Regression III: Computing a Good Estimator with Regularization

-Applied Multivariate Analysis-

Lecturer: Darren Homrighausen, PhD

Another way to choose the model

Let (X_0, Y_0) be a new observation that has the same properties as our sample D_n, but is independent of it.

Remember (prediction) risk: $\mathrm{pred}(\hat\beta) = \mathbb{E}(Y_0 - X_0^\top \hat\beta)^2$

The idea is to find a $\hat\beta$ from the sample D_n and then predict at a new observation to see how good of a job we've done.

We don't have any such new observation

So, we use some approximations to pred instead (AIC, BIC, etc.).

An intuitive idea

What if instead we tried a different idea?

Let's set aside one observation and predict it

Example: Set aside (X_1, Y_1) and fit $\hat{\beta}^{(1)}$ on $(X_2, Y_2), \ldots, (X_n, Y_n)$

(The notation $\hat{\beta}^{(1)}$ just symbolizes leaving out the first observation before fitting $\hat{\beta}$)

Now, let's look at the (test) MSE of $\hat{\beta}^{(1)}$

$$\mathrm{MSE}_1 = (Y_1 - X_1^\top \hat{\beta}^{(1)})^2$$

An intuitive idea

As the left off data point is independent of the data points used for estimation,

$$\mathbb{E}\mathrm{MSE}_1 = \mathrm{pred}(\hat{\beta}_{D_{\mathrm{train}}}) \approx \mathrm{pred}(\hat{\beta}_{D_n})$$

Where

- $D_{\mathrm{train}} = \{(X_2, Y_2), \ldots, (X_n, Y_n)\}$
- $D_{\mathrm{test}} = \{(X_1, Y_1)\}$
- $\hat{\beta}_{D_{\mathrm{train}}}$ is $\hat{\beta}$ trained only with observations in D_{train}
- $\hat{\beta}_{D_n} = \hat{\beta}$ is the estimator trained on all the data

An intuitive idea

Why stop there? We can do the same thing with the second observation as well:

$$\mathrm{MSE}_2 = (Y_2 - X_2^\top \hat{\beta}^{(2)})^2$$

Repeating the notation as for MSE_1....

An intuitive idea

$$\mathbb{E}\mathrm{MSE}_2 = \mathrm{pred}(\hat{\beta}_{D_{\mathrm{train}}}) \approx \mathrm{pred}(\hat{\beta}_{D_n})$$

Where

- $D_{\mathrm{train}} = \{(X_1, Y_1), (X_3, Y_3) \ldots, (X_n, Y_n)\}$
- $D_{\mathrm{test}} = \{(X_2, Y_2)\}$
- $\hat{\beta}_{D_{\mathrm{train}}}$ is $\hat{\beta}$ trained only with observations in D_{train}
- $\hat{\beta}_{D_n} = \hat{\beta}$ is the estimator trained on all the data

Cross-Validation

We can use this idea to form an estimate of pred

It is known as (leave-one-out) cross-validation[1]

$$\mathrm{CV}(\hat{\beta}) = \frac{1}{n}\sum_{i=1}^{n} \mathrm{MSE}_i = \frac{1}{n}\sum_{i=1}^{n}(Y_i - X_i^\top \hat{\beta}^{(i)})^2.$$

Now, we have another risk estimate minimize CV

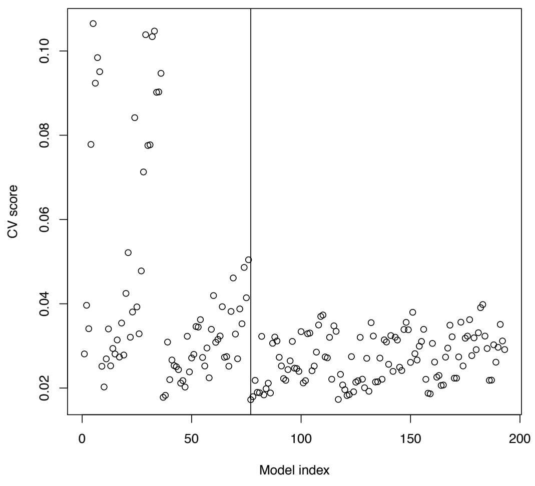
[1]We'll get to the leave-one-out part in a moment.

Let's look at CV in action

I wrote two functions, which are in the file 1_CVfunc.r (check the website) for doing model selection with cross-validation.

Here is an example on the Prostate data:

```
source('1_CVfunc.r')
validationSets = 1:n
cv = CVfunc(X,Y,n,validationSets,models)
```



Let's look at CV in action

Results:

```
> models[which.min(cv),]
    1      2      3      4      5      6      7      8
 TRUE   TRUE FALSE   TRUE   TRUE FALSE FALSE FALSE
> names(X)[models[which.min(cv),]]
[1] "lcavol"  "lweight" "lbph"    "svi"
```

In this case, we have come up with a model in between all subsets regression and its greedy approximations.

More general cross-validation procedures

There are two strong disadvantages to cross-validation as we defined it:

$$\mathrm{CV}(\hat{\beta}) = \frac{1}{n}\sum_{i=1}^{n}(Y_i - X_i^\top \hat{\beta}^{(i)})^2$$

These are:

- It is computationally demanding (we need to fit n different times).
- It is an unbiased estimator of $\mathrm{pred}(\hat{\beta}_{n-1})$
  (which means it can be very high variance)

K-Fold cross-validation

A commonly used compromise is to randomly divide your data into K groups.

Let $v_1, \ldots, v_K$ correspond to these groups.

For Example: If we have data Z_1, Z_2, Z_3, Z_4, Z_5, then we can have $K = 2$, and $v_1 = \{2, 5\}$ and $v_2 = \{1, 3, 4\}$

Then, we can form

$$CV_K(\hat{\beta}) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{|v_k|} \sum_{i \in v_k} (y_i - X_i^\top \hat{\beta}^{(v_k)})^2.$$

(For CV, $K = ?$ and $v_i = ?$)

K-Fold cross-validation

A commonly used compromise is to randomly divide your data into K groups.

Let $v_1, \ldots, v_K$ correspond to these groups.

For Example: If we have data Z_1, Z_2, Z_3, Z_4, Z_5, then we can have $K = 2$, and $v_1 = \{2, 5\}$ and $v_2 = \{1, 3, 4\}$

Then, we can form

$$CV_K(\hat{\beta}) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{|v_k|} \sum_{i \in v_k} (y_i - X_i^\top \hat{\beta}^{(v_k)})^2.$$

(For CV, $K = \ n$ and $v_i = \{i\}$)

Retrospective summary

In the previous slides, we took a set of p predictors and reduced them to smaller set of variables using AIC, AICc, BIC, CV,....

There are three main reasons for this:

- Interpretability: It is much easier (and convincing) to decide that a few variables are the 'main' contributors to a response variable of interest.
- Prediction accuracy: Including larger number of variables reduces bias but increases variance. If we include too many, we can't predict well.
- Parsimony: Some variables are unrelated to the response in any meaningful way and we would like to remove them.

Regularization

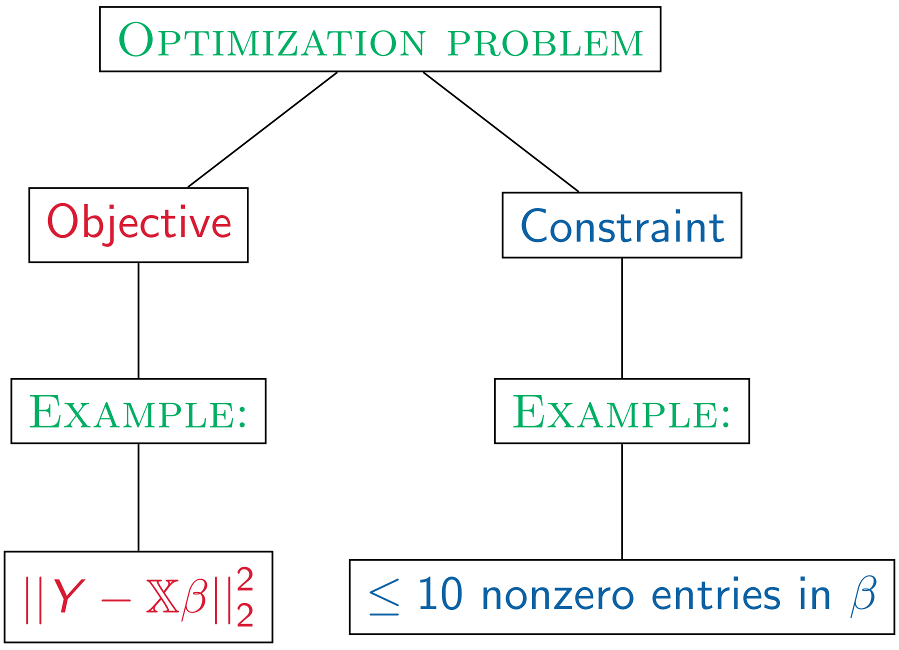
Regularization

Another way to control bias and variance is through regularization or shrinkage.

The idea is to make your estimates of β ‘smaller’, rather than set them to zero

(which is what all subsets does)

Some optimization terms



Optimization problem
Objective
Constraint
Example:
Example:
$||Y - \mathbb{X}\beta||_2^2$
$\leq$ 10 nonzero entries in β

A (contrained) optimization problem is phrased as

$$\min \ell(\beta) \text{ subject to } C(\beta)$$

where

- $\ell(\beta)$ is the objective function
- $C(\beta)$ is the constraint

Regularization

One way to do this for regression is via constraining squared error

$$\hat{\beta}_{\text{ridge},t} = \underset{||\tilde{\beta}||_2^2 \leq t}{\text{argmin}} ||Y - \mathbb{X}\tilde{\beta}||_2^2$$

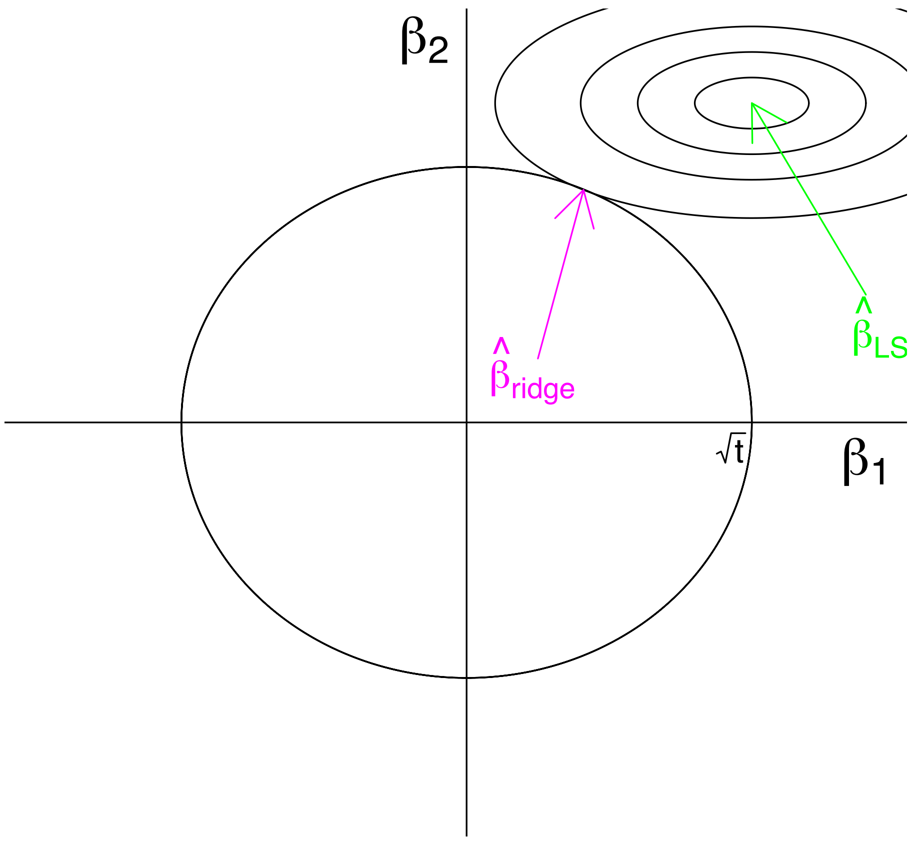
for any $t \geq 0$.

This procedure is called ridge regression

Compare this to least squares

$$\hat{\beta}_{LS} = \underset{\tilde{\beta} \in \mathbb{R}^p}{\text{argmin}} ||Y - \mathbb{X}\tilde{\beta}||_2^2$$

Geometry of ridge regression in $\mathbb{R}^2$



Ridge regression

An equivalent way to write

$$\hat{\beta}_{\text{ridge},t} = \underset{||\beta||_2^2 \leq t}{\text{argmin}} ||Y - \mathbb{X}\beta||_2^2 \tag{1}$$

is in the Lagrangian form

$$\hat{\beta}_{\text{ridge},\lambda} = \underset{\beta}{\text{argmin}} ||Y - \mathbb{X}\beta||_2^2 + \lambda||\beta||_2^2. \tag{2}$$

For every λ' there is a unique t' (and vice versa) that makes

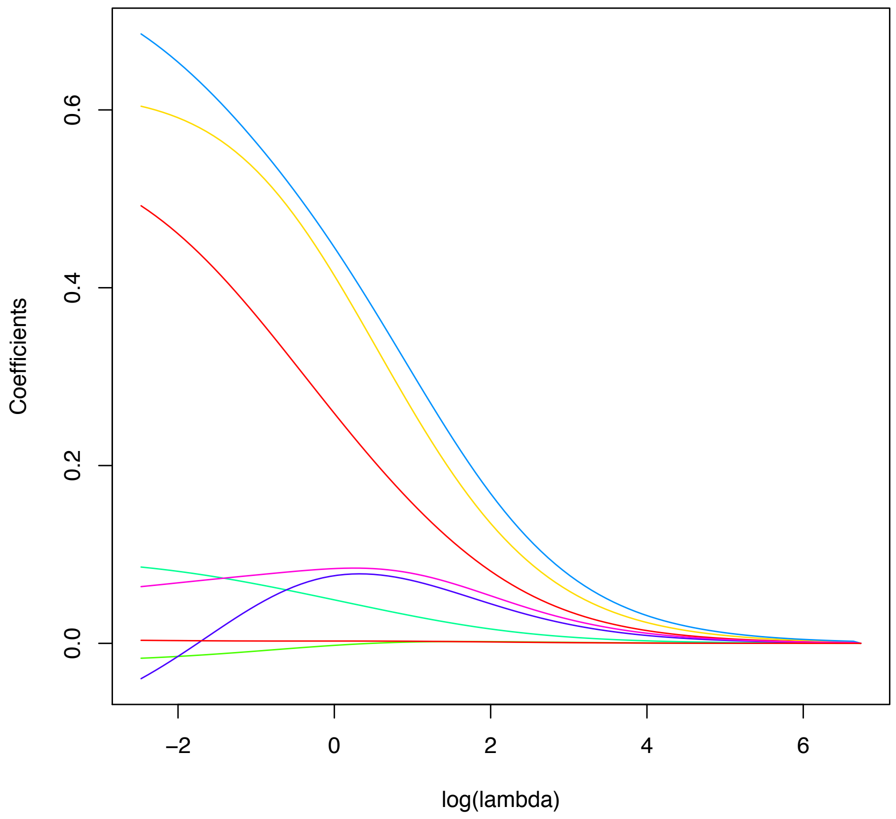
$$\hat{\beta}_{\text{ridge},\lambda'} = \hat{\beta}_{\text{ridge},t'}$$

Observe:

- $\lambda = 0$ (or $t = \infty$) makes $\hat{\beta}_{\text{ridge},\lambda=0} = \hat{\beta}_{LS}$
- Any $\lambda > 0$ (or $t < \infty$) penalizes larger values of β, effectively shrinking them.

Note: λ and t are known as tuning parameters

Ridge regression path



Regularization and Rescaling

Least squares is invariant to rescaling

Example: Let's multiply our design matrix by a factor of 10 to get $\tilde{\mathbb{X}} = 10\mathbb{X}$. Then:

$$\tilde{\beta}_{\text{OLS}} = (\tilde{\mathbb{X}}^\top \tilde{\mathbb{X}})^{-1}\tilde{\mathbb{X}}^\top Y = \frac{1}{10}(\tilde{\mathbb{X}}^\top \tilde{\mathbb{X}})^{-1}\tilde{\mathbb{X}}^\top Y = \frac{\hat{\beta}_{\text{OLS}}}{10}$$

So, multiplying our data by ten just results in our estimates being reduced by one tenth.

Hence, any prediction is left unchanged:

$$\tilde{\mathbb{X}}\tilde{\beta}_{\text{OLS}} = \mathbb{X}\hat{\beta}_{\text{OLS}}$$

This means, for instance, if we have a covariate measured in miles, then we will get the "same" answer if we change it to kilometers

Least squares is invariant to rescaling: example

```
n = 20
set.seed(1)
X = runif(n,0,1)
Y = X*1.5 + rnorm(n,0,.25)
Xtilde    = 2*X
Ytilde    = Y - mean(Y)
```

Least squares is invariant to rescaling: example

```
>summary(lm(formula = Y ~ X))
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   0.1065     0.1265   0.842    0.411
X             1.3341     0.2036   6.554  3.7e-06 ***

> summary(lm(formula = Y ~ Xtilde))
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   0.1065     0.1265   0.842    0.411
Xtilde        0.6671     0.1018   6.554  3.7e-06 ***

> summary(lm(formula = Ytilde ~ Xtilde))
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  -0.7407     0.1265  -5.857 1.51e-05 ***
Xtilde        0.6671     0.1018   6.554 3.70e-06 ***
```

Ridge regression is not invariant to rescaling

(See next few slides for how to compute the ridge solution via SVD as below)

```
u = X/sqrt(sum(X**2))
d = sqrt(sum(X**2))
lam = 1
betaHat   = (d/(d+lam))*u%*%Y
> print(betaHat)
        [,1]
[1,] 3.03864

u = Xtilde/sqrt(sum(X**2))
d = sqrt(sum(Xtilde**2))
lam = 1
betaTilde = (d/(d+lam))*u%*%Y
> print(betaTilde)
         [,1]
[1,] 7.004142
> print(betaHat*2)
        [,1]
[1,] 6.07728
```

Ridge regression is not invariant to rescaling

So, we need to choose a scale before we fit.

The agreed upon scale is to make each column of $\mathbb{X}$ have

- Zero (sample) mean and
- (sample) standard deviation 1.

This can be easily done in R via the 'scale' function:

```
X = scale(X,center=T,scale=T)
```

The scale function

Note: A nice part of about the scale function is that it keeps the scalings:

```
X = runif(20,0,1)
X = scale(X,center=T,scale=T)
> attributes(X)
$dim
[1] 20  1

$‘scaled:center‘
[1] 0.5551671

$‘scaled:scale‘
[1] 0.2861179

> attributes(X)$’scaled:center’
[1] 0.5551671
```

Ridge regression

Ridge regression

RECALL: The least squares solution can be written

$$\hat{\beta}_{\mathrm{LS}} = (\mathbb{X}^\top \mathbb{X})^{-1} \mathbb{X}^\top Y$$

It turns out through differential calculus, we can write out the ridge regression solution as well:

$$\hat{\beta}_{\mathrm{ridge},\lambda} = (\mathbb{X}^\top \mathbb{X} + \lambda I)^{-1} \mathbb{X}^\top Y$$

Quite similar!

However, the λ can make all the difference..

Regularization - Ridge Regression

Using the SVD[2] ($\mathbb{X} = UDV^\top$), we can look even deeper.

$$\hat{\beta}_{\mathrm{LS}} = (\mathbb{X}^\top\mathbb{X})^{-1}\mathbb{X}^\top Y = VD^{-1}U^\top Y \qquad = \sum_{j=1}^{p} \mathbf{v}_j \left(\frac{1}{d_j}\right) \mathbf{u}_j^\top Y$$

$$\hat{\beta}_{\mathrm{ridge},\lambda} = (\mathbb{X}^\top\mathbb{X} + \lambda I)^{-1}\mathbb{X}^\top Y = V(D^2 + \lambda I)^{-1}DU^\top Y \quad = \sum_{j=1}^{p} \mathbf{v}_j \left(\frac{d_j}{d_j^2 + \lambda}\right) \mathbf{u}_j^\top Y$$

Ridge shrinks the data by an additional factor of λ

To see this, note:

$$\begin{aligned}
(\mathbb{X}^\top\mathbb{X})^{-1}\mathbb{X}^\top &= (VD\underbrace{U^\top U}_{=I}DV^\top)^{-1}VDU^\top \\
&= (VD^2V^\top)^{-1}VDU^\top \\
&= VD^{-2}\underbrace{V^\top V}_{=I}DU^\top = VD^{-1}U^\top
\end{aligned}$$

[2]This is after centering/scaling

Ridge Regression: Computation

There are several ways to compute ridge regression

We can follow any conventional least squares solving technique (i.e.: QR factorization, Cholesky Decomposition, SVD,...):

$$(\mathbb{X}^\top \mathbb{X} + \lambda I)\beta = \mathbb{X}^\top Y$$

This can be computed via many techniques, for instance the solve function in R

$$Ax = b \;\Rightarrow\; \texttt{solve(A, b)}$$

Ridge Regression: Computation

Alternatively, we can actually solve it using lm in R if we make the following augmentation

$$\tilde{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \\ 0 \\ \vdots \\ 0 \end{bmatrix} \in \mathbb{R}^{n+p} \text{ and } \tilde{\mathbb{X}} = \begin{bmatrix} \mathbb{X} \\ \sqrt{\lambda} I \end{bmatrix}$$

```
lm(tildeY ~ ., data = Xtilde)
```

(To see this, multiply out $(\tilde{\mathbb{X}}^\top \tilde{\mathbb{X}})^{-1} \tilde{\mathbb{X}}^\top \tilde{Y}$ and note that it equals $(\mathbb{X}^\top \mathbb{X} + \lambda I)^{-1} \mathbb{X}^\top Y$)

Ridge Regression: Recap

Important:

- As the constraint set is a sphere, each direction is treated equally. You should standardize your coefficient before fitting.
- Likewise, if included, don't penalize the intercept. If the sample means of the covariates are zero, then make the response have mean zero as well (and don't include intercept)

  This means either

  - solve
  $$\min_{\beta} ||Y - (\beta_0 \mathbf{1} + \mathbb{X}\beta)||_2^2 + \lambda ||\beta||_2^2$$
  - or standardize $\mathbb{X}$ and center Y by $\overline{Y}$

Ridge Regression with glmnet

Another way in R to do ridge regression is through glmnet

```
install.packages('glmnet')
library(glmnet)

Y = prostate$lpsa
X = as.matrix(prostate[,names(prostate)!=c('lpsa','train')])
X.df = prostate[,names(prostate)!=c('lpsa','train')]

ridge.out = glmnet(x=X,y=Y,alpha=0)
```

Note: Turning $\mathbb{X}$ into a matrix data structure is crucial!

(Note that for lm, the opposite is true, $\mathbb{X}$ must be a data.frame)

```
> ridge.out = glmnet(x=X.df,y=Y,alpha=0)
Error in elnet(x, is.sparse, ix, jx, y, weights, offset, ...
  (list) object cannot be coerced to type 'double'
```

Ridge Regression with glmnet

```
> names(ridge.out)
 [1] "a0"         "beta"       "df"         "dim"        "lambda"
 [6] "dev.ratio"  "nulldev"    "npasses"    "jerr"       "offset"
[11] "call"       "nobs"

> length(ridge.out$lambda)
[1] 100

> ridge.out$lambda[c(1,2,3,4,99,100)]
[1] 843.42743826 768.49966923 700.22827669 638.02192650
[5]   0.09256606   0.08434274
```

Ridge Regression with glmnet

To get the ridge solution at a particular λ value, say 10, do not do:

```
ridge.out = glmnet(x=X,y=Y,alpha=0,lambda=10)
```

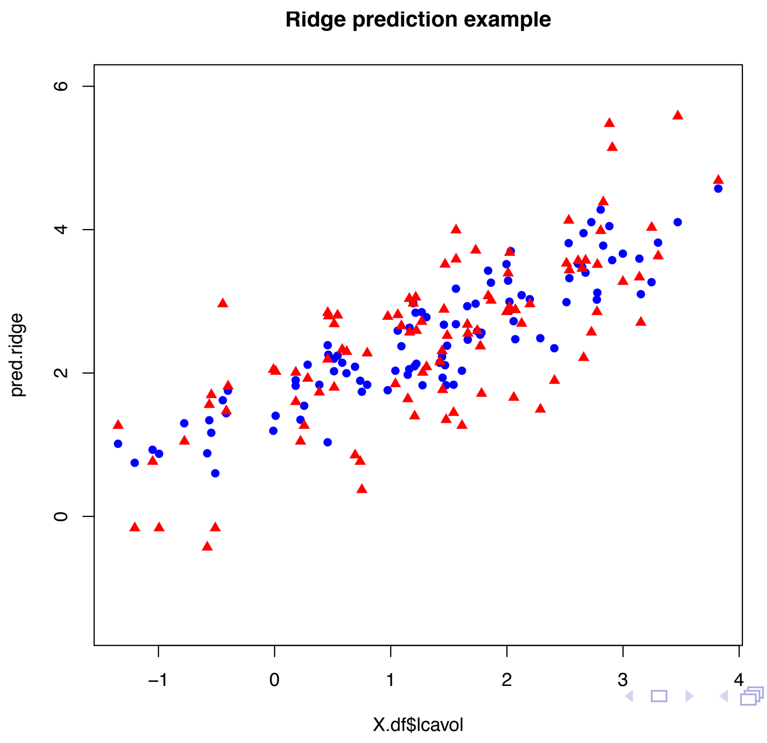
The numerical properties of glmnet require running over entire grid.

Instead, use the coef or predict functions

```
> coef(ridge.out,s=10)
9 x 1 sparse Matrix of class "dgCMatrix"
                      1
(Intercept) 1.535925340
lcavol      0.064472545
lweight     0.106714247
age         0.001718621
lbph        0.012833216
svi         0.135482215
lcp         0.036522691
gleason     0.044727284
pgg45       0.001325149
```

Ridge Regression with glmnet

```
pred.ridge = predict(ridge.out,X,s=.01)

plot(X.df$lcavol,pred.ridge,ylim=c(-5,5),pch=16,col='blue')
points(X.df$lcavol,Y,col='red',pch=17)
```



Choosing λ

Ridge Regression: picking the tuning parameter

The crucial choice with regularization is how large to set the tuning parameter λ.

While we can use AIC or BIC for this, conventionally people use cross-validation instead.

Think of CV_K as a function of λ, and pick its minimum:

$$\hat{\lambda} = \underset{\lambda \geq 0}{\text{argmin}}\, CV_K(\lambda)$$

and we will use the estimator $\hat{\beta}_{\text{ridge},\hat{\lambda}}$

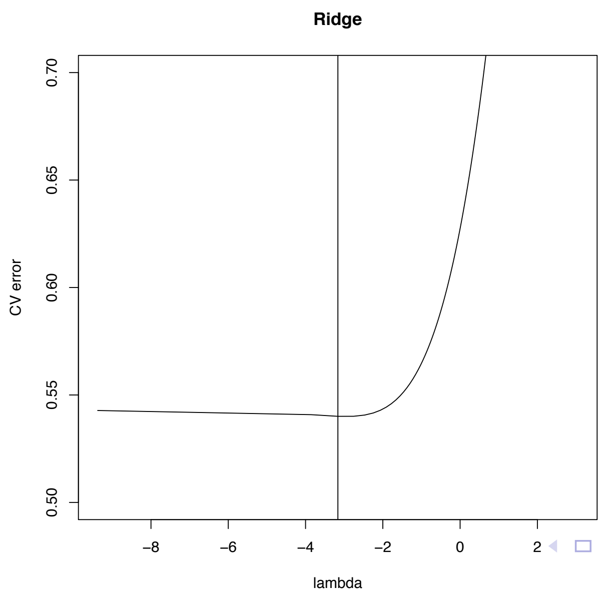
Ridge Regression: CV

We can do this easily with glmnet via the function cv.glmnet

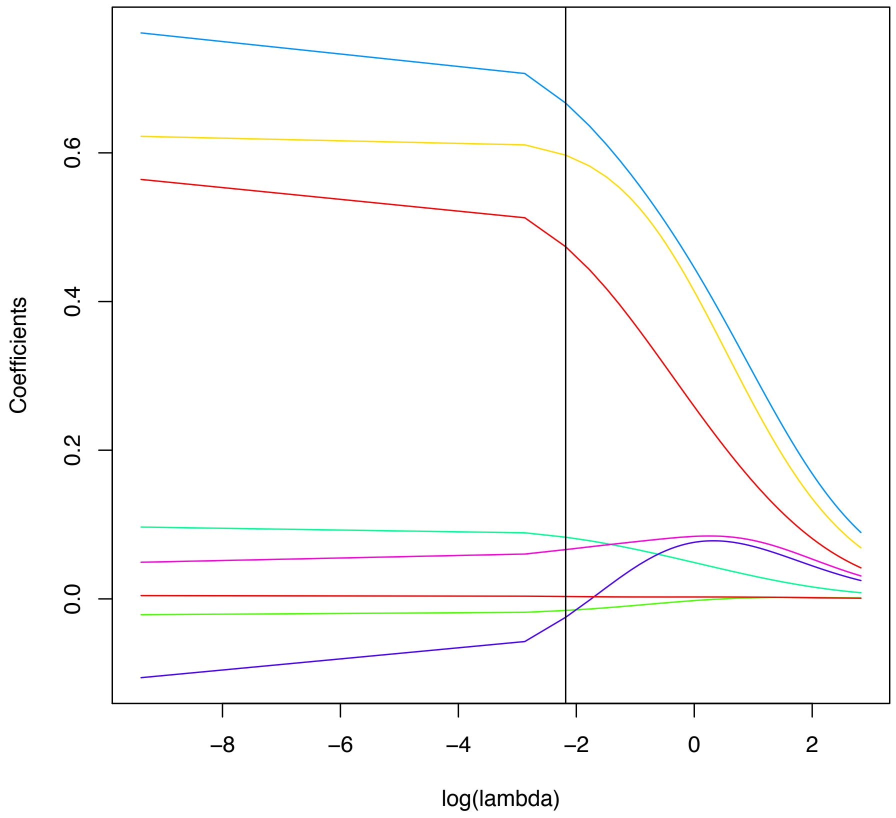
```
X = as.matrix(X)
> ridge.cv    = cv.glmnet(x=X,y=Y,alpha=0)
> names(ridge.cv)
 [1] "lambda"      "cvm"          "cvsd"         "cvup"
 [5] "cvlo"        "nzero"        "name"         "glmnet.fit"
 [9] "lambda.min"  "lambda.1se"
> ridge.out   = ridge.cv$glmnet.fit
```

Ridge Regression: CV

```
lambda.hat = ridge.cv$lambda[which.min(ridge.cv$cvm)]
plot(ridge.cv$lambda,ridge.cv$cvm,
     xlab='lambda',ylab='CV error',main='Ridge',type='l')
abline(v=lambda.hat)

> print(log(lambda.hat))
[1] -2.243919
```



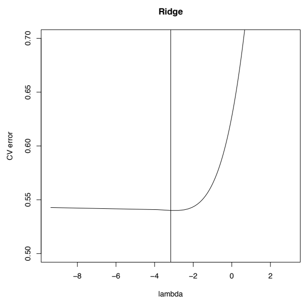
Ridge regression: CV



Some comments about glmnet

Some further details

- Note that in this figure:



  many solutions have almost the same CV error

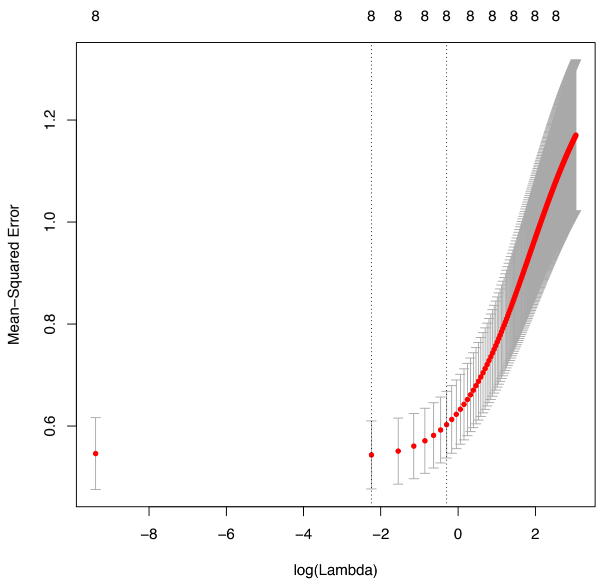
  In fact, since CV is a pred estimate, it is random
- The lower end point of the grid is somewhat arbitrary chosen

Some comments about glmnet

The function cv.glmnet comes with a plotting function

```
ridge.cv    = cv.glmnet(x=X,y=Y,alpha=0)
plot(ridge.cv)
```

Some comments about glmnet



- The left-most dashed, vertical line occurs at the *CV* minimum
- The right-most dashed, vertical line is the
  - largest value of λ ...
  - such that the error is within one standard-error of the minimum

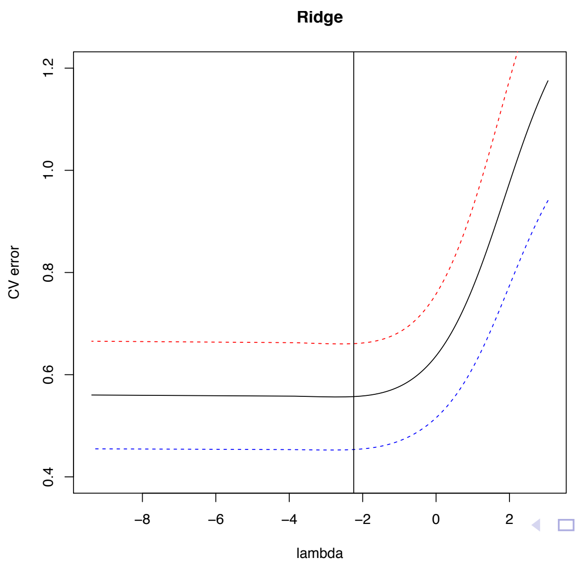
(the so called one-standard-error rule. We'll see this is more important with a related method soon)

Some comments about glmnet

Alternatively, you can demand a 'significant' amount of CV reduction to discard full model

(By full model, I mean the model with all covariates)

```
plot(log(ridge.cv$lambda),ridge.cv$cvm,
     xlab='lambda',ylab='CV error',main='Ridge',
     type='l',ylim=c(.4,1.2))
lines(log(ridge.cv$lambda),ridge.cv$cvup,col="red",lty=2)
lines(log(ridge.cv$lambda),ridge.cv$cvlo,col="blue",lty=2)
```



Some comments about glmnet

The way that glmnet works is to

1. form a grid of λ values,
2. find the cross-validation error for each ridge solution on that grid
3. compute the minimum cross-validated λ: $\hat{\lambda}$
4. report $\hat{\beta}_{\text{ridge},\hat{\lambda}}$ as the final solution

The important piece is that the final solution depends on which grid we choose

Some comments about glmnet

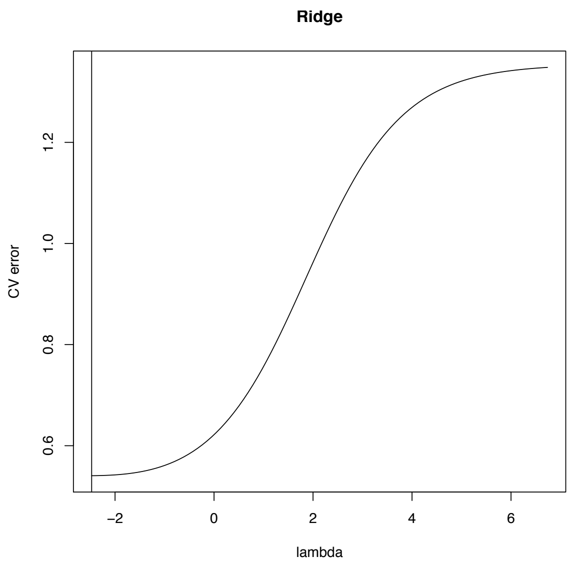
Unfortunately, there is not a good way to define both end points of this grid

(We will see later that for the lasso the grid is easier to define, but can have some of the same problems)

Important: The minimum value of the grid is chosen arbitrarily

Some comments about glmnet

Example of a bad minimum

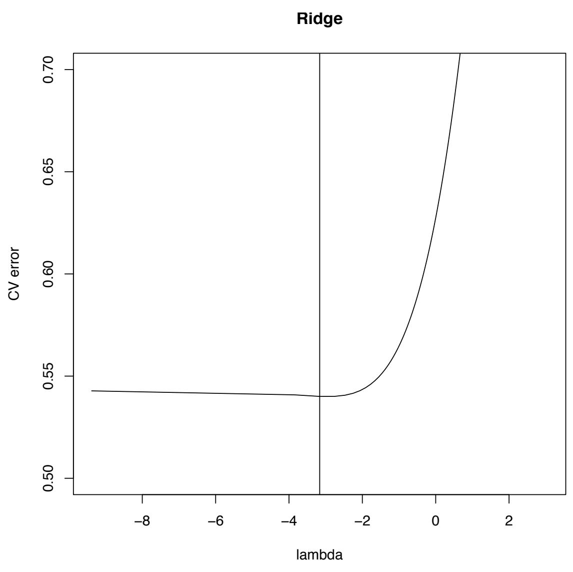


How to fix it:

```
ridge.cv    = cv.glmnet(x=X,y=Y,alpha=0)
min.lambda = min(ridge.cv$lambda)
lambda.new = seq(min.lambda*250,min.lambda*.001,length=1000)
ridge.cv    = cv.glmnet(x=X,y=Y,alpha=0,lambda=lambda.new)
lambda.hat = ridge.cv$lambda[which.min(ridge.cv$cvm)]
```

Some comments about glmnet

New minimum, after moving λ grid smaller:



Multicollinearity

Ridge regression and multicollinearity

Multicollinearity is a phenomenon in which a combination of predictor variables is extremely similar to another predictor variable. Some comments:

- A better term that is sometimes used is $\mathbb{X}$ is ill-conditioned
- It means that one of its columns is nearly (or exactly) a linear combination of other columns. This is sometimes known as '(numerically) rank-deficient'.
- If $\mathbb{X} = UDV^\top$ is ill-conditioned, then some elements of D are nearly zero

  (remember, D is a diagonal matrix with decreasing entries)
- If we form $\hat{\beta}_{LS} = (\mathbb{X}^\top\mathbb{X})^{-1}\mathbb{X}^\top Y = VD^{-1}U^\top Y$, then we see that the small entries of D are now huge (due to the inverse). This in turn creates a huge variance

  $(\mathbb{V}\hat{\beta}_{LS} = (\mathbb{X}^\top\mathbb{X})^{-1} = VD^{-2}V^\top)$

Ridge regression and multicollinearity

Ridge Regression fixes this problem by preventing the division by a near zero number

Example: If a is a really small number, and $\lambda > 0$ is another number, then

$$\frac{1}{a} \approx \infty \quad \text{while} \quad \frac{1}{a+\lambda} \text{ is much smaller.}$$

To wit, $1/0.0001 = 10,000$, while $1/(0.0001 + 0.1) \approx 10$

Conclusion: $(\mathbb{X}^\top \mathbb{X})^{-1}$ can be really unstable, while $(\mathbb{X}^\top \mathbb{X} + \lambda I)^{-1}$ is not.

Ridge regression and multicollinearity: Example

Consider the example of predicting blood pressure from a person's weight and body surface area.

```
blood = read.table('../data/bloodpress.txt',header=T)

Y = blood$BP
weight = blood$Weight #persons weight
bsa = blood$BSA

outBoth = lm(Y~bsa+weight)
summary(outBoth)
outBSA = lm(Y~bsa)
summary(outBSA)
outWeight = lm(Y~weight)
summary(outWeight)
```

Ridge regression and multicollinearity: Example

```
lm(formula = Y ~ bsa + weight)
            Estimate Std. Error t value Pr(>|t|)
(Intercept)    5.653      9.392   0.602    0.555
bsa           11.663     12.125   0.962    0.350
weight        -4.793      6.232  -0.769    0.452

lm(formula = Y ~ bsa)
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   2.7971     8.5284   0.328    0.747
bsa           2.3389     0.1792  13.052 1.29e-10 ***

lm(formula = Y ~ weight)
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.20531    8.66333   0.255    0.802
weight       1.20093    0.09297  12.917 1.53e-10 ***
```

Ridge Regression and Multicollinearity: Example

This code shows that we are estimating $(\hat{\alpha}, \hat{\beta})$ with

```
out = cv.glmnet(x=cbind(weight,bsa),y=Y,alpha=0,nfolds=4,
                             lambda=(1:100)/100)
out$lambda[which.min(out$cvm)]
[1] 0.35
> out$glmnet.fit$beta[,which.min(out$cvm)]
weight  bsa
0.574 1.1462
```

$$\hat{\beta}_{\text{ridge},\hat{\lambda}} = (0.574, 1.1462)^\top$$

and

```
> out$glmnet.fit$a0[which.min(out$cvm)]
     s65
6.059
```

$$\hat{\alpha}_{\text{ridge},\hat{\lambda}} = 6.059$$

A comparison

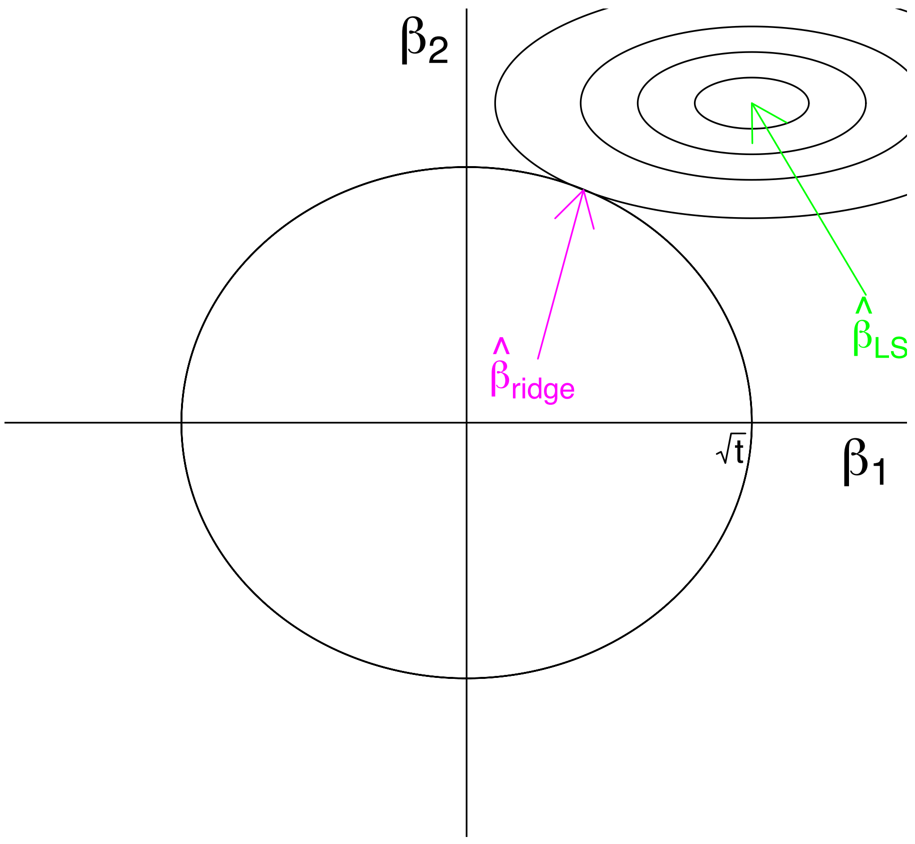
Ridge Regression: Using the λ

Here is the chosen fit (along with some previous methods):

```
#for predictor coefficient estimates
ridge.out$glmnet.fit$beta[,which.min(ridge.out$cvm)]
#for intercept
ridge.out$glmnet.fit$a0[which.min(ridge.out$cvm)]
```

Variable	Ridge	Full Linear Model	Forward and Backward
intercept	-0.017	0.181561	0.4947
lcavol	0.474	0.564341	0.543
lweight	0.597	0.622020	0.588
age	-0.015	-0.021248	-0.016
lbph	0.083	0.096713	0.101
svi	0.667	0.761673	0.715
lcp	-0.025	-0.106051	0
gleason	0.066	0.049228	0
pgg45	0.003	0.004458	0

Geometry of ridge regression in $\mathbb{R}^2$



Can we get the best of both worlds?

To recap:

- Forward, backward, and all subsets regression offer good tools for model selection.

  (but the optimization problem is nonconvex[3])

- Ridge regression provides regularization, which trades off bias and variance and also stabilizes multicollinearity.

  (problem is convex, but doesn't do model selection)

Ridge regression	$\min \|\|\mathbb{Y} - \mathbb{X}\beta\|\|_2^2$ subject to $\|\|\beta\|\|_2^2 \leq t$
Best linear regression model	$\min \|\|\mathbb{Y} - \mathbb{X}\beta\|\|_2^2$ subject to $\|\|\beta\|\|_0 \leq t$
	$(\|\|\beta\|\|_0 =$ the number of nonzero elements in $\beta)$

[3] In fact, it is NP-hard

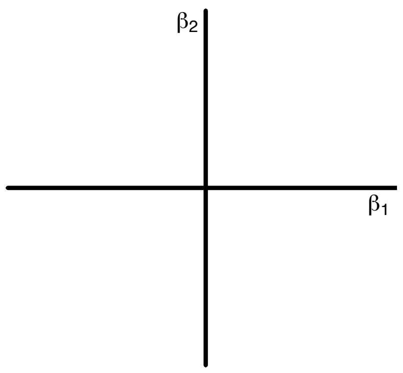
An intuitive idea

Ridge regression	$\min \|\|\mathbb{Y} - \mathbb{X}\beta\|\|_2^2$ subject to $\|\|\beta\|\|_2^2 \leq t$
Best linear regression model	$\min \|\|\mathbb{Y} - \mathbb{X}\beta\|\|_2^2$ subject to $\|\|\beta\|\|_0 \leq t$
	($\|\|\beta\|\|_0 =$ the number of nonzero elements in β)

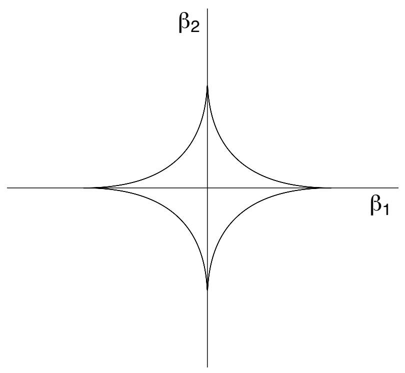
	Best linear regression model	Ridge regression
Computationally Feasible?	No	Yes
Does Model Selection?	Yes	No

Can we 'interpolate' $||\beta||_2$ and $||\beta||_0$ to find a method that does both?

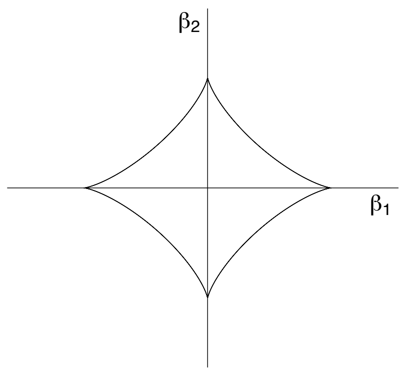
Geometry of regularization in $\mathbb{R}^2$: Convexity



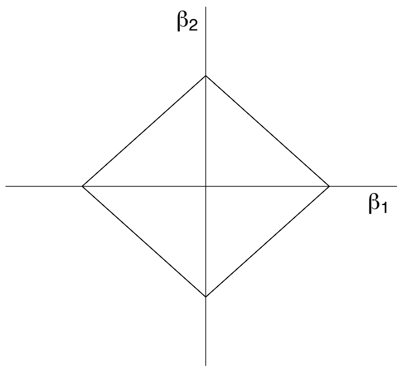
$||\beta||_0 \leq t$



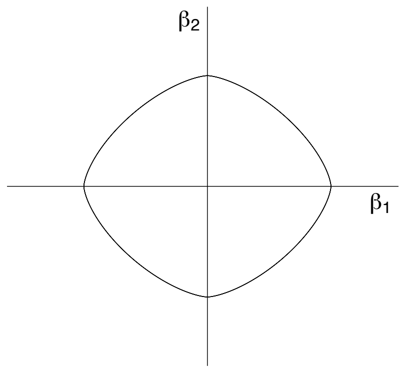
$||\beta||_{\frac{1}{2}} \leq t$



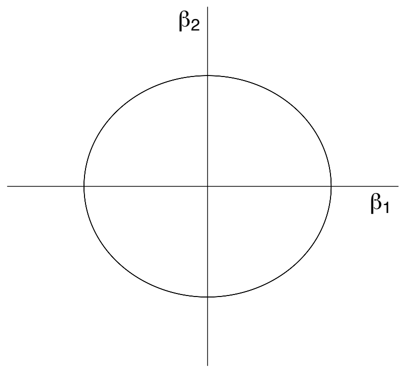
$||\beta||_{\frac{3}{4}} \leq t$



$||\beta||_1 \leq t$

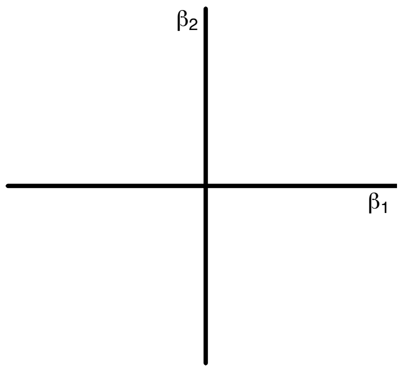


$||\beta||_{\frac{3}{2}} \leq t$

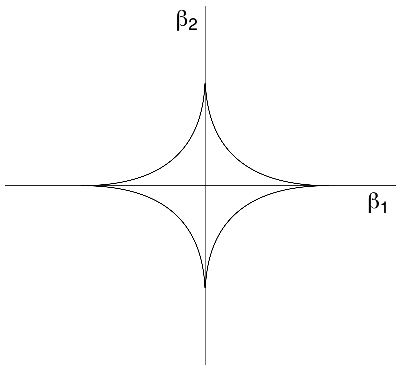


$||\beta||_2 \leq t$

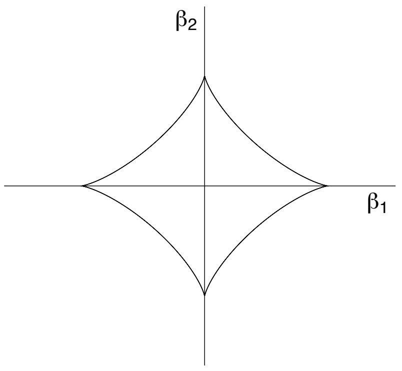
Geometry of regularization in $\mathbb{R}^2$: Convexity



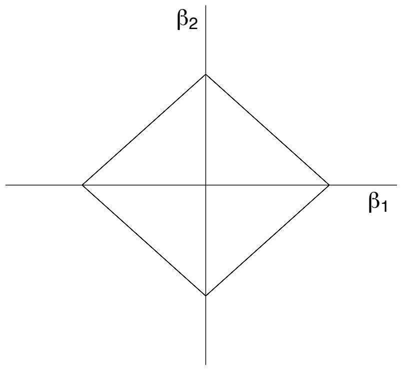
$||\beta||_0 \leq t$



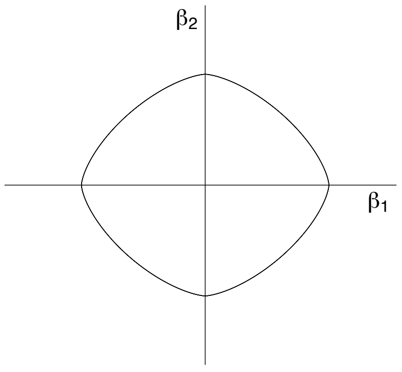
$||\beta||_{\frac{1}{2}} \leq t$



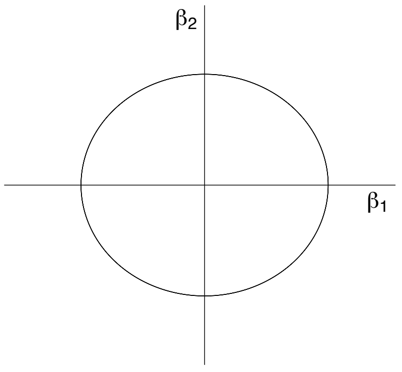
$||\beta||_{\frac{3}{4}} \leq t$



$||\beta||_1 \leq t$

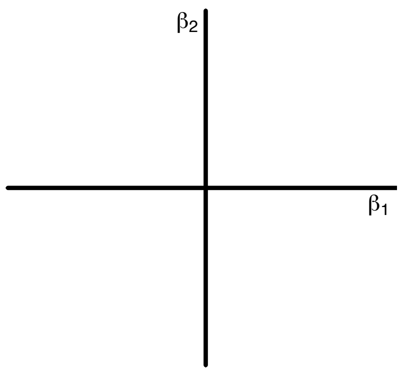


$||\beta||_{\frac{3}{2}} \leq t$

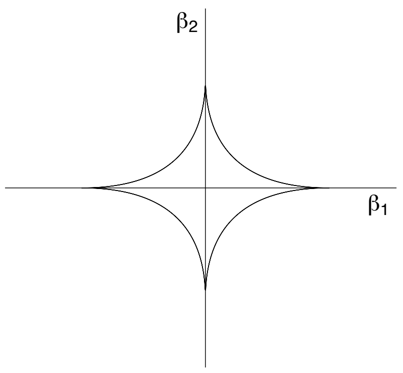


$||\beta||_2 \leq t$

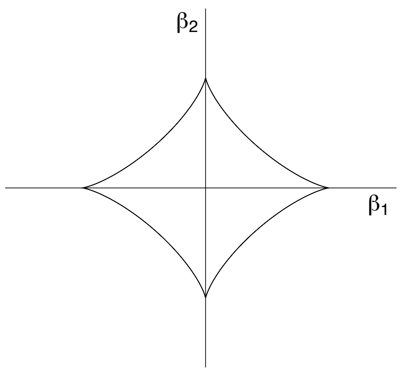
Geometry of regularization in $\mathbb{R}^2$: Convexity



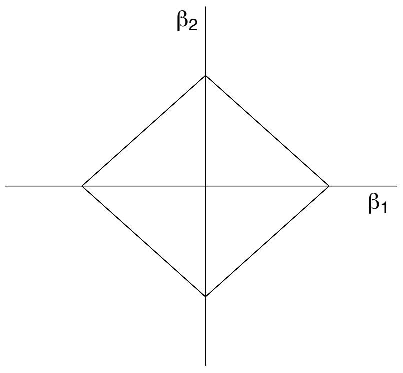
$||\beta||_0 \leq t$



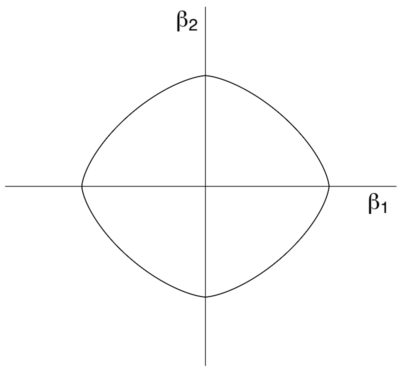
$||\beta||_{\frac{1}{2}} \leq t$



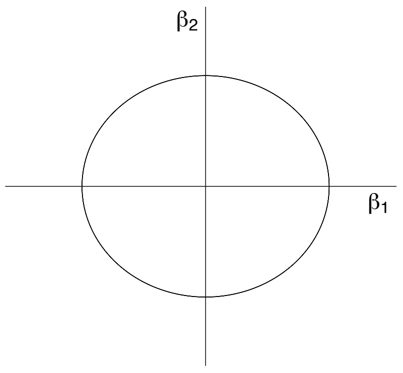
$||\beta||_{\frac{3}{4}} \leq t$



$||\beta||_1 \leq t$

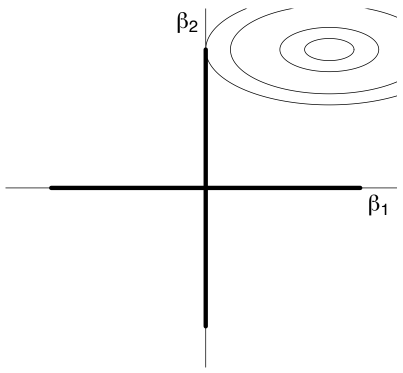


$||\beta||_{\frac{3}{2}} \leq t$

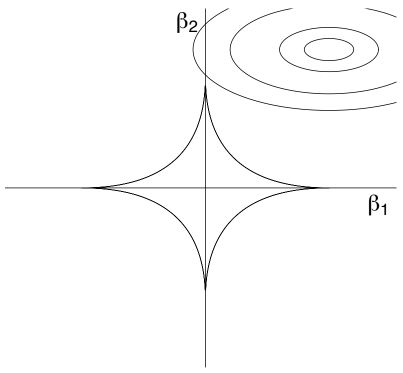


$||\beta||_2 \leq t$

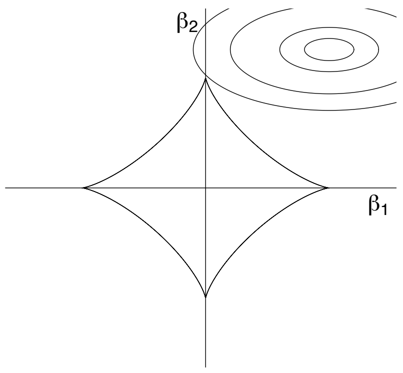
Geometry of regularization in $\mathbb{R}^2$: Model selection



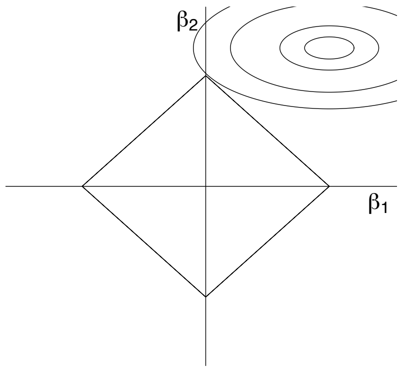
$||\beta||_0 \leq t$



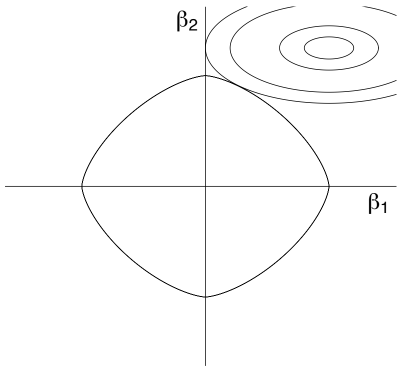
$||\beta||_{\frac{1}{2}} \leq t$



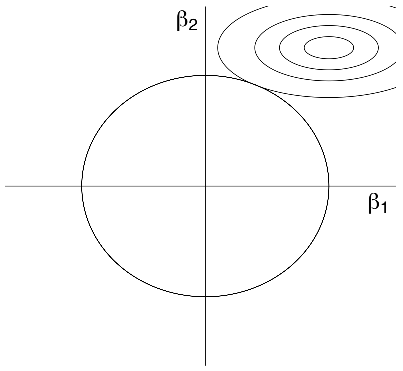
$||\beta||_{\frac{3}{4}} \leq t$



$||\beta||_1 \leq t$

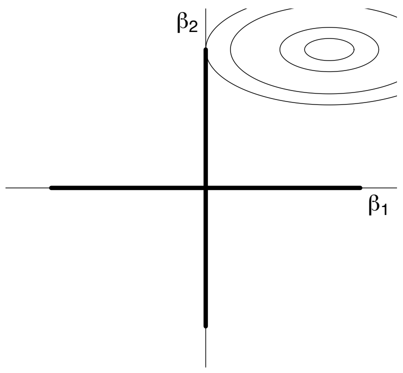


$||\beta||_{\frac{3}{2}} \leq t$

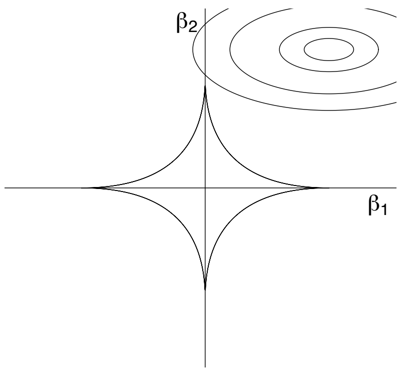


$||\beta||_2 \leq t$

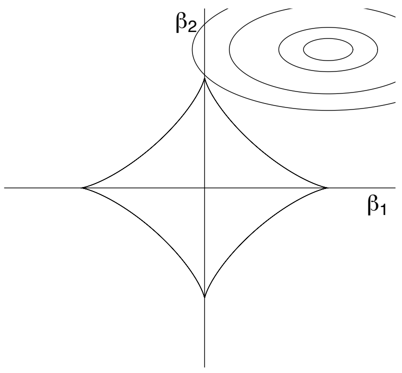
Geometry of regularization in $\mathbb{R}^2$: Model selection



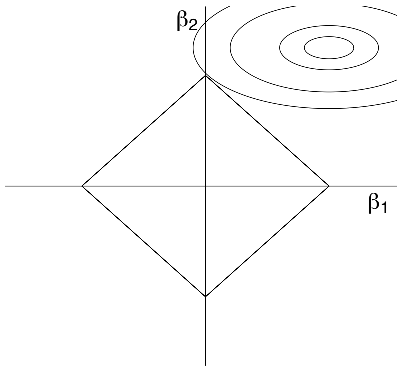
$||\beta||_0 \leq t$



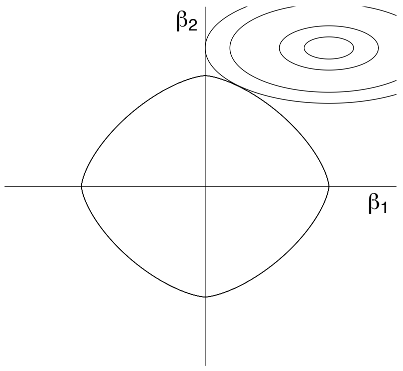
$||\beta||_{\frac{1}{2}} \leq t$



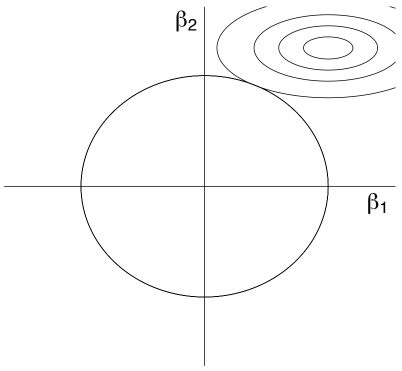
$||\beta||_{\frac{3}{4}} \leq t$



$||\beta||_1 \leq t$

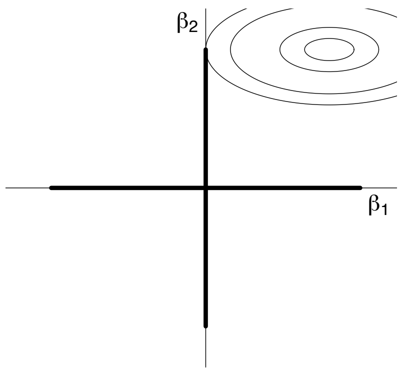


$||\beta||_{\frac{3}{2}} \leq t$

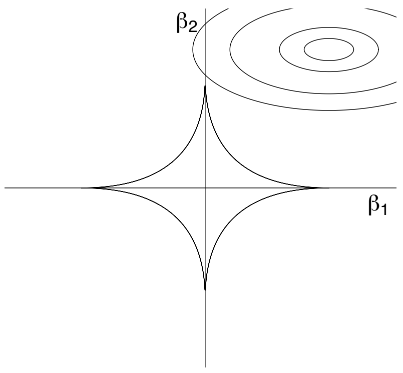


$||\beta||_2 \leq t$

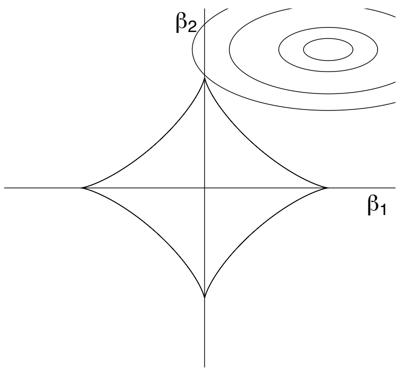
Geometry of regularization in $\mathbb{R}^2$: Model selection



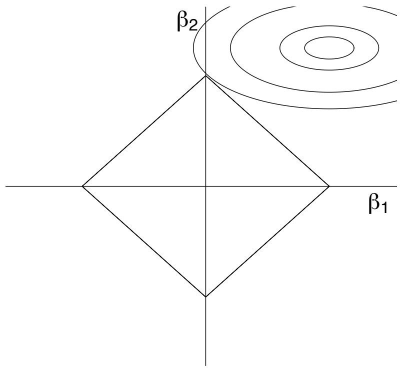
$||\beta||_0 \leq t$



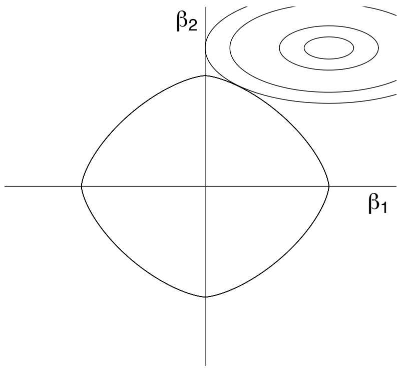
$||\beta||_{\frac{1}{2}} \leq t$



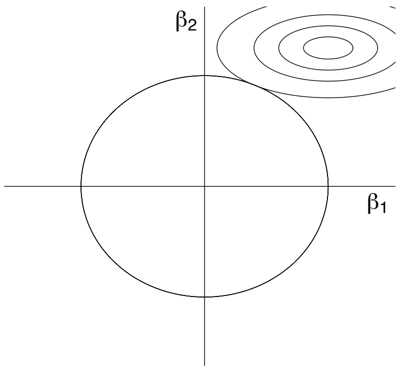
$||\beta||_{\frac{3}{4}} \leq t$



$||\beta||_1 \leq t$

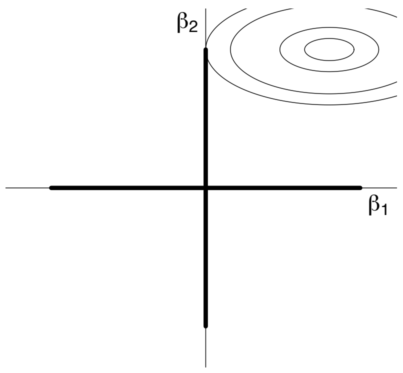


$||\beta||_{\frac{3}{2}} \leq t$

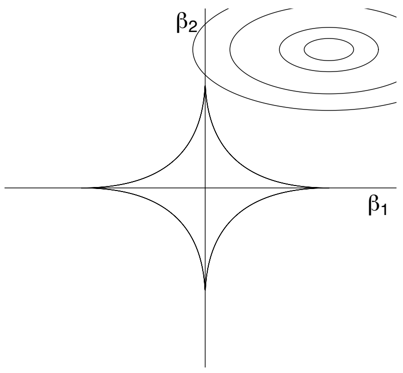


$||\beta||_2 \leq t$

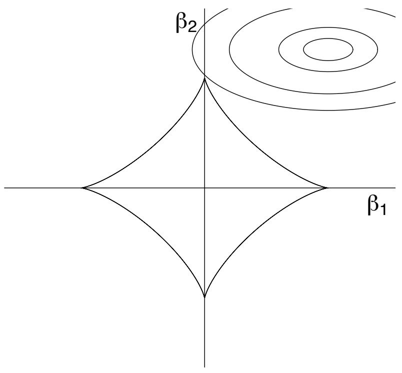
Geometry of regularization in $\mathbb{R}^2$: Both



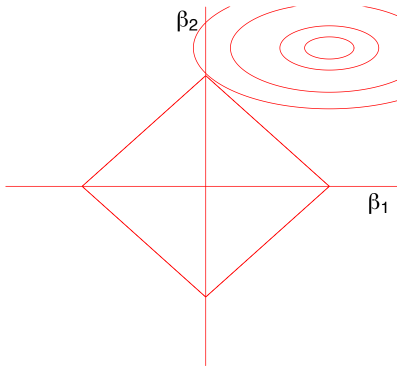
$||\beta||_0 \leq t$



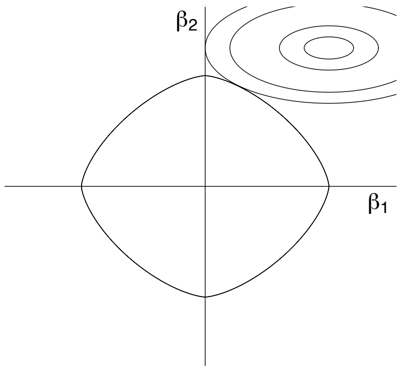
$||\beta||_{\frac{1}{2}} \leq t$



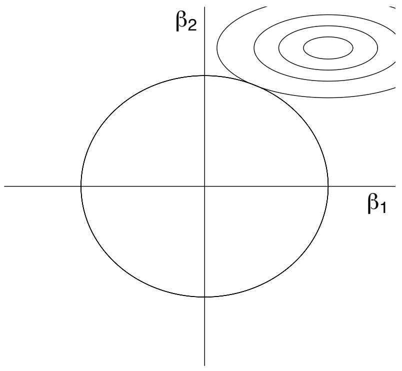
$||\beta||_{\frac{3}{4}} \leq t$



$||\beta||_1 \leq t$



$||\beta||_{\frac{3}{2}} \leq t$

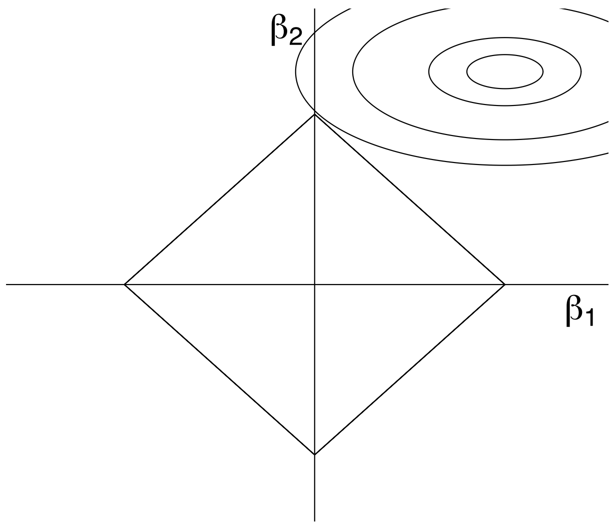


$||\beta||_2 \leq t$

Summary

	Convex?	Corners?	
$\|\|\beta\|\|_0$	No	Yes	
$\|\|\beta\|\|_{\frac{1}{2}}$	No	Yes	
$\|\|\beta\|\|_{\frac{3}{4}}$	No	Yes	
$\|\|\beta\|\|_1$	Yes	Yes	✓
$\|\|\beta\|\|_{\frac{3}{2}}$	Yes	No	
$\|\|\beta\|\|_2$	Yes	No	

The best of both worlds: $||\beta||_1$



This regularization set...

... is convex (computationally efficient)

... has corners (performs model selection)

The lasso

ℓ_1-REGULARIZED REGRESSION

Known as

- 'lasso'
- 'basis pursuit'

The estimator satisfies

$$\hat{\beta}_{lasso}(t) = \underset{||\beta||_1 \leq t}{\text{argmin}} \, ||\mathbb{Y} - \mathbb{X}\beta||_2^2$$

In its corresponding Lagrangian dual form:

$$\hat{\beta}_{lasso}(\lambda) = \underset{\beta}{\text{argmin}} \, ||\mathbb{Y} - \mathbb{X}\beta||_2^2 + \lambda ||\beta||_1$$

ℓ_1-REGULARIZED REGRESSION

While the ridge solution can be easily computed

$$\hat{\beta}_{ridge,\lambda} = \underset{\beta}{\text{argmin}} \, ||\mathbb{Y} - \mathbb{X}\beta||_2^2 + \lambda||\beta||_2^2 = (\mathbb{X}^\top \mathbb{X} + \lambda I)^{-1}\mathbb{X}^\top Y$$

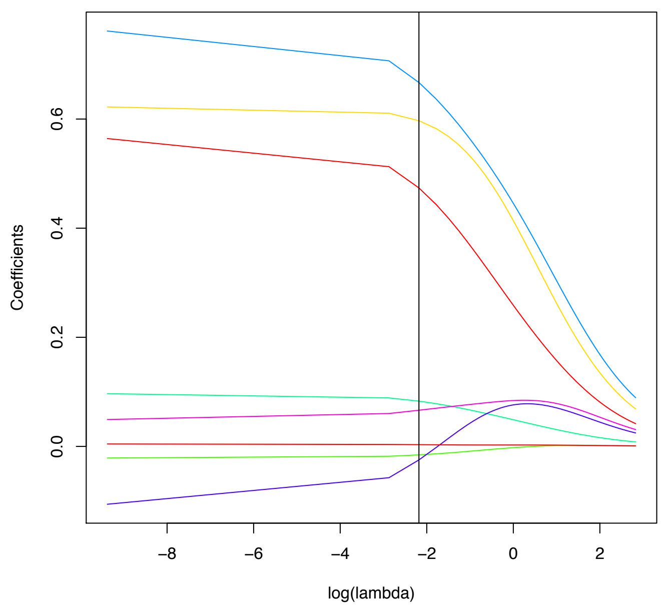
the lasso solution

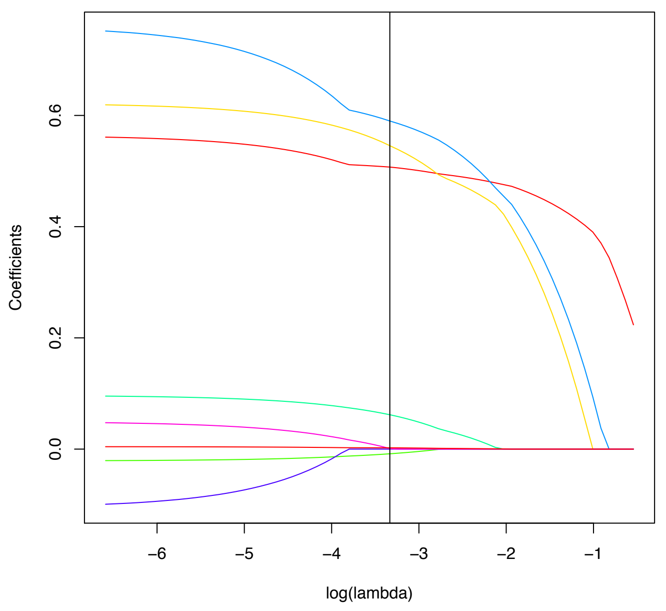
$$\hat{\beta}_{lasso,\lambda} = \underset{\beta}{\text{argmin}} \, ||\mathbb{Y} - \mathbb{X}\beta||_2^2 + \lambda||\beta||_1 = ??$$

doesn't have a closed form solution.

However, as the optimization problem is convex, there exist efficient algorithms for computing it

Coefficient path: Ridge vs. Lasso





Choosing the tuning parameter for lasso

There are two main R implementations for finding $\hat{\beta}_{lasso,\lambda}$

- Using glmnet. Just change the ‘alpha =0’ to ‘alpha =1’, and you’re lassoing:

  ```
  lasso.out = glmnet(x=X,y=Y,alpha=1)
  ```

- Alternatively, there is the lars package

(Technically, we will talk about a third way, called scaled sparse regression (SSR). It differs in how the tuning parameter λ is chosen, but still uses the lars algorithm for minimizing)

The lasso in R: glmnet

glmnet uses gradient descent to quickly fit the lasso solution

It can...

- handle other likelihoods than Gaussian

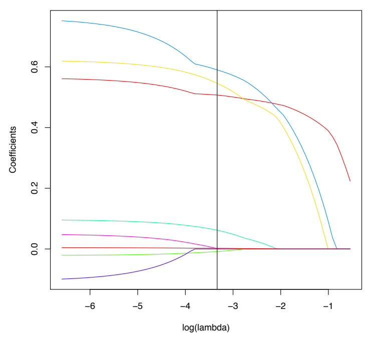
  (This will become more important when we talk about classification and generalized linear models (GLM))
- supports/exploits sparse matrices

  (We will cover this soon)
- uses warm restarts for the grid of λ to produce more stable fits/faster computations

  (You'll just have to believe me on this one)

The lasso in R: lars

The lars approach is a path algorithm



This means we can exploit the fact that the coefficient profiles are piecewise linear to:

- not need a grid of λ's
- make exact computations

To do this in R, we can do:

```
lasso.lars = lars(X,Y,type='lasso')
```

Comparison of lars and glmnet

There are two main problems with glmnet

- The same as with ridge, the λ grid can be poorly chosen

  (In practice, the λ interval looks like $\left[\epsilon||\mathbb{X}^\top Y||_\infty, ||\mathbb{X}^\top Y||_\infty\right)$ for a small ϵ. Sometimes, this results in finding a boundary solution)
- The gradient descent approach is approximate. Sometimes the thresh parameter needs to be adjusted to be smaller:

  ```
  fit     = glmnet(X,Y,alpha=1,thresh=1e-16)
  ```

There are three main problems with lars

- It is slow(er)
- It doesn't directly support other likelihoods (such as for doing classification)
- It doesn't automatically produce the lasso fit when doing cross-validation

Choosing the tuning parameter for lasso

Of course, just like in Ridge, we need a way of choosing this tuning parameter.

We can just use cross-validation again, though this is still an area of active research:

Homrighausen, D. and McDonald, D.J. *Leave-one-out cross-validation is risk consistent for lasso*, Machine Learning

Homrighausen, D. and McDonald, D.J. *Risk consistency of cross-validation for lasso-type procedures*, Journal of Machine Learning Research

Homrighausen, D. and McDonald, D.J. *The lasso, persistence, and cross-validation*, (2013) International Conference on Machine Learning, JMLR 28(3), 1031–1039.

Choosing the tuning parameter for lasso

For cross-validation, the heavy lifting has been done for us

```
lasso.cv.glmnet = cv.glmnet(x=as.matrix(X),y=Y,alpha=1)

lasso.cv.lars   = cv.lars(x=as.matrix(X),y=Y,type='lasso')
```

We can also get the predictions:

$$\hat{Y}_0 = X_0^\top \hat{\beta}_{\mathrm{lasso},\hat{\lambda}}$$

and coefficient estimates

$$\hat{\beta}_{\mathrm{lasso},\hat{\lambda}}$$

with the following code..

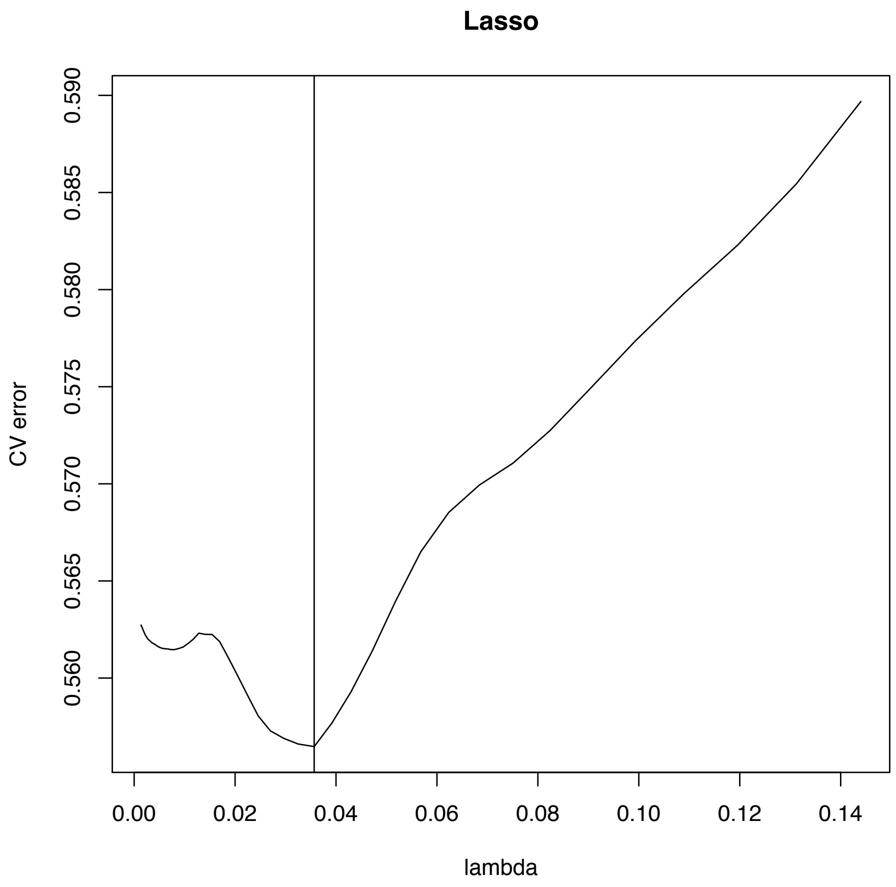
Predictions and coefficients: glmnet

```
###
# glmnet
###
lasso.cv.glmnet = cv.glmnet(X,Y,alpha=1,standardize=F)
lasso.glmnet    = lasso.cv.glmnet$glmnet.fit

Yhat.glmnet    = predict(lasso.cv.glmnet,X_0,s='lambda.min')
betaHat.glmnet = coef(lasso.cv.glmnet,s='lambda.min')
```

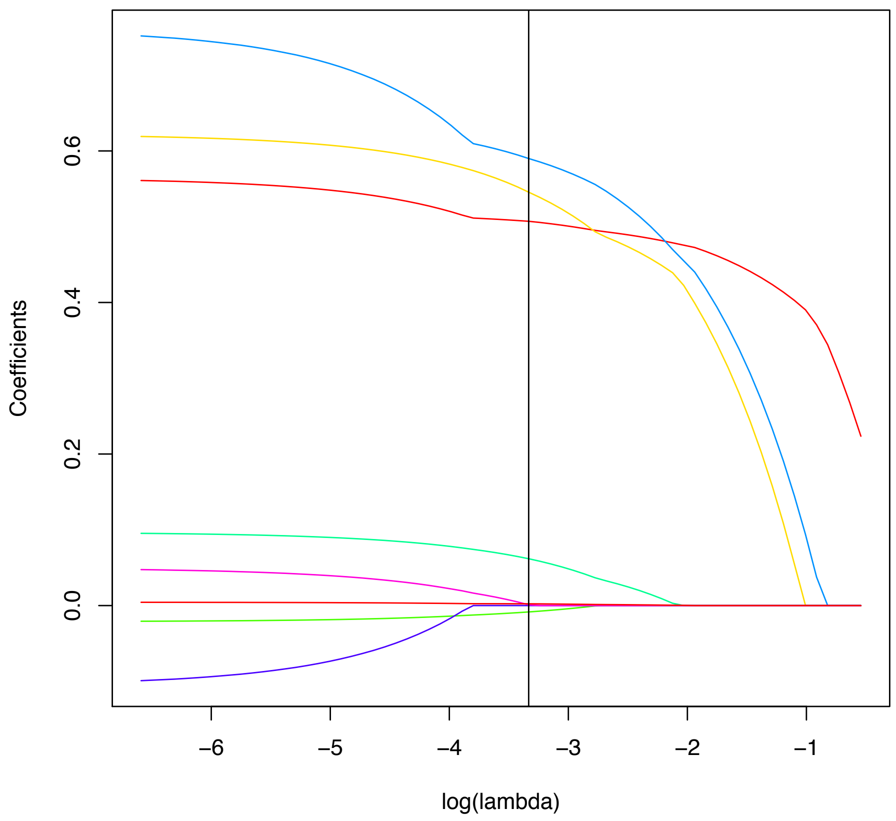
Predictions and coefficients: lars

```
###
# lars
###
lasso.lars    = lars(X,Y,type='lasso')
lasso.cv.lars = cv.lars(X,Y,type='lasso',mode='fraction')

frac.hat  = lasso.cv.lars$index[which.min(lasso.cv.lars$cv)]
Yhat.lars = predict(lasso.lars,X_0,type='fit',
                        mode='fraction',s=frac.hat)$fit
betaHat   = coef(lasso.lars,mode='fraction',s=frac.hat)
```

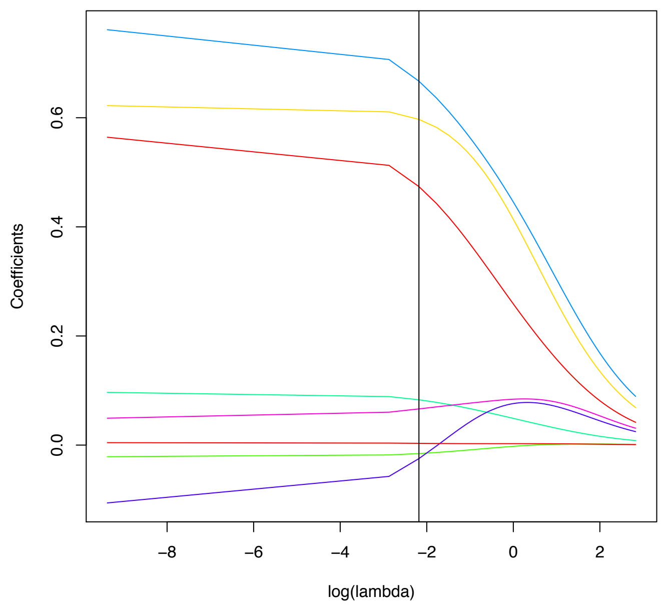
The lasso in R

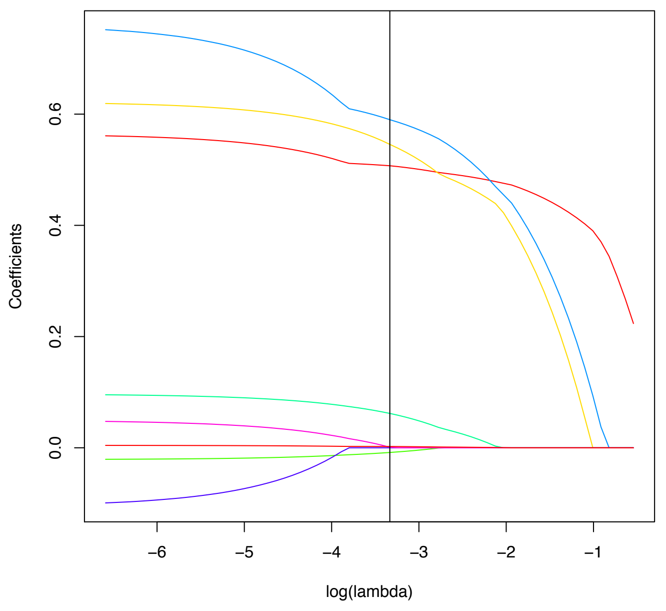


Lasso regression path



Comparison: Regression path





Vertical line at minimum CV tuning parameter