Linear Models and Regularization

Some of the figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani

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1. Linear Regression

Part of the exciting part of modern ‘machine learning” is a set of relatively new methods with the ability to fit complex relationships (*nonlinearity*, *interaction*).

However,

the time honored linear model is still a major player:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip} + \epsilon$$

Why?

In high dimensions (big p), it may be very hard to look for complex relationships.

The linear model may have *acceptable bias* and *low variance*.

We can also make the linear model more flexible by throwing in a lot of transformations of the original x's.

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

"Throw in" squares and cross product: $\Rightarrow$

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5\, x_1 x_2 + \epsilon$$

Example:

Start with $p = 10$. Throw in all squares and cross products.
Now have $10 + 10 + (10*9/2) = 65$ variables.

Also, a linear model, without too many transformations thrown in, may be more interpretable.

It may also be useful to have a simple mathematical representation of $f(x)$, because you may want to use it as one input to a more complex decision, in which case being able to manipulate it or easily optimize it may be important.

So, basically, we will make regression interesting by having lots of x's !!

However, if we just throw in a lot of x's we could have a high variance overfit situation.

We will explore ways to *constrain the fit* so that we do not overfit.

Complex Model: Lot's of x's, not very constrained.

Simpler Model: Lot's of x's, constrained.

What does constrained mean??
Set some β_j to 0 and/or *shrink* some β_j towards 0.

This kind of shrinkage is known as **regularization**.

2. Linear Regression Review

In this section we present the linear Regression model in matrix form and review some its basic properties.

The linear model has a lot of nice simple properties.
These properties will also figure in some more complex models (e.g. iteratively reweighted least squares).

Note that sometimes we will include an intercept in which case I may use p to mean the number of x's$+1$ or sometimes I may use p for just the number of x's.

Matrix notation for the linear model

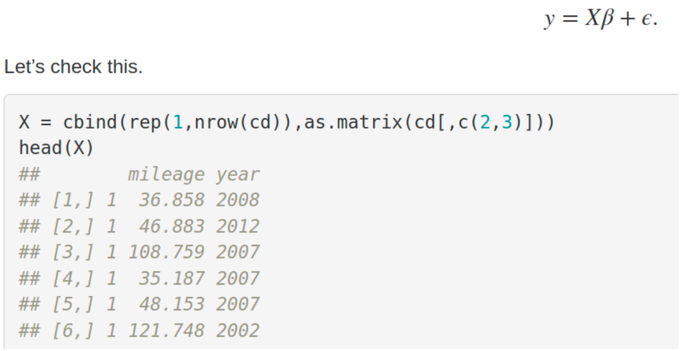
$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \varepsilon_i$$
$$i = 1, 2, \cdots n$$

$$x_i' = [1, x_{i1}, x_{i2}, \cdots x_{ip}] \qquad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

$$X = \begin{bmatrix} x_1' \\ x_2' \\ \vdots \\ x_n' \end{bmatrix} \quad (n \times (p+1))$$

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \qquad \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix} \qquad Y = X\beta + \varepsilon$$

Cut from R Hello world:



$$y = X\beta + \epsilon.$$

Let's check this.

```
X = cbind(rep(1,nrow(cd)),as.matrix(cd[,c(2,3)]))
head(X)
##        mileage year
## [1,] 1  36.858 2008
## [2,] 1  46.883 2012
## [3,] 1 108.759 2007
## [4,] 1  35.187 2007
## [5,] 1  48.153 2007
## [6,] 1 121.748 2002
```

We also write $X = [X_1, X_2, \ldots, X_p]$ so that X_j is a column of n values for the j^{th} x.

X_1 may or may not be a column of 1's.

p can mean *either* the number of x variables or the number of columns.

So if an intercept is included, p could be number of x's or number of x's $+1$.

You can tell from the context and I don't want to write $(p + 1)$ half the time.

2 x's + intercept

$$x_i = \begin{bmatrix} 1 \\ x_{i1} \\ x_{i2} \end{bmatrix} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

$$x_i' \beta = [1 \; x_{i1} \; x_{i2}] \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2}$$

$$X = \begin{bmatrix} x_1' \\ x_2' \\ \vdots \\ x_n' \end{bmatrix} = [\underline{1} \quad X_1 \quad X_2]$$

$$\underline{1} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \quad X_1 = \begin{bmatrix} x_{11} \\ x_{21} \\ \vdots \\ x_{n1} \end{bmatrix} \quad X_2 = \begin{bmatrix} X_{12} \\ X_{22} \\ \vdots \\ X_{n2} \end{bmatrix}$$

$$X\beta = \begin{bmatrix} x_1'\beta \\ x_2'\beta \\ \vdots \\ x_i'\beta \\ \vdots \\ x_n'\beta \end{bmatrix}$$

$$X\beta = [\underline{1} \; X_1 \; X_2] \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$
$$= \beta_0 \underline{1} + \beta_1 X_1 + \beta_2 X_2$$

Given training data, how do we estimate β?

Minimize the in-sample mean-square-error (MSE) which we will denote by L for "loss".

$$\min_{\beta} \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 = L(\beta)$$

To minimize we solve

$$\nabla L(\beta) = 0$$

$$\nabla L(\beta) = \left[\frac{\partial L}{\partial \beta_1}(\beta), \frac{\partial L}{\partial \beta_2}(\beta), \dots \frac{\partial L}{\partial \beta_p}(\beta) \right]$$

To minimize we will set the gradient to 0.
Note that the gradient is a row vector.

Quick Review: The Chain Rule

Chain Rule

$$f : \mathbb{R} \to \mathbb{R}$$

$$h : \mathbb{R} \to \mathbb{R}$$

Composition $\quad g(x) = f \circ h(x) \equiv f(h(x))$

$$g'(x) = f'(h(x))\, h'(x)$$

Alternative Notation $\quad y = y(z) \quad z = z(x)$

$$y(x) = y(z(x)) \qquad \frac{dy}{dx} = \frac{dy}{dz}\frac{dz}{dx}$$

$$x \to z \to y$$

$$\Delta x \to \Delta z = z'(x)\Delta x \to y'(z)\Delta z = y'(z) z'(x)\, \Delta x$$

Example of Chain Rule

$x^T = [1, x_1, x_2]$

$\beta^T = [\beta_0, \beta_1, \beta_2]$

$\beta_1 \rightarrow y - \beta_0 - \beta_1 x_1 - \beta_2 x_2 = e(\beta_1)$

(e for "error")

$e \rightarrow e^2 = L(e)$ (L for "loss")

$f(\beta_1) = L(e(\beta_1))$

$f(\beta_1) = (y - \beta_0 - \beta_1 x_1 - \beta_2 x_2)^2 = (y - x^T\beta)^2$

$f'(\beta_1) = L'(e)\, e'(\beta_1) = 2e[-x_1]$

$= -2(y - x^T\beta)x_1$

$\ell(\beta) = (y - \beta_0 - \beta_1 x_1 - \beta_2 x_2)^2$ $\quad \frac{\partial \ell(\beta)}{\partial \beta_1} = -2(y - x^T\beta)x_1$

Let's compute the gradient:

For a single observation (x, y),
the loss is

$$\ell(\beta) = (y - x^T\beta)^2$$

$$\frac{\partial \ell}{\partial \beta_j} = 2(y - x^T\beta)\{-x_j\}$$

(could be a 1)

$$x_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{bmatrix}$$

Summing over observations:

$$L(\beta) = \sum_{i=1}^{n} (y_i - x_i^T\beta)^2 = \sum_{i=1}^{n} (y_i - \beta_1 x_{i1} - \beta_2 x_{i2} \cdots - \beta_p x_{ip})^2$$

$$\frac{\partial L}{\partial \beta_j} = -2\sum_{i=1}^{n} (y_i - x_i^T\beta)x_{ij} = -2 \langle y - X\beta, X_j \rangle$$

$$\nabla L(\beta) = -2(y - X\beta)^T X$$

where the inner product is

$$< x, y >= \sum x_i y_i$$

Let's unpack that last step from the previous slide.

$$(Y - X\beta)^T X = (Y - X\beta)^T [x_1, x_2, \cdots x_p]$$

$$= [(Y-X\beta)^T x_1, (Y-X\beta)^T x_2, \cdots (Y-X\beta)^T x_p]$$

$$(Y-X\beta)^T x_j = \sum_{i=1}^{n} (y_i - x_i^T \beta) x_{ij}$$

Recall that two vectors are “orthogonal” (perpendicular) if their inner product is 0.

We call $y - X\beta$ the “residuals”.

$\nabla L = 0$ means the resids are orthogonal to each column of X!!!!!

Now we set the gradient equal 0 and solve.

$$\nabla L(\beta) = 0$$

$$X^T(Y - X\beta) = 0$$

$$X^T Y = X^T X \beta$$

$$\Rightarrow \quad \hat{\beta} = (X^T X)^{-1} X^T Y$$

Note

Geometrically we talk about x and y being orthogonal:

$$< x, y >= x'y = y'x = \sum x_i y_i = 0.$$

If we demean the variables so that we use $x_i - \bar{x}$ and $y_i - \bar{y}$, then we have

$$\sum (x_i - \bar{x})(y_i - \bar{y})$$

and the sample covariance is

$$\frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n-1}$$

So, after you demean, saying they are orthogonal is the same as saying they are uncorrelated.

3. Maximum Likelihood Estimation

For some things that we do it will be helpful to view the least squares estimator as a maximum likelihood estimate.

Recall that if we have parametric model for observable y with parameter θ

$$p(y \mid \theta)$$

then, we obtain the maximum likelihood estimate (MLE) of θ by solving:

$$\max_{\theta} p(y \mid \theta).$$

This is very intuitive, find the parameter value which makes what you have seen (the y) most likely.

To compute an MLE for regression we again need an assumption about the errors.

Again, let's use normal errors:

$$Y_i = x_i'\beta + \epsilon_i, \;\; \epsilon_i \sim N(0, \sigma^2), \; \epsilon_i \text{ iid.}$$

or,

$$Y_i \sim N(x_i'\beta, \sigma^2), \;\; \textit{independent}$$

Our parameter is (β, σ) and the likelihood has the form

$$p(y \mid \beta, \sigma^2) = \prod_{i=1}^{n} p(y_i \mid \beta, \sigma^2)$$

We will maximize this over (β, σ^2).

$$p(y_1, y_2, \ldots, y_n \mid \beta, \sigma) = \prod_{i=1}^{n} \, \frac{1}{\sqrt{2\pi}} \, \frac{1}{\sigma} \exp(-\frac{1}{2\sigma^2}(y_i - x_i'\beta)^2$$
$$= (2\pi)^{-n/2} \, \sigma^{-n} \, \exp(-\frac{1}{2\sigma^2}||\,Y - X\beta||^2).$$

So for any σ, the likelihood is minimized at the least squares $\hat{\beta} = (X'X)^{-1}X'y$.

Let $v = \sigma^2$. Let $S = ||y - X\hat{\beta}||^2$.

$log(L(v, \hat{\beta})) = -\frac{n}{2}\log(v) - \frac{1}{2v}S + C$.

$-2log(L(v, \hat{\beta})) = n\log(v) + \frac{1}{v}S + C$.

Taking the derivative wrt v and setting it equal to 0, we have:

$\frac{n}{v} - \frac{S}{v^2} = 0, \Rightarrow \hat{v} = \frac{S}{n}$.

And, $-2log(L(\hat{v}, \hat{\beta})) = n\log(\hat{v}) + n + C$.

4. Subset Selection

If we just "throw in a ton of x's" our model may be too complex, we may overfit.

Often, we try to start with a "ton of x's" and then see how many we can throw out and still have good fit.

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip} + \epsilon$$

Throwing out an x is equivalent to setting its coefficient to 0.

Which coefficients do we set to 0?

The key idea is *the bias variance trade-off !!!*

If we set too many coefficients to 0, we may be throwing out some variables that do important work in explaining Y, $\Rightarrow$ *bias*.

If we keep too many variables, it may be difficult to get good estimates of all the corresponding coefficients $\Rightarrow$ *variability*.

Our basic problem is that there are a lot of possible ways to pick a subset of variables to keep!!

Let k denote the number of variables kept.

How many ways can you choose k from p: $\left(\begin{array}{c} p \\ k \end{array} \right) = \frac{p!}{k!\,(p-k)!}$.

And, summing over possible $k = 0, 1, 2, \ldots, p$, there are 2^p possible regression models.

Example, p=20,k=10:

2^{20} = 1,048,576
choose(20,10)= 184,756

What we need is a simple way to move from simpler models to more complex models (recall k in kNN).

In subset selection, we will **let k denote the number of variables used**, so that k goes from 0 to p.

Big k: complex model, Small k: simple model !!

For each k we will choose a single regression model from the $\binom{p}{k}$ possible models.

Two possible ways of choosing a subset (a model) given k are:

small p:

All subsets:

For p less than about 40, it is possible to run all the possible regressions.

Given the number of variables k, we will pick the subset of variables of size k with the highest R^2.

big p:

Forward Stepwise Selection:

- Start with k=0, no variables selected.
- Given a current k and corresponding subset, add in the new variable which gives you the biggest increase in R^2.
- Stop at $k = p$.

This is a greedy forward search!!

We can now choose k, the number of variables, the same way we chose k in kNN.

A simple validation set approach simply splits the data into train and validate, and sees which value of k gives the best prediction.

Or, we could use cross validation.

Hitters Example

Let's look at the "Hitters" example used in the Lab in the ISLR book.

Each observation corresponds to a baseball player.

Y: `Salary`:
1987 annual salary on opening day in thousands of dollars.

x1: `AtBat`:
Number of times at bat in 1986

...

x19: `NewLeague`:
A factor with levels 'A' and 'N' indicating player's league at the beginning of 1987.

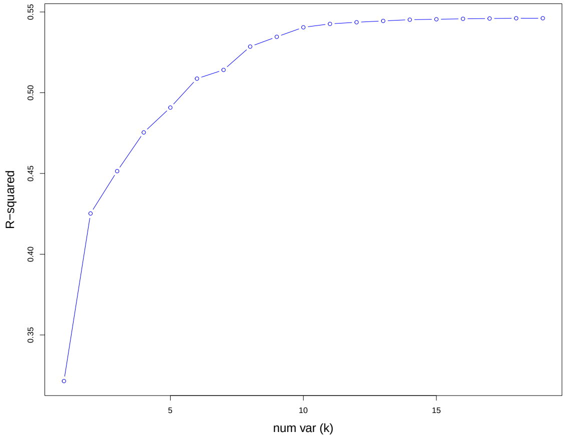
For $k = 1, 2, 3, 4, 5$,
here are the variables that give you the highest R^2:

```
  (Intercept) AtBat  Hits HmRun  Runs   RBI Walks Years CAtBat CHits CHmRun
1        TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  FALSE FALSE  FALSE
2        TRUE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  FALSE FALSE  FALSE
3        TRUE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  FALSE FALSE  FALSE
4        TRUE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  FALSE FALSE  FALSE
5        TRUE  TRUE  TRUE FALSE FALSE FALSE FALSE FALSE  FALSE FALSE  FALSE
  CRuns CRBI CWalks LeagueN DivisionW PutOuts Assists Errors NewLeagueN
1 FALSE TRUE  FALSE   FALSE     FALSE   FALSE   FALSE  FALSE      FALSE
2 FALSE TRUE  FALSE   FALSE     FALSE   FALSE   FALSE  FALSE      FALSE
3 FALSE TRUE  FALSE   FALSE     FALSE    TRUE   FALSE  FALSE      FALSE
4 FALSE TRUE  FALSE   FALSE      TRUE    TRUE   FALSE  FALSE      FALSE
5 FALSE TRUE  FALSE   FALSE      TRUE    TRUE   FALSE  FALSE      FALSE
```

So, if $k = 3$, you use `Hits`, `CRBI`, and `PutOuts`.

‘Hits’: Number of hits in 1986
‘CRBI’: Number of runs batted in during his career
‘PutOuts’: Number of put outs in 1986

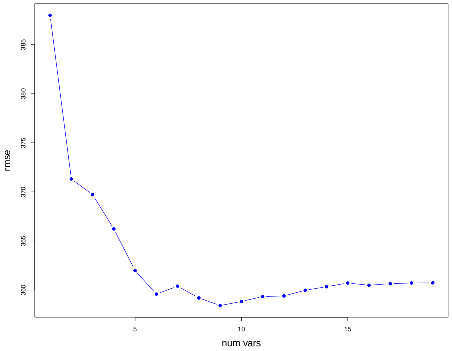
Here is a plot of k vs. the R^2 for the model having the highest R^2 out of all models of size k.



Of course, we may not want the model with the highest in-sample R^2 !!!

Split the data 50/50 into train/validate. Get the best subset for each k using the train, and then predict on the validate.

I repeated the train/validate split 100 times and then averaged the results. Maybe better to do 10-fold cross validation.



I'll choose $k = 6$.

Given the choice $k = 6$, we then get the best subset of size 6, using all the data. Here is the regression.

```
Call:
lm(formula = Salary ~ ., data = ddfsub)

Residuals:
    Min      1Q  Median      3Q     Max 
-873.11 -181.72  -25.91  141.77 2040.47 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept)   91.51180   65.00006   1.408 0.160382    
AtBat         -1.86859    0.52742  -3.543 0.000470 ***
Hits           7.60440    1.66254   4.574 7.46e-06 ***
Walks          3.69765    1.21036   3.055 0.002488 ** 
CRBI           0.64302    0.06443   9.979  < 2e-16 ***
DivisionW   -122.95153   39.82029  -3.088 0.002239 ** 
PutOuts        0.26431    0.07477   3.535 0.000484 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1 

Residual standard error: 319.9 on 256 degrees of freedom
Multiple R-squared:  0.5087,Adjusted R-squared:  0.4972 
F-statistic: 44.18 on 6 and 256 DF,  p-value: < 2.2e-16
```

5. AIC and BIC in Linear Regression

Suppose we have a parametric model $f(y \mid \theta)$.

For example, in our regression model (supressing x) we have $\theta = (\beta_0, \beta_1, \ldots, \beta_p, \sigma)$.

Now suppose we have two parametric models for the same y with two corresponding parameters:

$$p(y \mid \theta_1) \text{ and } p(y \mid \theta_2).$$

For example, in our regression model we could have $\theta_1 = (\beta_0, \beta_1, \ldots, \beta_p, \sigma)$ and $\theta_2 = (\beta_0, \beta_1, \sigma)$

Given observed data y how can we decide which model is better?

Well, we could compare the maximized likelihoods:

$$L_1 = L(\hat{\theta}_1) \text{ and } L_2 = L(\hat{\theta}_2)$$

where the parameter estimates are the MLEs.

But, if we just choose the model with the largest maximized likelihood, we could overfit.

Rather than use a train/test strategy to choose the models, AIC and BIC compare the maxmimized log Likelihoods but subtract off a "penalty term" which depends on the number of parameters in the model.

Let m be the number of parameters in the model.

AIC: $-2\log(\hat{L}) + 2m$
BIC: $-2\log(\hat{L}) + \log(n)m$.

The idea is that you choose the model which has the *smallest* AIC or BIC.

So, AIC charges you 2 per parameter and BIC charges you $\log(n)$.

BIC selects a simpler model since in charges more per parameter.

AIC: $-2\log(\hat{L}) + 2m$
BIC: $-2\log(\hat{L}) + \log(n)m$.

For example the model $\theta_1 = (\beta_0, \beta_1, \ldots, \beta_p, \sigma)$ has $p+2$ parameters and the model $\theta_2 = (\beta_0, \beta_1, \sigma)$ has 3 parameters.

This is not quaranteed to work as a lot of approximations and assumptions go into their derivations.

What does "work" mean?

Choose a model that gives good out-of-sample predictions!!!

AIC and BIC for Regression:

Let $\hat{L}$ denote the maximized likelihood
(the likelihood evaluated at the MLE's).

Suppose we include the intercept and use k x variables:

AIC:

$$n \log(\hat{\sigma}^2_{MLE,k}) + 2\,k + C(n)$$

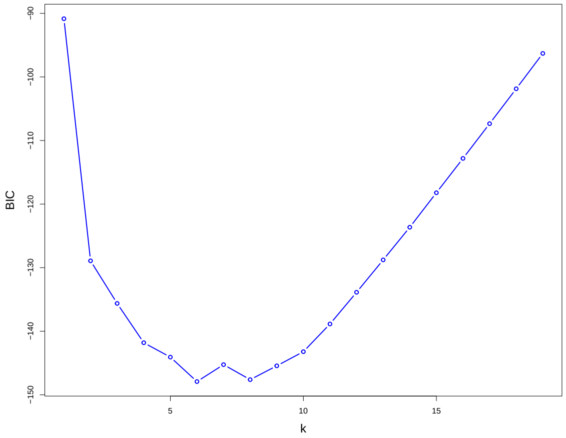
BIC:

$$n \log(\hat{\sigma}^2_{MLE,k}) + \log(n)\,k + C(n)$$

You are supposed to prefer the model which has the smallest AIC or BIC.

$C(n)$ is a constant that only depends on n, since this is fixed, we can ignore it.

Here is a plot of k vs. BIC.



This suggests k of about 6 which is what we got using our of-of-sample expermiment.

The Deviance

The basic idea behind AIC and BIC is the $L(\hat{\theta})$ can be used as measure of fit on the training data.

The is often expressed in terms of the deviance:

$$D = -2\,\log(L(\hat{\theta}))$$

So, a *small deviance means a good fit*.

$$\text{AIC: } D + 2k, \quad \text{BIC: } D + \log(n)\,k$$

We choose the model with the smallest AIC or BIC.

Warning: D or $D + c$ where c is an constant that does not depend on the model, so when you see a deviance computed it may be $\pm c$.

6. Regularized Linear Regression - L2, Ridge Regression

Our variable selection approach set some of the coefficients in a multiple regression to 0.

This helped keep our model simple so that we do not overfit.

Another way to keep our model “simple” is to *push* or *shrink* the coefficient towards 0.

This way a coefficient will only be large if the data demands it!

Ridge Regression:

Recall that least squares works by picking the coefficients to minimize

$$RSS = \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2.$$

Ridge regression works by mimimizing:

$$\sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} \beta_j^2.$$

For large λ you pay a price to make a coefficient large !!

Minimize:

$$\sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j \, x_{ij})^2 + \lambda \sum_{j=1}^{p} \beta_j^2 .$$

λ will be our "walk the bias-variance trade-off" parameter.

small λ: can have big coefficient $\Rightarrow$ *complex model.*

big λ: can't have many big coefficients $\Rightarrow$ *simple model.*

So, for every λ, you will get a different optimizing β:

$$\lambda \Rightarrow \hat{\beta}^R_\lambda.$$

For example $\hat{\beta}^R_0$ is just the least squares estimator.

How do you choose λ ?

cross-validation, or another out-of-sample criterion!!.

Note:

We are minimizing

fit: $\sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j \, x_{ij})^2$

$+$

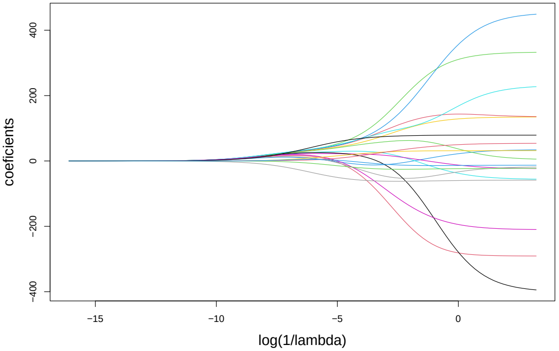
penalty: $\lambda \sum_{j=1}^{p} \beta_j^2$.

Since the penalty treats all the β_j the same you have to be thinking about all the x's the same. What are the units of β_j?

Usually people *standardize* the x's before the do this kind of shrinkage.

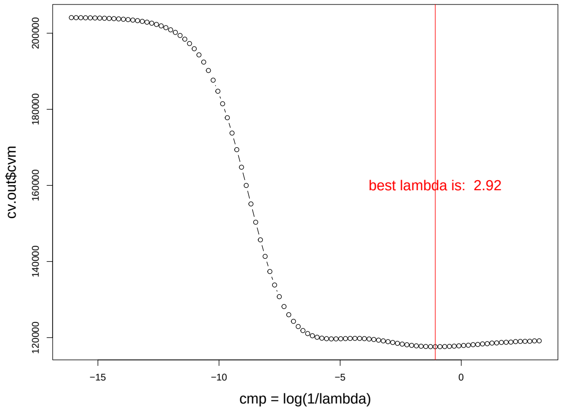
Let's try Ridge regression with the Hitters data.
I standardized all the x's.

Here we plot $\log(1/\lambda)$ vs. $\hat{\beta}^R_\lambda$.

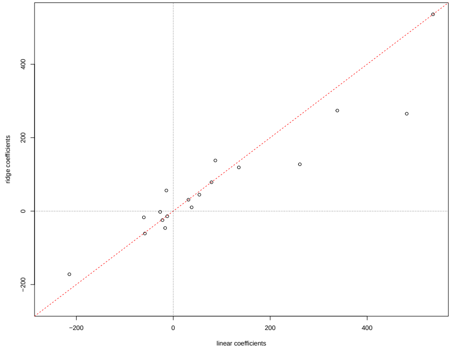


A *complex* model is one where the coefficients are allowed to be big.

Here is the cross-validation estimate of the out of sample loss.

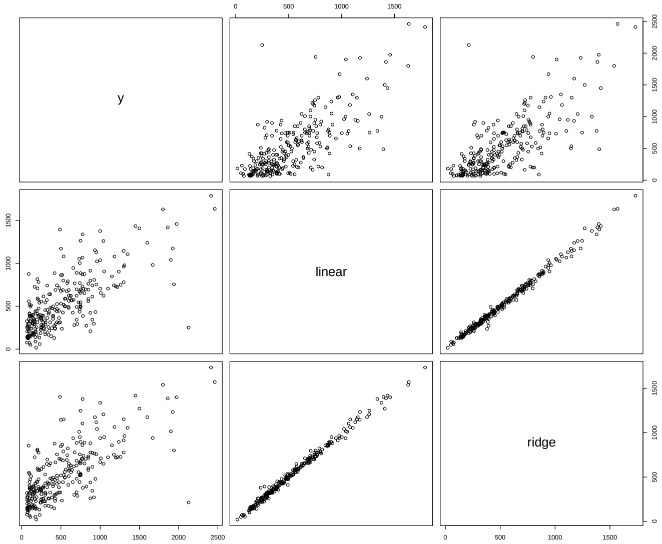


Here we plot the coefficients from linear regression against those we get using ridge regression with the optimal λ.



They are not too different in this case.
You can see some of the bigger coefficients are shrunk a bit.
A lot of the coeficients are close to 0, (we standardized the x's).
The x's with absolute values bigger than 100 are "AtBat" "Hits" "Walks" "CAtBat" "CHits" "CRuns" "CRBI" "CWalks"

Here we compare the in-sample fits from regression and ridge.



What is the ridge regression $\hat{\beta}^R_\lambda$?

Let's assume that we have subracted the mean from y and each x.

We don't shrink the intercept so we can go ahead and just use $\bar{y}$ to estimate it.

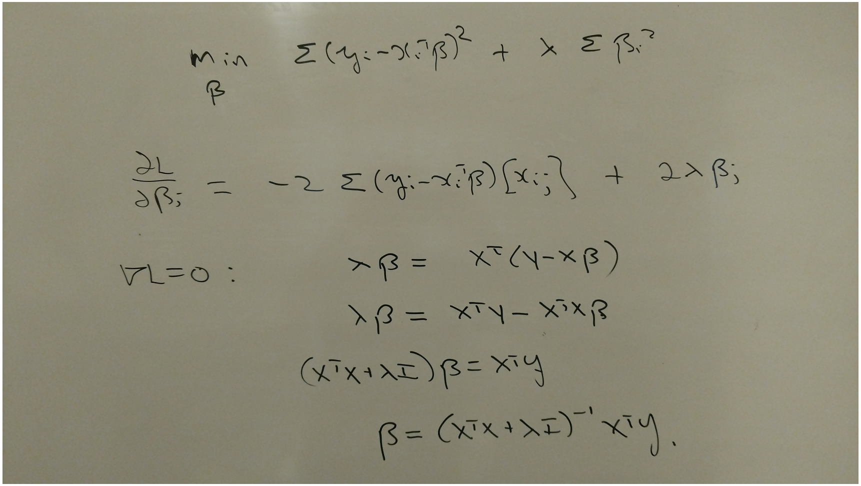
So, now our problem is just:
minimize:

$$\sum_{i=1}^{n} (y_i - \sum_{j=1}^{p} \beta_j \, x_{ij})^2 + \lambda \sum_{j=1}^{p} \beta_j^2 .$$

or

$$\sum_{i=1}^{n} (y_i - x_i' \beta)^2 + \lambda \sum \beta_i^2 = ||y - X\beta||^2 + \lambda ||\beta||_2^2$$

What is the ridge regression $\hat{\beta}^R_\lambda$?



$$\min_{\beta} \ \Sigma(y_i - x_i^T\beta)^2 + \lambda \, \Sigma \beta_i^2$$

$$\frac{\partial L}{\partial \beta_j} = -2 \, \Sigma(y_i - x_i^T\beta)[x_{ij}] + 2\lambda\beta_j$$

$$\nabla L = 0 : \quad \lambda\beta = X^T(Y - X\beta)$$

$$\lambda\beta = X^TY - X^TX\beta$$

$$(X^TX + \lambda I)\beta = X^Ty$$

$$\beta = (X^TX + \lambda I)^{-1} X^Ty.$$

What happens if the x's are orthogonal (uncorrelated) so that $X'X =$ is diagonal?

If $X'X = diag(x_j'x_j)$
then

$$\hat{\beta}_j = \frac{< y, x_j >}{< x_j, x_j > + \lambda}$$

which is an extremely simple and intuitive version of *shrinkage*.

If $\lambda = 0$ we have the usual OLS solution, but at as λ increases, our solution is pushed towards 0.

Regularization and Constrained Optimization

If we let $f(\beta) = ||y - X\beta||^2$ and $p(\beta) = ||\beta||^2$ then we are minimizing

$$f(\beta) + \lambda p(\beta)$$

More generally if f is our "fit" and p is our "penalty" we have a very general approach to walking the bias-variance trade-off as we vary λ .

As long as p does not like big β, then large λ will give us "simple" models.

This approach is often called *regularization*.

It is also useful to view the problem as a constrained fit.

Minimizing the unconstrained

$$f(\beta) + \lambda p(\beta)$$

is related to solving the *constrained optimization*

$$\min \; f(\beta) \; \text{ subject to } \; p(\beta) \leq k$$

min fit + penalty, *or* min fit subject to penalty not big.

Clearly if β^* minimizes $f(\beta) + \lambda\, p(\beta)$ then it must also solve

$$\min \ f(\beta) \ \text{ subject to } \ p(\beta) = p(\beta^*)$$

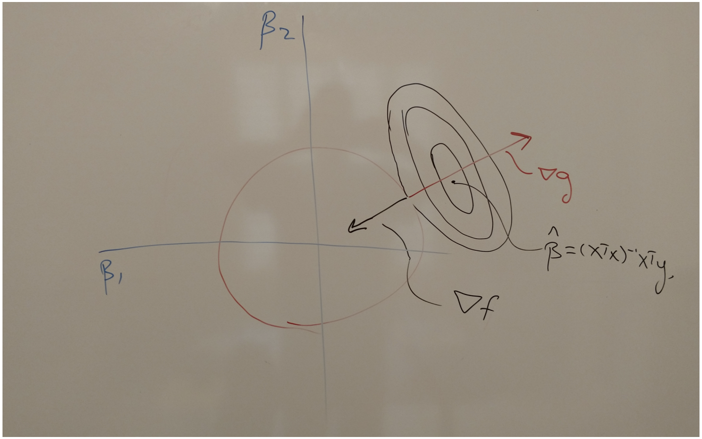
For our Ridge regression problem we have $f(\beta) = ||y - X\beta||^2$ and $g(\beta) = ||\beta||^2 - k$ where k is a positive constant.

In this case the contours $f(\beta) = c$ are ellipses and the contours $g(\beta) = c$ are circles.

We have a very nice picture which makes the lagrangian FOC inutitive.

Here is the key picture for the case where the constraint is binding.

Remember, ∇f is the direction in which f goes up the fastest!!
∇f points perpendicularly to the contour of f.



It is intuitive that $\nabla f + \alpha \nabla g = 0$ with $\alpha > 0$.

To solve our Ridge regularization as a constrained problem we have:

$-\nabla f' = 2X'(Y - X\beta)$.

$\nabla g' = 2\beta$.

$2\alpha\beta = 2X'(Y - X\beta)$.

$\beta^*_\alpha = (X'X + \alpha I)^{-1}X'Y$.

We would then solve (the easy problem) of finding the α such that $||\beta^*_\alpha||^2 = k$.

Regularization in Machine Learning

We can think of ridge regression as a basic example of a general setup we see in Machine Learning.

We have a "model" the defines our *action* given the information in the observed vector of features x.

Our action is characterized by a vector of parameters θ.

Let's denote our action by $f(x, \theta)$.

Given our action and the then observed y we incur a *loss* $L(y, f(x, \theta))$.

In our linear regression example, θ is β and

$$f(x, \beta) = x' \beta, \quad L(y, f(x, \beta)) = (y - x' \beta)^2.$$

We have “complexity measure” $C(\theta)$.

In ridge regression, $C(\beta) = ||\beta||_2^2$.

Given training observation observation (x_i, y_i) and parameter θ we “learn” θ by

$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{n} L(y_i, f(x_i, \theta)) + \lambda\, C(\theta)$$

The parameter λ walks you from simple to complex models.

7. Shrinkage: The Lasso

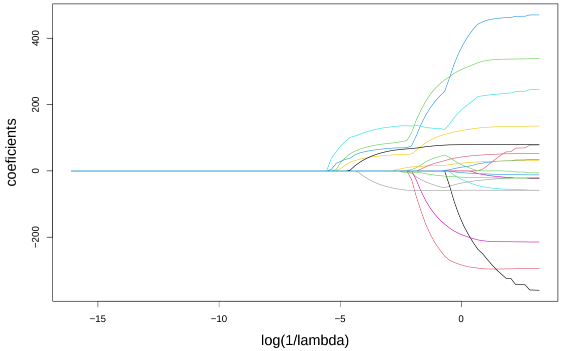
The Lasso (least absolute shrinkage and selection operator) changes the form of the penalty.

Now, we minimize:

$$\sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j \, x_{ij})^2 + \lambda \sum_{j=1}^{p} |\beta_j|.$$

This may not seem like a big deal, but it turns out the solution to this problem can set a β_j exactly to 0, so that you get variable selection.

Here are the lasso solutions as λ varies.

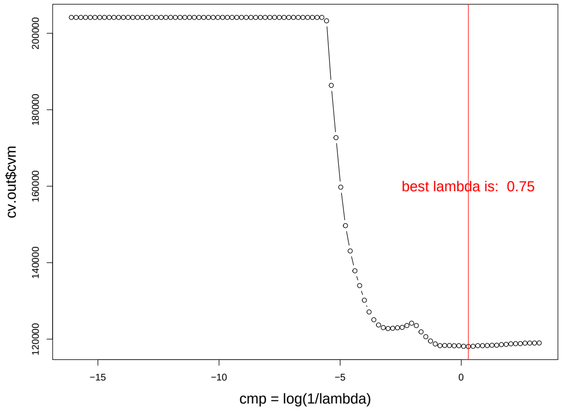


The point is, that for big λ, coefficients get set to 0.

In the Lasso, there is shrinkage as well as selection and the shrinkage takes on a different form than in L2 regularization.

Also, with the Lasso, variables can to out as λ decreases, whereas with forward, once you are in, you are always in.

As usual, we can choose λ using cross-validation.



For big enough λ, all the coefficients are set to 0.

Here are the $\hat{\beta}^L_\lambda$ for the best CV lambda.

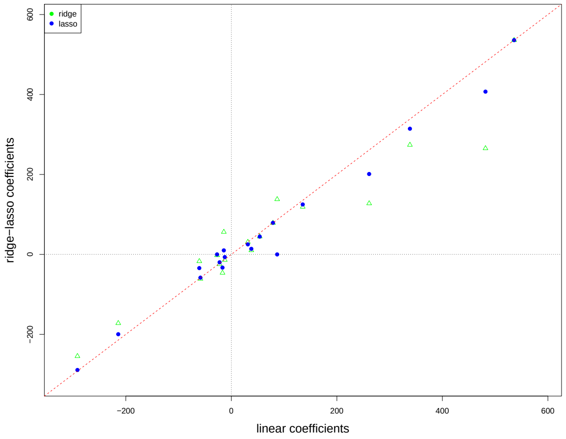
```
(Intercept)       AtBat        Hits       HmRun        Runs         RBI
 535.925882 -289.109678  314.374161   13.916703  -34.239618    0.000000
      Walks       Years      CAtBat       CHits      CHmRun       CRuns
 124.971379  -33.041086 -191.538897    0.000000   10.072782  407.092162
       CRBI      CWalks     LeagueN   DivisionW     PutOuts     Assists
 201.114077 -199.619610   25.169164  -58.149563   79.100366   44.502170
     Errors  NewLeagueN
 -19.688952   -6.704629
```

We see that a couple are 0.

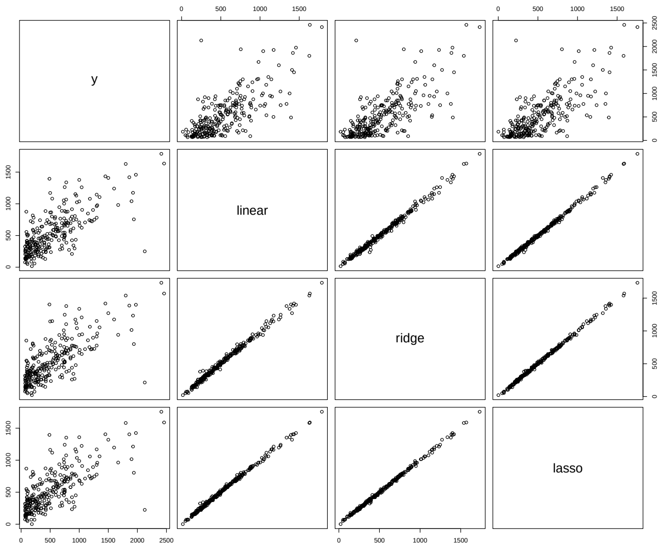
Plot Ridge and Lasso coefficients vs the least squares coefficients.

A couple of the Lasso coefficients are 0.

A big coefficent is shrunk less under Lasso than Ridge.



Fits are not actually too different.



Why do people like the Lasso?

- Simple way to walk the bias variance trade-off.
- Zero coefficients give variable selection, can get more interpretable models.
- Computationally fast.

Stewise compared to Lasso

Lasso is a quadratic (and hence convex and differentiable) loss function optimized under a convex constraint.
Hence, the Lasso problem has a guaranted global optimum and we have very efficient algorithms for finding that optimum.

The step wise algorithms are greedy searches so there is no guarantee the global optimum has been found.

But, since they do not shrink, the step wise methods can find more parisimonious solutions (use fewer x's) faster!!

In our Hitters example, the allsubsets method ended up using just 6 x's but the lasso only set two coefficients to 0!!

8. Understanding the Lasso Solution

Why does the Lasso give solutions with coeficients at 0?

How is Ridge different from Lasso?

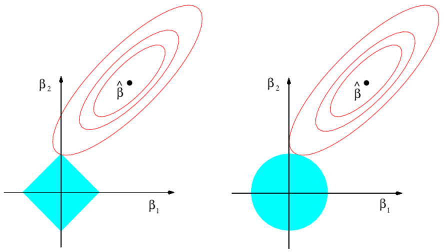
To get a good simple intuition, it is helpful to consider the constrained optimization view of Lasso and Ridge.

Ridge:

$$\begin{aligned}
&\underset{\beta_0,\beta}{\text{minimize}} \quad \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j \, x_{ij})^2 \\
&\text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq t^2
\end{aligned}$$

Lasso:

$$\begin{aligned}
&\underset{\beta_0,\beta}{\text{minimize}} \quad \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j \, x_{ij})^2 \\
&\text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq t
\end{aligned}$$



At left we have the Lasso problem, where the constraint set looks like a diamond.

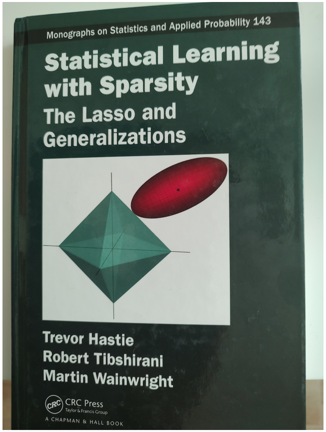
At right we have the Ridge problem, where the constraint set looks like a circle.

The diamond constraint can give solutions at an axis.

This is a very famous picture !!!!!

"Sparcity" is another term you often hear.

The Lasso give sparcity because some the coefficients are set to 0.

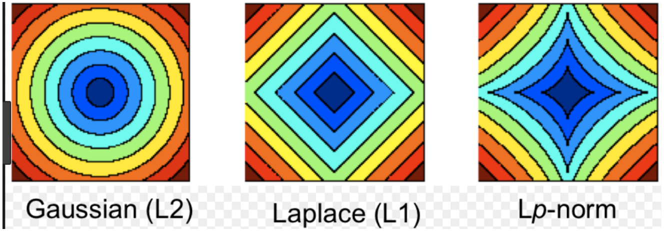

Monographs on Statistics and Applied Probability 143
Statistical Learning with Sparsity
The Lasso and Generalizations
Trevor Hastie
Robert Tibshirani
Martin Wainwright
CRC Press
Taylor & Francis Group
A CHAPMAN & HALL BOOK

sparcity, regularization, shrinkage ......

With L2 and L1 you have a convex optimization problem.

You are minimizing a convex function on a convex constraint set.

If you go L_p, $p < 1$, you get even more variable selection, but you lose the convexity.



$$||x||_p = (\sum |x_i|^p)^{1/p}$$

The Simplest Version

Let's consider the simplest possible version of our problems back in the "Lagrangian" formulation:

Ridge:

$$\underset{\beta}{\text{minimize}}\ \ (y-\beta)^2 + \lambda\,\beta^2$$

Lasso:

$$\underset{\beta}{\text{minimize}}\ \ \tfrac{1}{2}\,(y-\beta)^2 + \lambda\,|\beta|$$

Adding the $1/2$ for the Lasso changes nothing and makes the expressions look nicer.

$$\underset{\beta}{\text{minimize}} \;\; (y-\beta)^2 + \lambda\, \beta^2$$

For the Ridge version we are minimizing a quadatric so we can easily find the global miniumum by setting the derivative equal to 0:

$$2(y-\beta)(-1) + 2\lambda\beta = 0 \Rightarrow \hat{\beta}^R = \frac{y}{1+\lambda}.$$

Of course the unconstrained solution is $\hat{\beta} = y$ so we can very nicely see how a choice of λ shrinks the estimate towards 0.

For the Lasso problem, we suddenly have a basic technical problem.

The function

$$g(\beta) = |\beta|$$

is not differentiable at 0!!

Our function is convex, so there is a global minimum, but can we find it in a simple way?

We can, and the solution will shed light on the Lasso and on how to solve the general regression problem.

$$\underset{\beta}{\text{minimize}} \;\; \frac{1}{2}\left(y-\beta\right)^2 + \lambda\left|\beta\right|$$

To derive the Lasso solution, suppose the optimal β is greater than 0.

Then, locally, our differential first order conditions apply *and* our criterion is differentiable since we know $|\beta| = \beta$.

$$(y-\beta)(-1) + \lambda = 0 \Rightarrow \hat{\beta}^L = y - \lambda.$$

Similarly, if the optimal is less than 0, then $|\beta| = -\beta$ so,

$$(y-\beta)(-1) - \lambda = 0 \Rightarrow \hat{\beta}^L = y + \lambda.$$

Shrink towards 0 by an amount λ !!

Now we only have three posibilities for the optimal β and you can just check that the minimum is obtained with

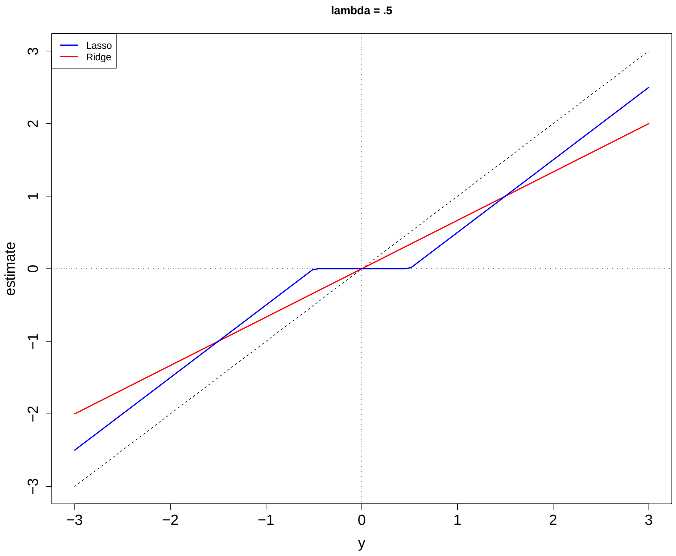
$$\hat{\beta}^L = \begin{cases} y - \lambda & y > \lambda \\ \\ 0 & |y| \leq \lambda \\ \\ y + \lambda & y < -\lambda \end{cases}$$

For example, suppose $0 < y < \lambda$.
Which is better, $\beta = 0$ or $\beta = y - \lambda$?.
At $y - \lambda$ we have

$$\begin{aligned} (y - (y - \lambda))^2 + \lambda|y - \lambda| &= \lambda^2 + \lambda|y - \lambda| \\ &\geq (y - 0)^2 + \lambda|0|. \end{aligned}$$

Intuitively, if $0 < y < \lambda$, there is no way I want negative estimate $y - \lambda$.

Here is a plot of the Lasso and Ridge shrinkage.



We can express these solutions succintly using the *soft threshholding function* S_λ.

$$\hat{\beta}^R = \frac{y}{1+\lambda}.$$

$$\hat{\beta}^L = S_\lambda(y)$$

where

$$S_\lambda(y) = \text{sign}(y)(|y| - \lambda)_+$$

with $x_+ = x$ if x is positive and 0 otherwise.

Let's see how it works out in practice.

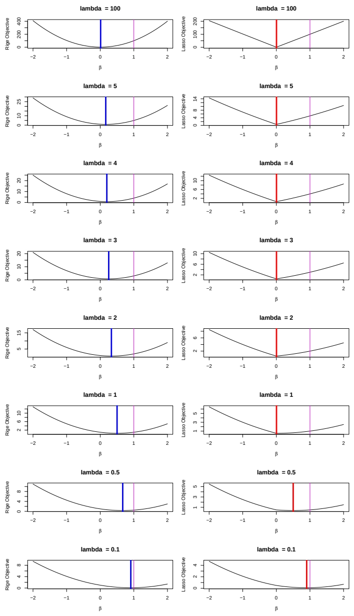
Let's say $y = 1$.
We plot y with the solid magenta line.

λ decreases as we go down the plots.

At left we have the Ridge criterion plotted with the minimizing β indicated by the solid blue line.

At right we have the Lasso criterion plotted with the minimizing β indicated by the solid red line.

Each estimate moves from 0 to 1, but the Lasso estimate sticks at 0 for a while and then moves faster to 1.



Standardization:

Ok, now let's try Lasso with some x's !!

But first, we emphasize again that for this to make sense you have to put the x's on the same scale by standarizing them.

The Lasso literature strongly favors standardization using the sample mean and variance.

Since we are not trying to regularize (shrink) the intercept, it is usual to start by demeaning y and x:

$$y_i \rightarrow y_i - \bar{y}; \;\; x_{ij} \rightarrow x_{ij} - \bar{x}_j .$$

Recall that if you run a regression using the demeaned variables, you get the same slope estimates.

We then scale the x's:

$$x_{ij} \to \frac{x_{ij}}{s_j}$$

where

$$s_j^2 = \frac{\sum x_{ij}^2}{n}$$

Note that after you do this standardization $\sum_i x_{ij}^2 = n$ for each $j = 1, 2, \ldots, p$.

Lasso with one x

Let's now see what happens when we just have one x variable.

After standardizing we miminize:

$$\frac{1}{2n}\sum_{i=1}^{n}(y_i-\beta\,x_i)^2+\lambda\,|\beta|.$$

Dividing by $2n$ does not change the problem, but makes the formulas turn out nicer.

Again if the solution were positive, we must have

$$\frac{1}{n}\sum(y_i - \beta x_i)(-x_i) + \lambda = 0 \to \hat{\beta}^L = \frac{1}{n} < x, y > -\lambda.$$

And if negative,

$$\frac{1}{n}\sum(y_i - \beta x_i)(-x_i) - \lambda = 0 \to \hat{\beta}^L = \frac{1}{n} < x, y > +\lambda.$$

So that,

$$\hat{\beta}^L = S_\lambda(\frac{1}{n} < x, y >).$$

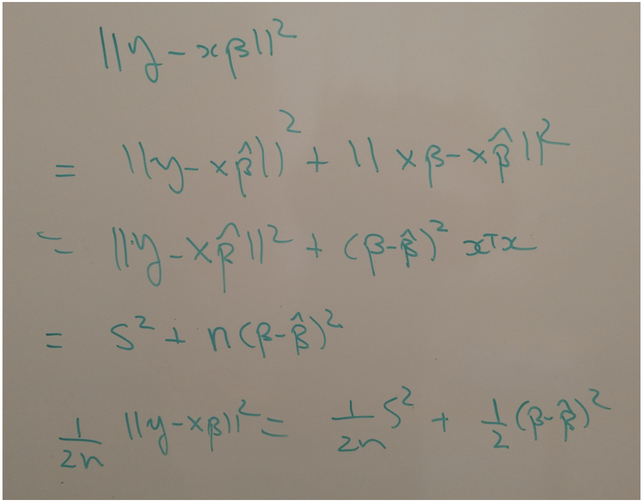
Note that with our standardization, we are basically soft-thresholding the least-squares $\hat{\beta}$.

$$\hat{\beta} = \frac{< x, y >}{< x, x >} = \frac{< x, y >}{n}$$

so

$$\hat{\beta}^L = S_\lambda(\hat{\beta}).$$

How about this way??



$$\|y - x\beta\|^2$$

$$= \|y - x\hat{\beta}\|^2 + \|x\beta - x\hat{\beta}\|^2$$

$$= \|y - X\hat{\beta}\|^2 + (\beta - \hat{\beta})^2 x^T x$$

$$= S^2 + n(\beta - \hat{\beta})^2$$

$$\frac{1}{2n}\|y - x\beta\|^2 = \frac{1}{2n}S^2 + \frac{1}{2}(\beta - \hat{\beta})^2$$

Then by the result we got in our simplest problem $\hat{\beta}^L = S_\lambda(\hat{\beta})$.

The General Problem, p Variables:

$$\underset{\beta}{\text{minimize}}\ \frac{1}{2n}\sum_{i=1}^{n}(y_i - \sum_j \beta_j x_{ij})^2 + \lambda \sum_j |\beta_j|.$$

or,

$$\underset{\beta}{\text{minimize}}\ \frac{1}{2n}||y - X\beta||^2 + \lambda\,||\beta||_1$$

Cyclic Coordinate Descent:

Given a choice of λ, suppose we knew all of the coefficients except β_j.

We can write our objective as:

$$\underset{\beta_j}{\text{minimize}}\ \frac{1}{2n}\sum_{i=1}^{n}(y_i - \sum_{k\neq j}\beta_k\, x_{ik} - \beta_j x_{ij})^2 + \lambda|\beta_j| + \lambda\sum_{k\neq j}|\beta_k|.$$

Which is the same problem as

$$\underset{\beta_j}{\text{minimize}}\ \frac{1}{2n}\sum_{i=1}^{n}(r_i^{(j)} - \beta_j x_{ij})^2 + \lambda|\beta_j|$$

with

$$r_i^{(j)} = y_i - \sum_{k\neq j}\beta_k\, x_{ik}$$

The $r_i^{(j)}$ are the *partial residuals*.

$$\underset{\beta_j}{\text{minimize}}\ \frac{1}{2n}\sum_{i=1}^{n}(r_i^{(j)} - \beta_j x_{ij})^2 + \lambda|\beta_j|$$

But we know how to solve this problem:

$$\hat{\beta}_j = S_\lambda(\frac{1}{n} < x_j, r^{(j)} >).$$

This gives us a very simple *cyclic coordinate descent algorithm*

- Pick a fixed order for the coefficients (variables), e.g $1, 2, \ldots, p$.
- Cycle through the coefficient updating each with the soft thresholding formula: $\hat{\beta}_j = S_\lambda(\frac{1}{n} < x_j, r^{(j)} >)$.
- Repeat until covergence.

Simple !!!

Note:

We often want to do this for a set of λ values.

If we start with all the β_j at 0, then our initial $r^{(j)} = y$.

Thus we know that if we set

$$\lambda_{max} = max_j \ |\frac{1}{n} < x_j, y > |$$

then for that λ, and all larger, no matter what coefficient we attempted to update, we would get 0. So, there is no need to consider $\lambda > \lambda_{max}$.

So, we can,

- Start at $\lambda = \lambda_{max}$.
- Slowly decrease, λ.
- At each λ, find a solution using cyclic coordinate descent.
- *warm start*, each cyclic descent by starting at the solution from the previous λ.

Note:

Suppose our x's are orthogonal:

$$< x_i, x_j > = \; x_j' x_i = \; 0, \quad i \neq j.$$

Since we have demeaned, this is equivalent to the x's being uncorrelated.

Then,

$$< x_j, r^{(j)} > = < x_j, y >$$

So our cyclic alorgithm converges immediately to

$$\hat{\beta}_j = S_\lambda(\frac{1}{n} < x_j, y >).$$

Just as in least squares regression, we can fit the model one x at a time if the x's are uncorrelated.

9. The Elastic Net

Once you have the idea of penalized regression, you can imagine cooking up lots of different penalty specifications.

There are lots of variations in the literature, let's look at the *Elastic Net* which simply combines L1 and L2 penalties.

The motivation for the Elastic Net comes from the observation that if x's are highly corrrelated then the Lasso may behave erratically.

To see this, consider a regression where

$$y = \beta_1 x_1 + \epsilon$$

Suppose $\hat{\beta}_1 \approx 1$ works pretty well.

Suppose $x_2 \approx x_1$ and we run the regression

$$y = \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

what will happen?

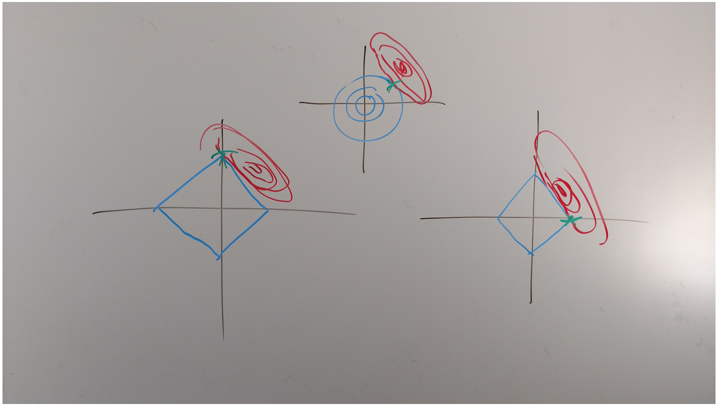
In this case any regression where $\beta_1 + \beta_2 = 1$ will fit pretty well.

Thus, we *almost* have a lack of identification.

The contours of the of the likelihood will be ellipses along the line $\beta_2 = 1 - \beta_1$ which will align with the Lasso constraint.

Thus, small changes in the data, or introduction of other x variables could swing the solution from $\beta = (1, 0)$ to $\beta = (0, 1)$ erratically.

What will the L2 penalty do?



“Elastic Net at Dawn”, McCulloch 2017.

The L2 penalty would divy up the fit 50/50 preferring a solution with $\beta = (.5, .5)$.

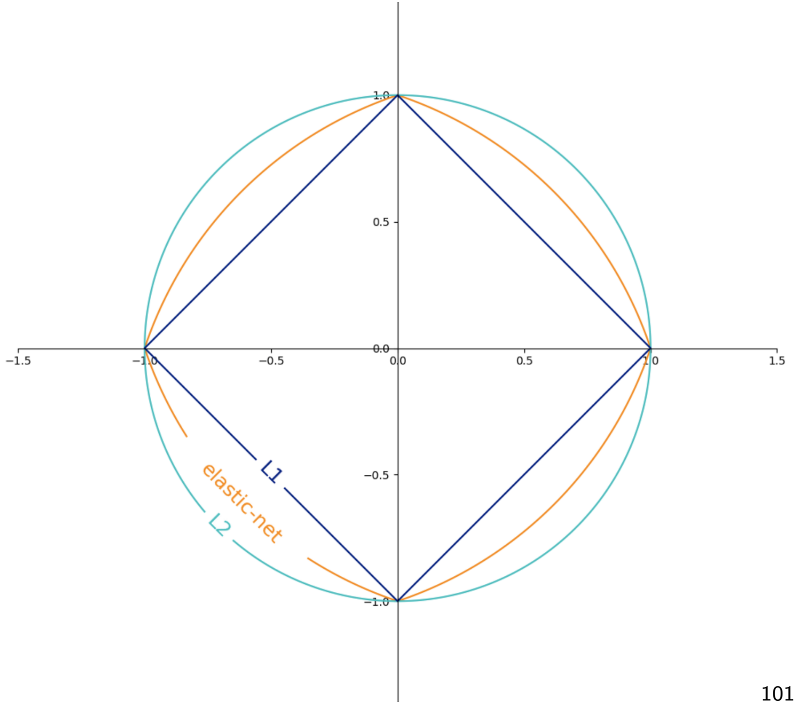
This motivates the Elastic net which just mixes in the L1 with the L2:

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ \frac{1}{2} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_j \beta_j \, x_{ij})^2 + \lambda \, [\tfrac{1}{2}(1-\alpha)||\beta||_2^2 + \alpha||\beta||_1] \right\}$$

For an individual coefficient, the penalty is then

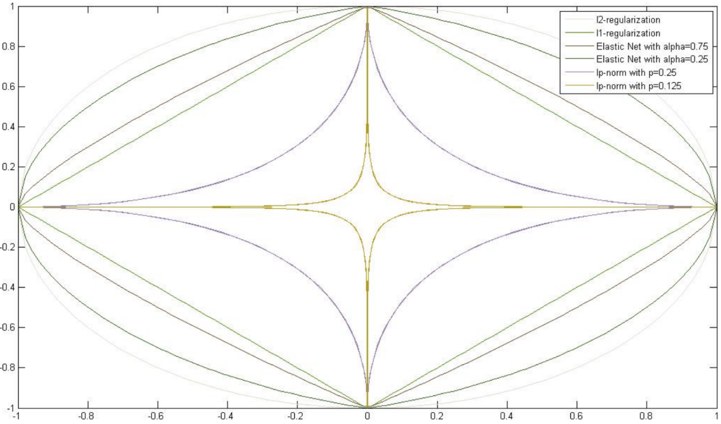
$$\lambda \, [\tfrac{1}{2} \, (1-\alpha) \, \beta_j^2 + \alpha \, |\beta_j|].$$

With the elastic net, we can still get solutions with zero coefficients, but the solution for highly correlated x variables is stabilized.

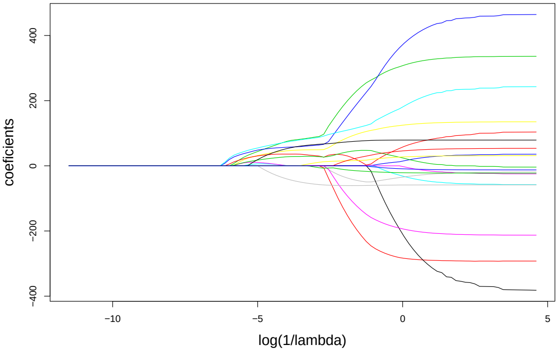


1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
L1
elastic-net
L2

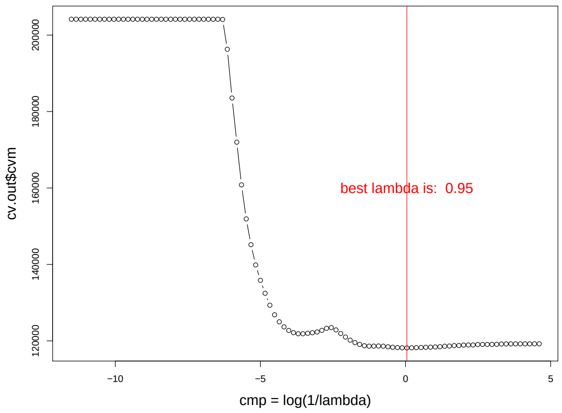
Cornell computer science:



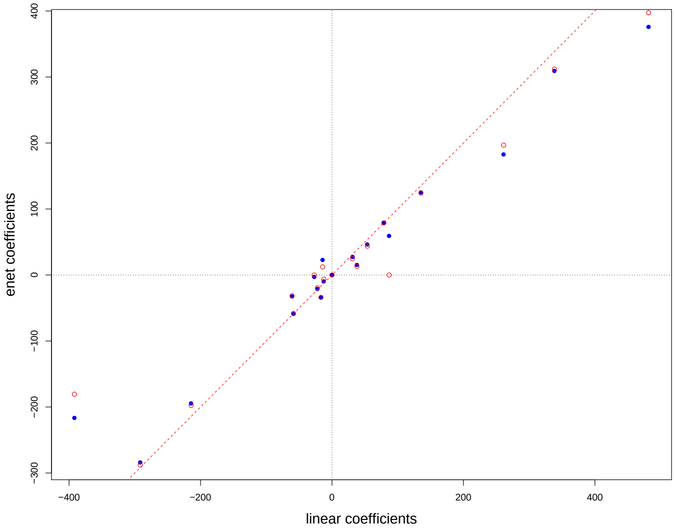
Hitters Data, Elastic net ($\alpha = .5$) solution path.



CV for elastic net.



Elastic net coefficients vs linear (blue).
Lasso net coefficients vs linear (red).



10. The Diabetes Data

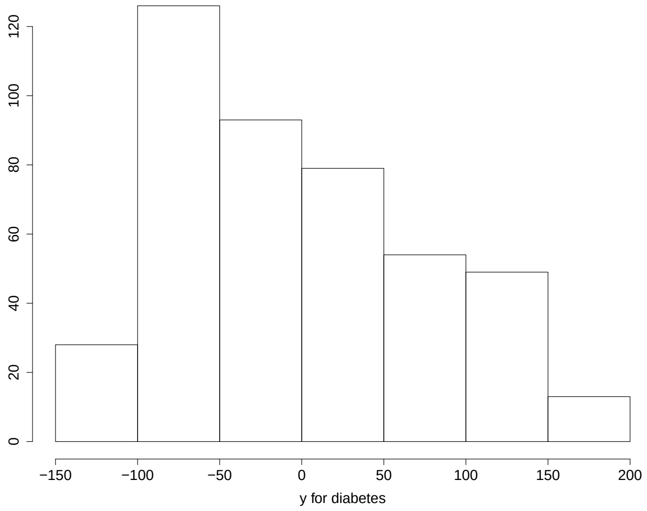
Let's look at all this stuff with the Diabetes data.

```
http://web.stanford.edu/~hastie/StatLearnSparsity/data.html

 Diabetes data
These data consist of observations on 442 patients,
with the response of interest being a quantitative
measure of disease progression one year after baseline.

There are ten baseline variables---
age, sex, body-mass index, average blood pressure,
and six blood serum measurements
---plus quadratic terms, giving a total of 64 features.
```

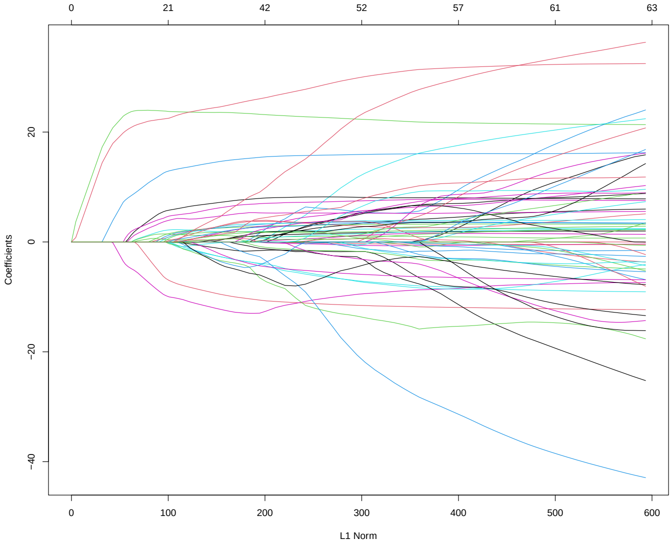
```
> 10+10+10*9/2 #linear + quadratic + interactions
[1] 65
```

But you don't square sex because it is a binary dummy so you get 64 variables.

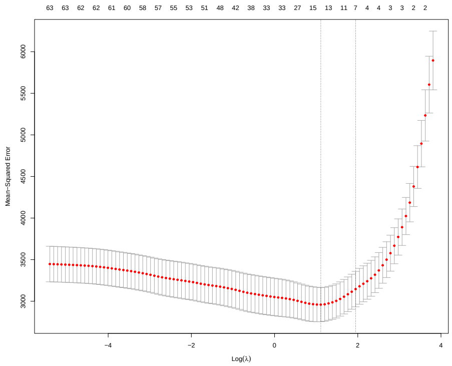
Here is the response.



Here is the Lasso coefficient plot.



Here is the Lasso cv plot.



```
[1] "minlam and minlam (1se) are:  3.0377 7.0175"
```

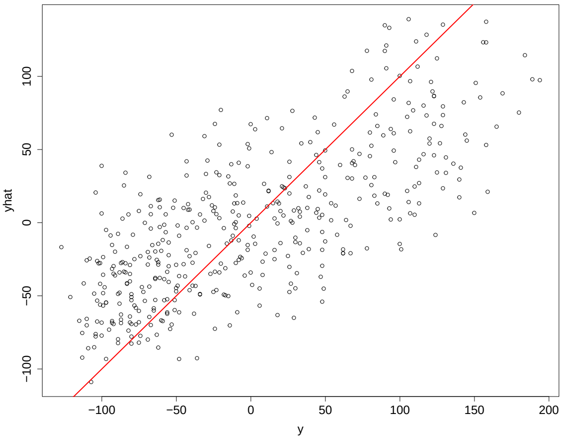
Here are the non-zero coefficents:

```
       sex        bmi        map        hdl        ltg        glu      age.2 
-5.3240588 23.8840329 11.9768009 -8.9267013 22.2766341  0.8536991  0.3510477 
     bmi.2      glu.2    age.sex    age.map    age.ltg    age.glu    bmi.map 
 1.8401302  3.3142418  5.1180918  1.4271455  0.4050495  0.5559682  4.0729018 
```

Wow.

This corresponds to a very simple nonlinear function using the 7 variables sex, bmi, map, hdl, ltg, glu, age.

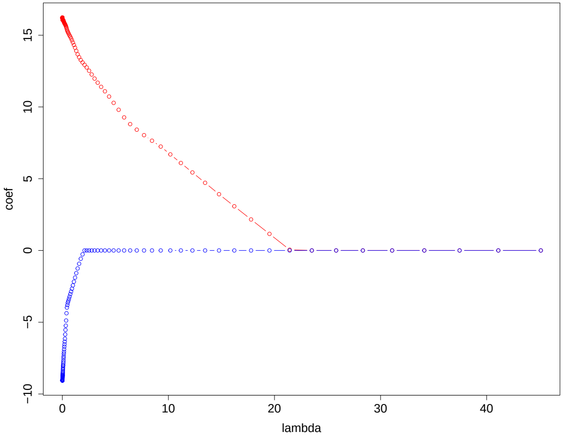
Here are the in-sample fits at the λ chosen by cv.



Can we see the effect of the shrinkage??!!

Seeing the Lasso Fit:

Here are the map and tc coefficients as functions of λ.



Notice how they look linear between knots.

Compare to Least-squares:

Suppose you do it the old multiple regression output way.

Note that *we all know you can't do variable selection by seeing which coefficients are significant*.

But that is what most people do.

```
Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept) -3.710e-08  2.532e+00   0.000   1.0000    
age          2.415e+00  3.120e+00   0.774   0.4393    
sex         -1.273e+01  3.108e+00  -4.096 5.15e-05 ***
bmi          2.194e+01  4.029e+00   5.446 9.32e-08 ***
map          1.633e+01  3.450e+00   4.734 3.13e-06 ***
tc          -1.717e+02  2.885e+03  -0.060   0.9526    
ldl          1.444e+02  2.535e+03   0.057   0.9546    
hdl          5.263e+01  1.078e+03   0.049   0.9611    
tch          3.568e+00  1.313e+01   0.272   0.7860    
ltg          8.715e+01  9.483e+02   0.092   0.9268    
glu          2.988e+00  3.352e+00   0.891   0.3733    
age.2        3.223e+00  3.308e+00   0.974   0.3305    
bmi.2        2.183e+00  3.966e+00   0.550   0.5823    
map.2       -4.028e-01  3.412e+00  -0.118   0.9061    
tc.2         3.175e+02  3.361e+02   0.945   0.3455    
ldl.2        1.706e+02  2.536e+02   0.673   0.5016    
hdl.2        8.246e+01  7.574e+01   1.089   0.2770    
tch.2        3.683e+01  2.890e+01   1.274   0.2034    
ltg.2        6.913e+01  8.239e+01   0.839   0.4019    
glu.2        5.436e+00  4.482e+00   1.213   0.2260    
age.sex      7.080e+00  3.496e+00   2.025   0.0435 *  
age.bmi     -8.596e-01  3.791e+00  -0.227   0.8208    
age.map      8.825e-01  3.633e+00   0.243   0.8082    
age.tc      -7.566e+00  2.939e+01  -0.257   0.7969    
age.ldl     -3.204e+00  2.355e+01  -0.136   0.8919    
age.hdl      9.964e+00  1.336e+01   0.746   0.4563    
age.tch      8.808e+00  1.002e+01   0.879   0.3798    
age.ltg      5.937e+00  1.066e+01   0.557   0.5778    
age.glu      2.980e+00  3.827e+00   0.779   0.4367    
```

```
sex.bmi       3.077e+00  3.710e+00   0.829   0.4074
sex.map       4.213e+00  3.559e+00   1.184   0.2373
sex.tc        2.065e+01  2.813e+01   0.734   0.4634
sex.ldl      -1.680e+01  2.233e+01  -0.752   0.4523
sex.hdl      -5.940e+00  1.304e+01  -0.455   0.6491
sex.tch      -6.249e+00  9.510e+00  -0.657   0.5115
sex.ltg      -5.666e+00  1.079e+01  -0.525   0.5996
sex.glu       2.179e+00  3.507e+00   0.621   0.5348
bmi.map       7.368e+00  4.111e+00   1.792   0.0739 .
bmi.tc       -1.438e+01  3.181e+01  -0.452   0.6514
bmi.ldl       1.150e+01  2.672e+01   0.431   0.6670
bmi.hdl       5.807e+00  1.571e+01   0.370   0.7118
bmi.tch      -1.593e+00  1.099e+01  -0.145   0.8849
bmi.ltg       5.461e+00  1.219e+01   0.448   0.6544
bmi.glu       1.113e+00  4.335e+00   0.257   0.7975
map.tc        2.278e+01  3.249e+01   0.701   0.4837
map.ldl      -1.556e+01  2.735e+01  -0.569   0.5698
map.hdl      -8.919e+00  1.474e+01  -0.605   0.5455
map.tch      -2.776e+00  9.457e+00  -0.294   0.7693
map.ltg      -7.371e+00  1.295e+01  -0.569   0.5696
map.glu      -6.356e+00  4.348e+00  -1.462   0.1447
tc.ldl       -4.435e+02  5.605e+02  -0.791   0.4294
tc.hdl       -1.872e+02  1.817e+02  -1.030   0.3036
tc.tch       -1.050e+02  8.390e+01  -1.252   0.2113
tc.ltg       -1.810e+02  6.270e+02  -0.289   0.7730
tc.glu       -8.395e+00  2.836e+01  -0.296   0.7673
ldl.hdl       1.258e+02  1.508e+02   0.835   0.4045
ldl.tch       5.747e+01  7.002e+01   0.821   0.4124
ldl.ltg       1.320e+02  5.219e+02   0.253   0.8004
ldl.glu       4.077e+00  2.405e+01   0.170   0.8655
hdl.tch       5.659e+01  4.773e+01   1.186   0.2365
hdl.ltg       6.988e+01  2.195e+02   0.318   0.7504
hdl.glu       1.036e+01  1.413e+01   0.733   0.4640
tch.ltg       1.856e+01  2.975e+01   0.624   0.5330
tch.glu       1.122e+01  1.119e+01   1.003   0.3167
ltg.glu       3.977e+00  1.261e+01   0.316   0.7525
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

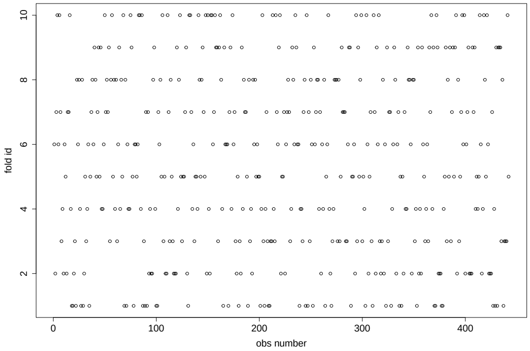
Only 4 variables are “significant”

Comparing Lasso, Ridge, and Elastic-Net:

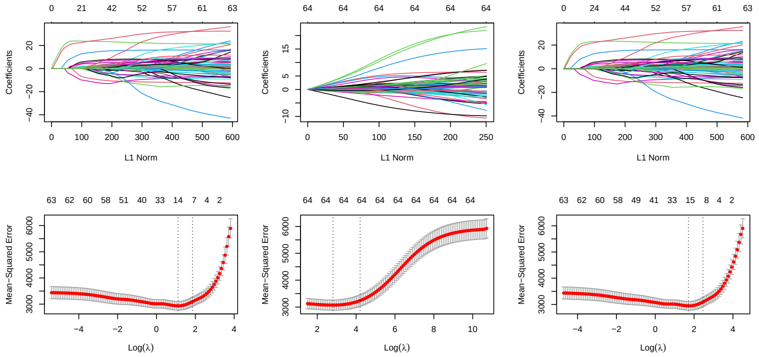
Let's try Lasso, Ridge, and elastic-net with $\alpha = .5$ and see which seems to work best.

To do this we will have to give cv.glmnet a prechosen set of cv folds.

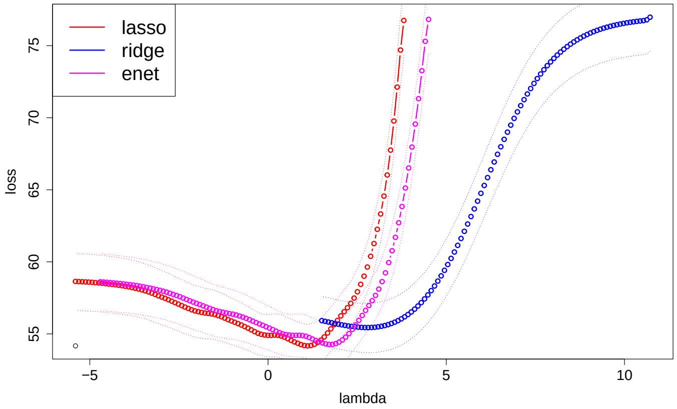
Here is a set of folds for 10-fold cv.



Left to right, Lasso, Ridge, Elastic(.5).



I took the square root of the loss measures so that we are looking at RMSE.



It looks like Lasso and Enet are similar and better than Ridge, but, as a *practical matter* they are all about the same.

Seeing the Ridge Fit:

To check our understanding of the Ridge fit, we let $x_1 = bmi$ and $x_{2.1}$ be the standardized residuals from regressing map on bmi.

```
x1 = x[,3]; x2 = x[,4]
x2.1 = x2-(sum(x1*x2)/sum(x1^2))*x1
x2.1 = scale(x2.1)
```

Then we should have

$$\hat{\beta}_\lambda = \frac{\hat{\beta}}{(1 + c\,\lambda)}$$

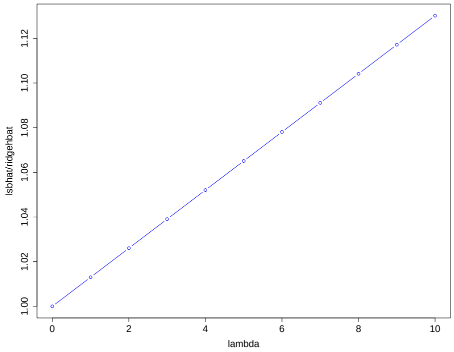
where

$$\hat{\beta} = \frac{< x, y >}{< x, x >}$$

and c depends on exactly how the penalty was scaled.

Below is a plot of

$$\frac{\hat{\beta}}{\hat{\beta}_\lambda} \text{ versus } \lambda.$$



Does indeed look like

$$\frac{\hat{\beta}}{\hat{\beta}_\lambda} = 1 + c\,\lambda.$$

BIC and Forward Step-Wise:

Let's try BIC and forward stepwise.

First note that if you run the regression without the transformations, that is with just the 10 x variables, then

BIC$=$ 3584.648 (with 11 parameters).

With all the transformations

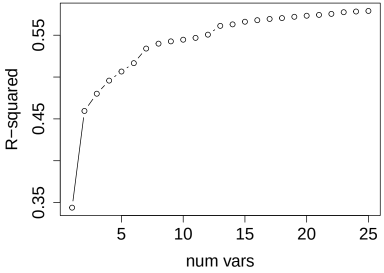
BIC $=$ 3839.201 (with 65 parameters, counting the intercept).

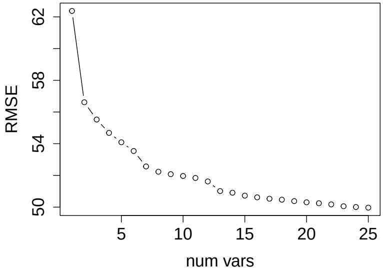
If we run forwards step-wise using BIC as our greedy loss and stopping criterion we get the model:

```
Call:
lm(formula = y ~ bmi + ltg + map + age.sex + bmi.map + hdl +
    sex, data = ddf)

Residuals:
     Min       1Q   Median       3Q      Max
-150.077  -39.269   -1.481   32.423  139.891

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -3.710e-08  2.523e+00   0.000 1.000000
bmi          2.481e+01  3.039e+00   8.165 3.53e-15 ***
ltg          2.406e+01  3.069e+00   7.840 3.53e-14 ***
map          1.477e+01  2.952e+00   5.004 8.16e-07 ***
age.sex      8.892e+00  2.552e+00   3.484 0.000545 ***
bmi.map      8.385e+00  2.552e+00   3.286 0.001100 **
hdl         -1.324e+01  3.063e+00  -4.323 1.91e-05 ***
sex         -1.133e+01  2.811e+00  -4.029 6.61e-05 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 53.05 on 434 degrees of freedom
Multiple R-squared:  0.534,Adjusted R-squared:  0.5265
F-statistic: 71.05 on 7 and 434 DF,  p-value: < 2.2e-16
```

which has 7 terms and the variables bmi, ltg, map, age, sex, hdl.
Almost the same as Lasso!
BIC for forward model is 3551.2, with 8 parameters.

Here are the in-sample R-squared and RMSE from the foward-stepwise:

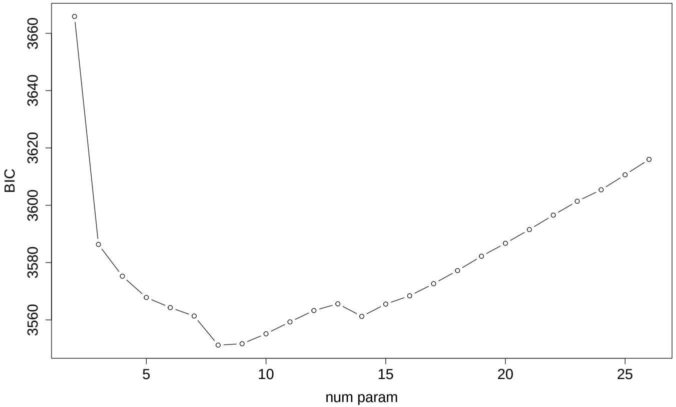




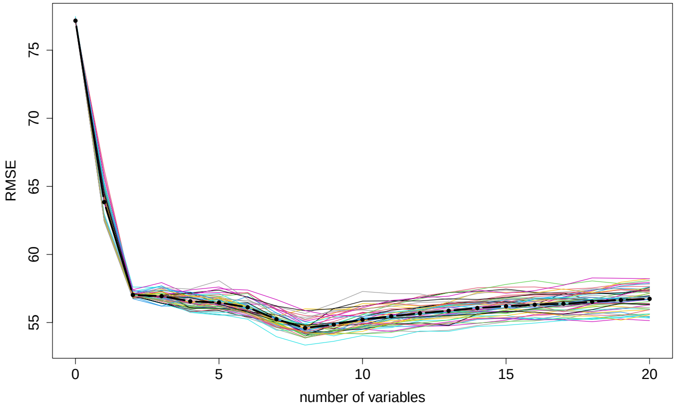
And the names of the variables as they come in:

```
 [1] "bmi"      "ltg"      "map"      "age.sex" "bmi.map" "hdl"      "sex"
 [8] "glu.2"    "age.2"    "map.glu" "tc"       "ldl"      "ltg.2"    "age.ldl"
[15] "age.tc"   "sex.map" "glu"      "tch"      "sex.tch" "sex.bmi" "tc.tch"
[22] "tch.glu" "hdl.glu" "map.tc"   "bmi.ltg"
```

Here are the BIC's of the models found by forward stepwise.



Here are the RMSE's from 50 runs of 10-fold cv using forwards step.
Remember, our knob is how many steps to take = number of variables



55 again !!!

So, the methods are giving very similar results,

except for the p-values stuff.