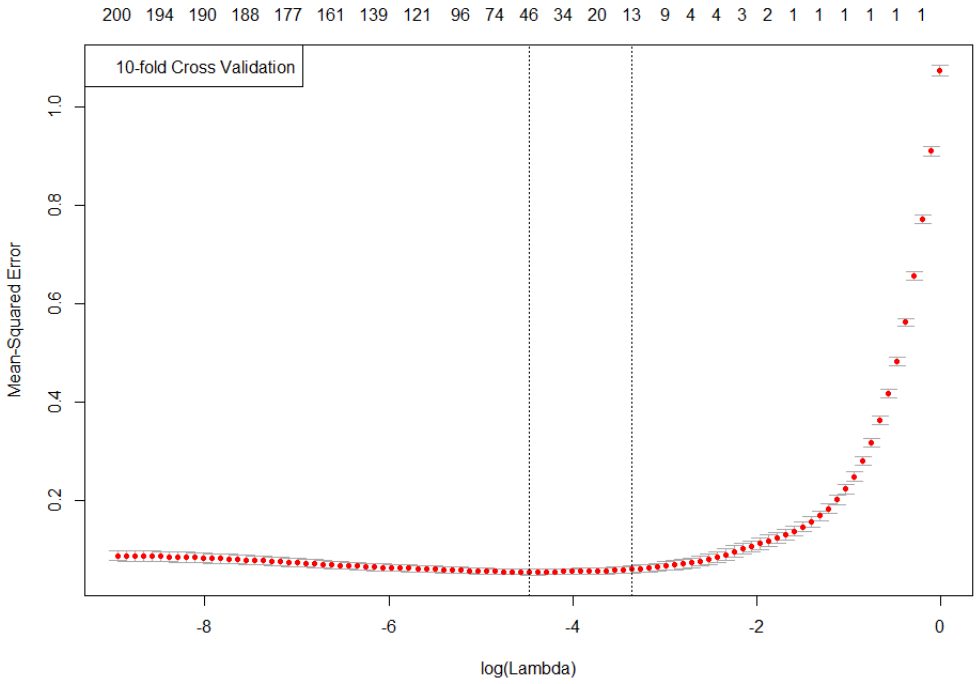
```
fit <- glmnet(hiv.train$x,hiv.train$y, alpha=0.2) #Elastic Net penalty
```



Cross-Validation

Ten-fold cross-validation shows us that the number of active variables are approximately 30.

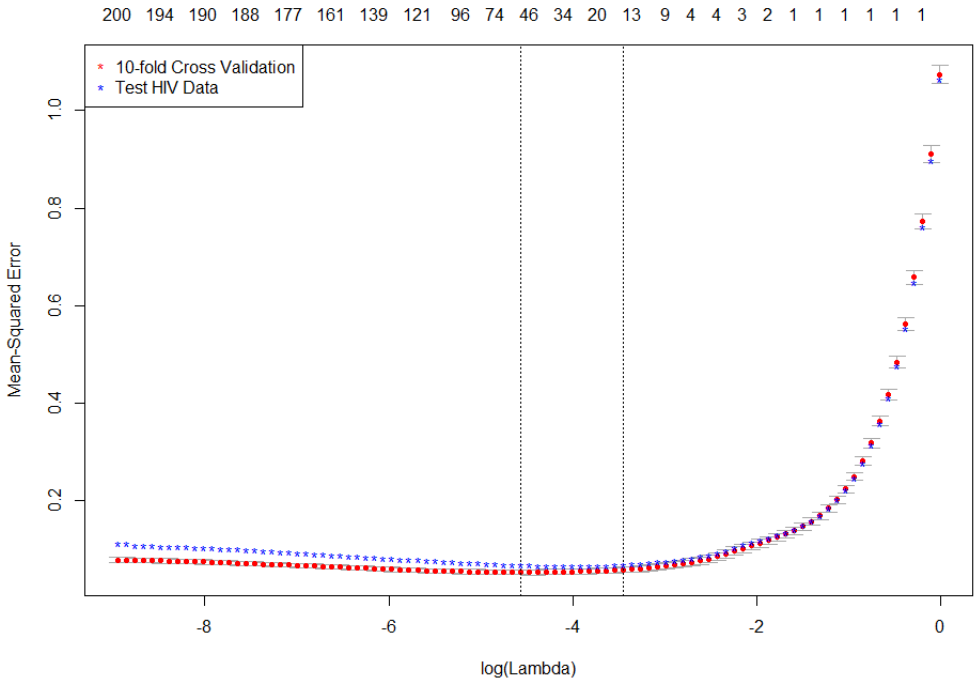
```
cv.fit <- cv.glmnet(hiv.train$x,hiv.train$y) #10-fold cross-validation
plot(cv.fit)
legend("topleft",legend=c("10-fold Cross Validation"))
```



Predicting the Test Data with the Model

The code snippet below predicts the error at every value of λ.

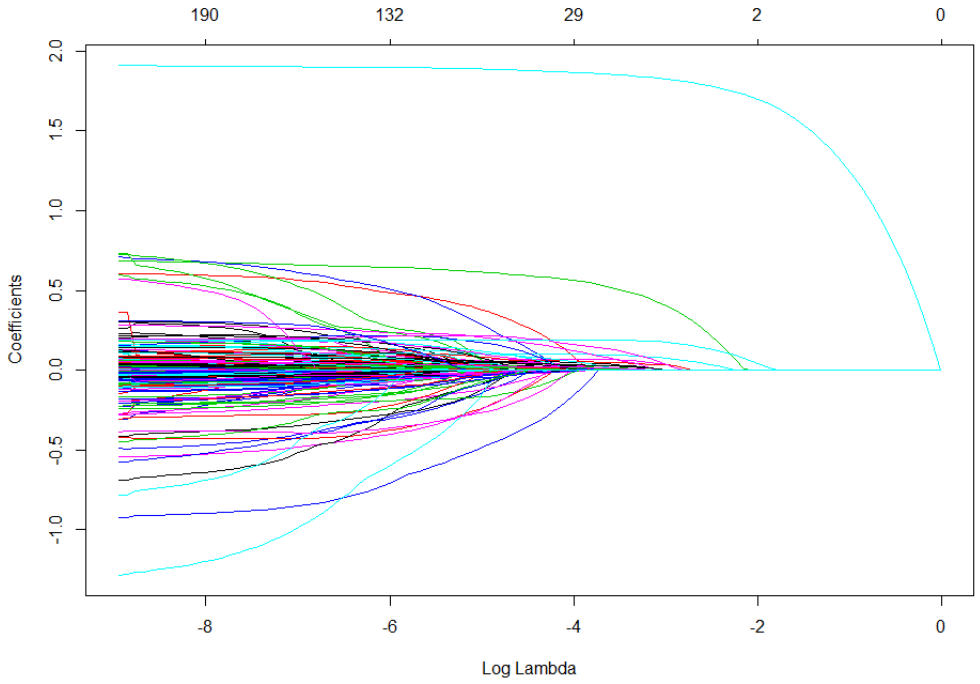
```
pred.y <- predict(fit, hiv.test$x) #predict the test data
mean.test.error <- apply((pred.y - hiv.test$y)^2,2,mean)
points(log(fit$lambda), mean.test.error, col="blue",pch="*")
legend("topleft",legend=c("10-fold Cross Validation","Test HIV Data"),pch="*",col=c("red","blue"))
```



Plotting the Regularization Path

The code snippet below shows the regularization path by plotting the coefficients against (log of) λ. Each curve represents a coefficient in the model. As λ gets smaller, more coefficients enter the model from a zero value. (see to the left).

```
plot(fit,xvar="lambda")
```



Code

```
# Author Auro Tripathy, auro@shatterline.com
# Adapted from ...Trevor Hastie's talk
rm(list=ls())

visualize.matrix <- function(mat) {
  print(names(mat))

  image(1:nrow(mat$x), 1:ncol(mat$x), z=mat$x,
        col = c("darkgreen", "white"),
        xlab = "Observations", ylab = "Attributes")

  title(main = "Visualizing the Sparse Binary Matrix",
        font.main = 4)
  return (dim(mat$x)) #returns the dimensions of the matrix
}

#---main---#
library(glmnet)
?glmnet
download.file("http://www.shatterline.com/MachineLearning/data/hiv.rda",
              "hiv.rda", mode="wb")
load("hiv.rda",
     verbose=TRUE) #contains hiv.train & hiv.test
visualize.matrix(hiv.train)
visualize.matrix(hiv.test)

print(length(hiv.train$y)) #length of response variable

fit <- glmnet(hiv.train$x,hiv.train$y, alpha=0) #Ridge penalty
plot(fit)
legend("bottomleft",legend=c("Ridge Penalty, alpha=0"))

fit <- glmnet(hiv.train$x,hiv.train$y, alpha=1) #Lasso penalty
plot(fit)
legend("bottomleft",legend=c("LASSO Penalty, alpha=1"))

fit <- glmnet(hiv.train$x,hiv.train$y, alpha=0.2) #ElasticNet penalty
plot(fit)
legend("bottomleft",legend=c("Elastic Net, alpha=0.2"))

cv.fit <- cv.glmnet(hiv.train$x,hiv.train$y) #10-fold cross-validation
plot(cv.fit)
legend("topleft",legend=c("10-fold Cross Validation"))
pred.y <- predict(fit, hiv.test$x) #predict the test data
mean.test.error <- apply((pred.y - hiv.test$y)^2,2,mean)
points(log(fit$lambda), mean.test.error, col="blue",pch="*")
```

```
legend("topleft",legend=c("10-fold Cross Validation","Test HIV Data"), pch="*", col=c("red","blue"))
plot(fit,xvar="lambda")
plot(fit,xvar="dev")
```

References

1. Prof Trever Hastie's talk
2. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*, Trevor Hastie , Robert Tibshirani , Jerome Friedman

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