Regularization

-Introduction to Data Science-

ISL 6.2

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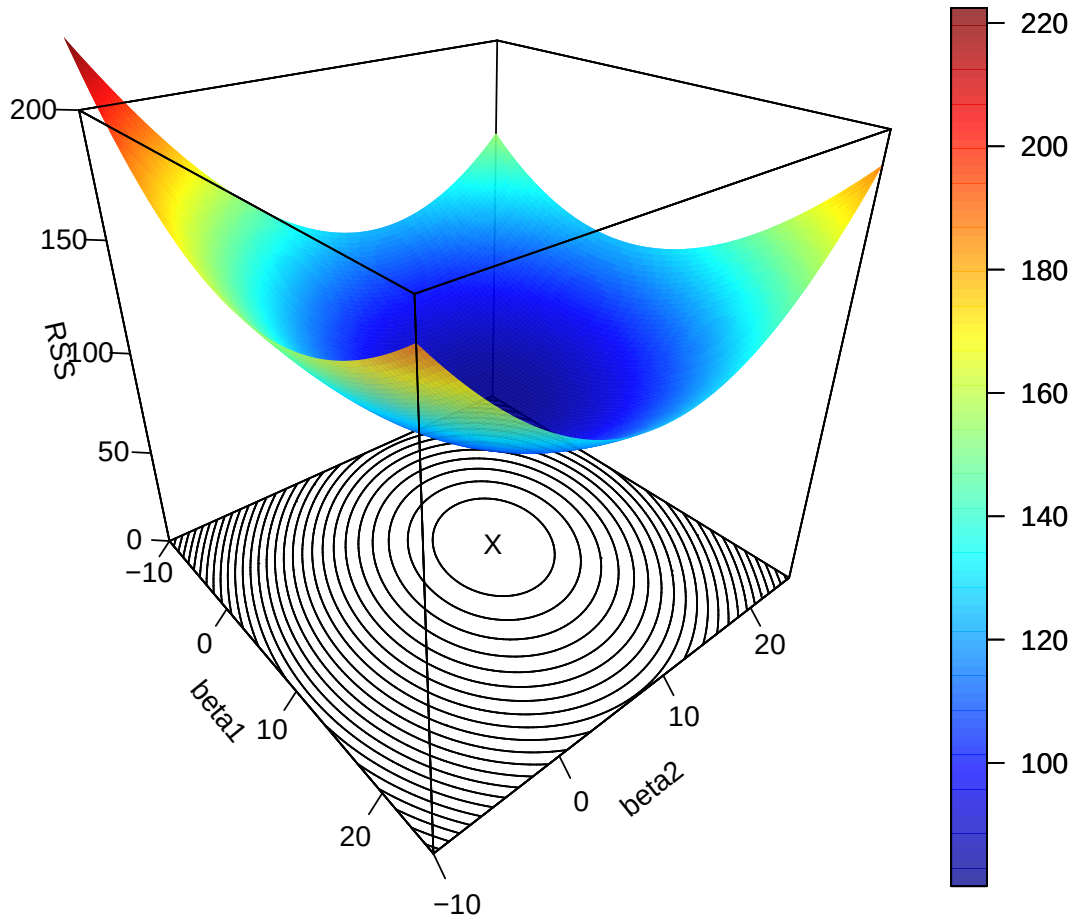
Preamble:

- All subsets and its stepwise approximations involve trading of between global & slow and local & fast
- Instead, we approach this problem via convex relaxation, which means solving a nearby problem in a global & fast way.
- Different relaxations result in different procedures

Least squares



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

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)

One way to do this is called ridge regression[1]:

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

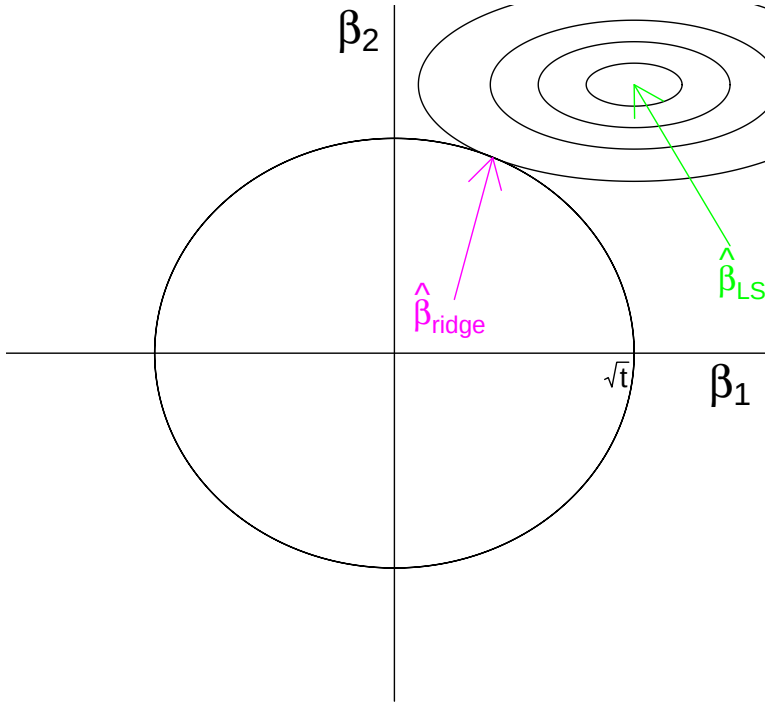
for any $t \geq 0$.

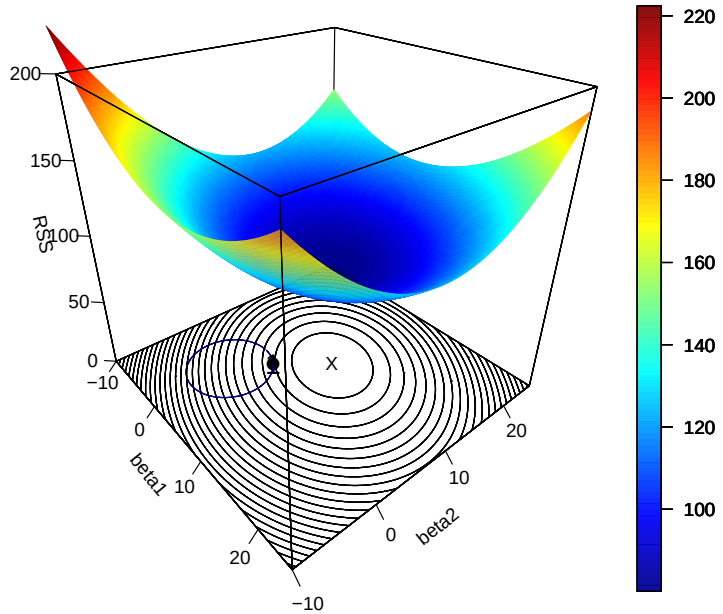
Compare this to least squares

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

[1] Hoerl, Kennard (1970)

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

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

Regularization and standardization

The coefficient vector isn't invariant to rescaling

If an intercept is included, do not penalize it:

$$\min_{\beta_0,\beta} \sum_{i=1}^{n} (Y_i - \beta_0 + \beta^\top X_i)^2 + \lambda ||\beta||_2^2$$

The usual way of addressing this in regression is:

- Standardize all features for which scale is meaningful:

$$x_j \leftarrow \frac{(x_j - \text{mean}(x_j))}{\text{sd}(x_j)}$$

  (So, don't standardize indictor variables, for instance)

- Standardize the supervisor $Y \leftarrow Y - \text{mean}(Y)$
- Don't include an intercept

Ridge regression

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

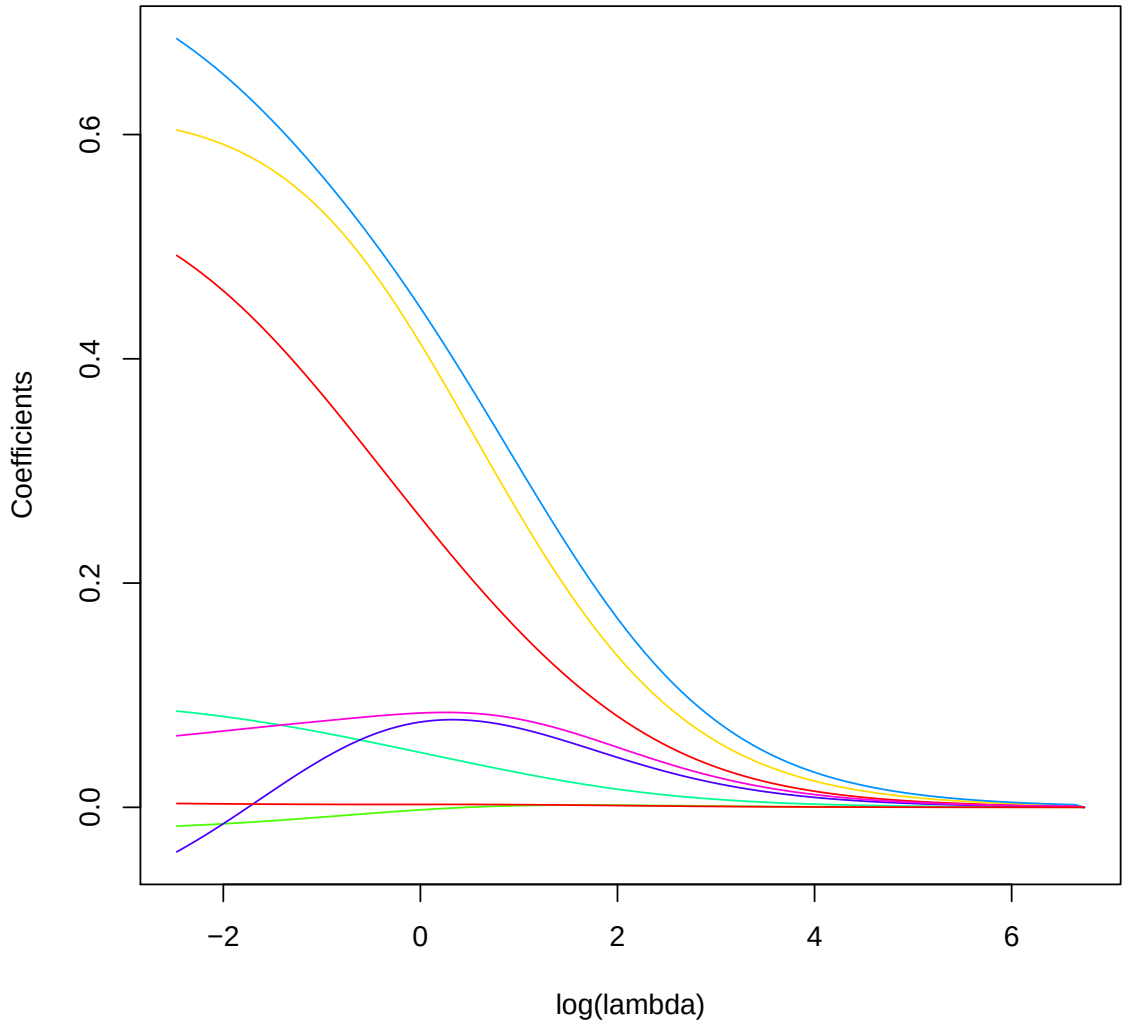
(Alternatively, hyper-parameters)

However we think about it, we have produced a suite of solutions

$$\{\hat{\beta}_{\text{ridge}}(\lambda) : \lambda \in [0, \infty)\}$$

What do these solutions look like?

Ridge regression path



Ridge regression

Reminder: The least squares solution can be written:

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

However, if $\text{rank}(\mathbb{X}) < p$, then $\hat{\beta}_{\text{LS}}$ is not unique. In fact,

$$\text{for any } b \text{ such that } \mathbb{X}b = 0$$

$\hat{\beta}_{\text{LS}} + b$ is a valid least squares solution.

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

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

Quite similar. However, the λ can make all the difference..

Regularization - Ridge Regression

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

$$\hat{\beta}_{\text{LS}} = VD^{-1}U^\top Y \qquad = \sum_{j=1}^{p} v_j \left(\frac{1}{d_j}\right) u_j^\top Y$$

$$\hat{\beta}_{\text{ridge}}(\lambda) = V(D^2 + \lambda I)^{-1} DU^\top Y \qquad = \sum_{j=1}^{p} v_j \left(\frac{d_j}{d_j^2 + \lambda}\right) u_j^\top Y.$$

Similarly for predictions:

$$\mathbb{X}\hat{\beta}_{\text{LS}} = UU^\top Y \qquad = \sum_{j=1}^{p} u_j u_j^\top Y$$

$$\mathbb{X}\hat{\beta}_{\text{ridge}}(\lambda) = UD(D^2 + \lambda I)^{-1} DU^\top Y \qquad = \sum_{j=1}^{p} u_j \left(\frac{d_j^2}{d_j^2 + \lambda}\right) u_j^\top Y.$$

$\Rightarrow$ **Ridge shrinks the data by an additional factor of λ.**

Regularization - Ridge Regression

Computationally, we need the ridge solution at many values of λ

Naively, that would mean solving the normal equations many times

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

However, with the SVD form, we can compute $\mathbb{X} = UDV^\top$ once and "solve" with only matrix multiplications

$$\hat{\beta}_{\text{ridge}}(\lambda) = \sum_{j=1}^{p} v_j \left(\frac{d_j}{d_j^2 + \lambda} \right) u_j^\top Y$$

Ridge in a new space

Note the matrix identity

$$(A - BC^{-1}E)^{-1}BC^{-1} = A^{-1}B(C - EA^{-1}B)^{-1}$$

Then,

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

This seemingly innocuous change can have large implications

Ridge in a new space: Computations

The ridge solution solves either the normal equations

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

or the alternative:

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

The 'heavy lifting' in each case is done with the inversion

- $\mathbb{X}^\top \mathbb{X} \in \mathbb{R}^{p \times p} \Longrightarrow$ takes p^3 computations, p^2 space
- $\mathbb{X}\mathbb{X}^\top \in \mathbb{R}^{n \times n} \Longrightarrow$ takes n^3 computations, n^2 space

Conclusion: Depending on the relative size of n and p, this could be a substantial savings

However, a much deeper realization is possible..

(Kernel) ridge regression

Suppose we want to predict at X, then

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

Also,

$$\mathbb{X}\mathbb{X}^\top = \begin{bmatrix} \langle X_1, X_1 \rangle & \langle X_1, X_2 \rangle & \cdots & \langle X_1, X_n \rangle \\ & \vdots & & \\ \langle X_n, X_1 \rangle & \langle X_n, X_2 \rangle & \cdots & \langle X_n, X_n \rangle \end{bmatrix}$$

and

$$X^\top \mathbb{X}^\top = [\langle X, X_1 \rangle, \langle X, X_2 \rangle, \cdots, \langle X, X_n \rangle]$$

where $\langle X, X' \rangle = X^\top X'$ is the Euclidean inner product.

If we transform $X_i \mapsto \Phi(X_i)$ then we use $\langle \Phi(X_i), \Phi(X_{i'}) \rangle$

Inserting Φ is known as kernelization or a kernel trick

(Kernel) ridge regression

Example: Suppose $X = (\text{income}, \text{height})^\top$

Then we could specify the map

$$\begin{aligned}\Phi(X)^\top &= (\phi_1(X), \phi_2(X), \phi_3(X), \phi_4(X), \phi_5(X)) \\ &= (\text{income}, \text{height}, \text{income} * \text{height}, \text{income}^2, \text{height}^2)\end{aligned}$$

where, for instance, $\phi_2(X) = x_2 = \text{height}$

The induced feature matrix is then

$$\mathbb{X} = \begin{bmatrix} \Phi(X_1) \\ \vdots \\ \Phi(X_n) \end{bmatrix} \in \mathbb{R}^{n \times 5}$$

(Kernel) ridge regression

Ordinarily, this would mean we need to solve the normal equation inversion for $p = 5$

- $\mathbb{X}^\top \mathbb{X} \in \mathbb{R}^{p \times p} \implies$ takes p^3 computations, p^2 space

However, using the kernel trick we can solve instead

- $\mathbb{X}\mathbb{X}^\top \in \mathbb{R}^{n \times n} \implies$ takes n^3 computations, n^2 space

which is fixed in p

Implication: We can add essentially arbitrary nonlinearity without paying higher computational, storage cost!

We will return to this again with support vector machines (SVM)

Ridge in practice

Ridge Regression: The tuning parameter

We can use a degrees of freedom based risk estimator to choose λ

The degrees of freedom of $\hat{\beta}_{\text{ridge}}(\lambda)$ can be seen to be

$$\text{df} = \text{trace}\left[\mathbb{X}(\mathbb{X}^\top\mathbb{X} + \lambda I)^{-1}\mathbb{X}^\top\right] = \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda}$$

(As $\lambda \to 0$, we get the number linearly independent columns of X)

We can plug this into any of the GIC measures or..

Note that a common choice is generalized cross-validation (GCV), which has the form:

$$\text{GCV}(\hat{\beta}) = \frac{\left\|Y - \mathbb{X}\hat{\beta}\right\|_2^2}{(1 - \text{df}(\hat{\beta})/n)^2}$$

Ridge Regression: The tuning parameter

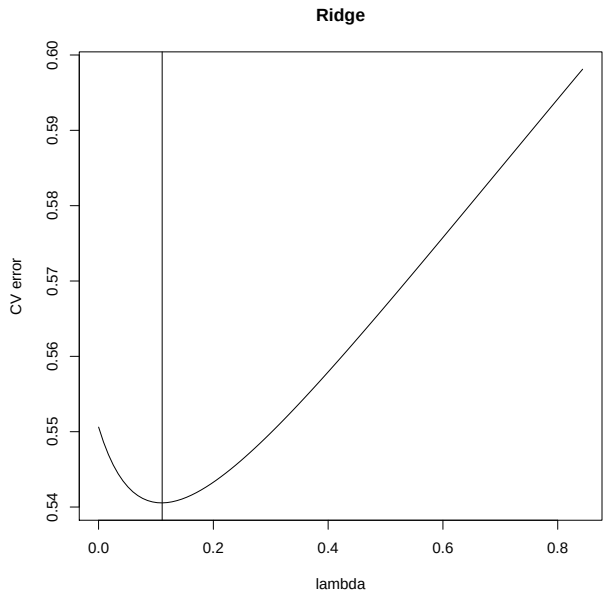
Nowadays, using K-fold cross-validation is common

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

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

Now, we report $\hat{\beta}_{\text{ridge}}(\hat{\lambda})$ as our estimator

Ridge Regression: Cross-validation plot



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,...):

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

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

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

Ridge Regression in R

We will concentrate on a slightly more obtuse way, as it will make things easier later.

```
if(!require(glmnet)){install.packages('glmnet');require(glmnet)}
ridge.out = cv.glmnet(x=X,y=Y,alpha=0)
```

glmnet automatically scales X, unless you set

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

Note:

- The function cv.glmnet computes CV_K for a grid of λ values as well as the ridge solutions
- The function glmnet just computes the ridge solutions over a grid of λ values
- The feature matrix X must be a "matrix" data structure

```
> class(X)
[1] "matrix"
```

Ridge computations

Ridge Regression: Compare

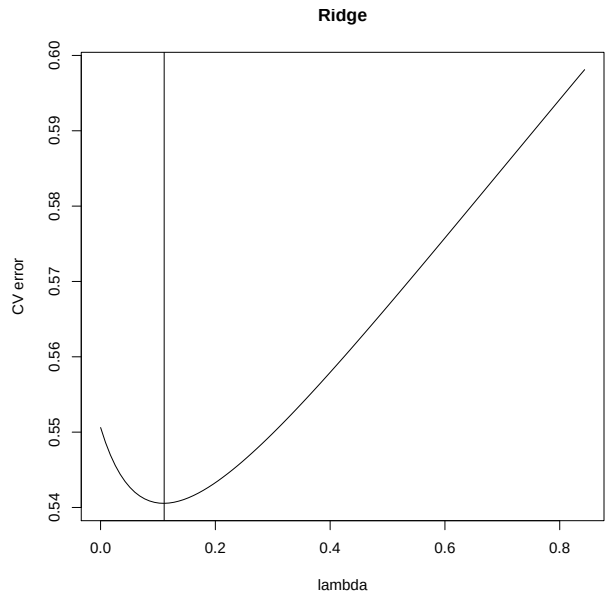
```
lam = 1
svd.out   = svd(X)
ridge.svd = svd.out$v %*%
                  diag(svd.out$d/(svd.out$d**2 + lam)) %*%
                  t(svd.out$u) %*% Y

Ytilde   = c(Y,rep(0,p))
Xtilde   = rbind(X,diag(sqrt(lam),p))
ridge.lm = lm(Ytilde~Xtilde-1)

library(glmnet)
ridge.glmnet = glmnet(x=X,y=Y,alpha=0,
                      standardize=FALSE,intercept=FALSE,
                      lambda = seq(1.1/n,.9/n,length.out = 1000))
```

Ridge Regression: Compare

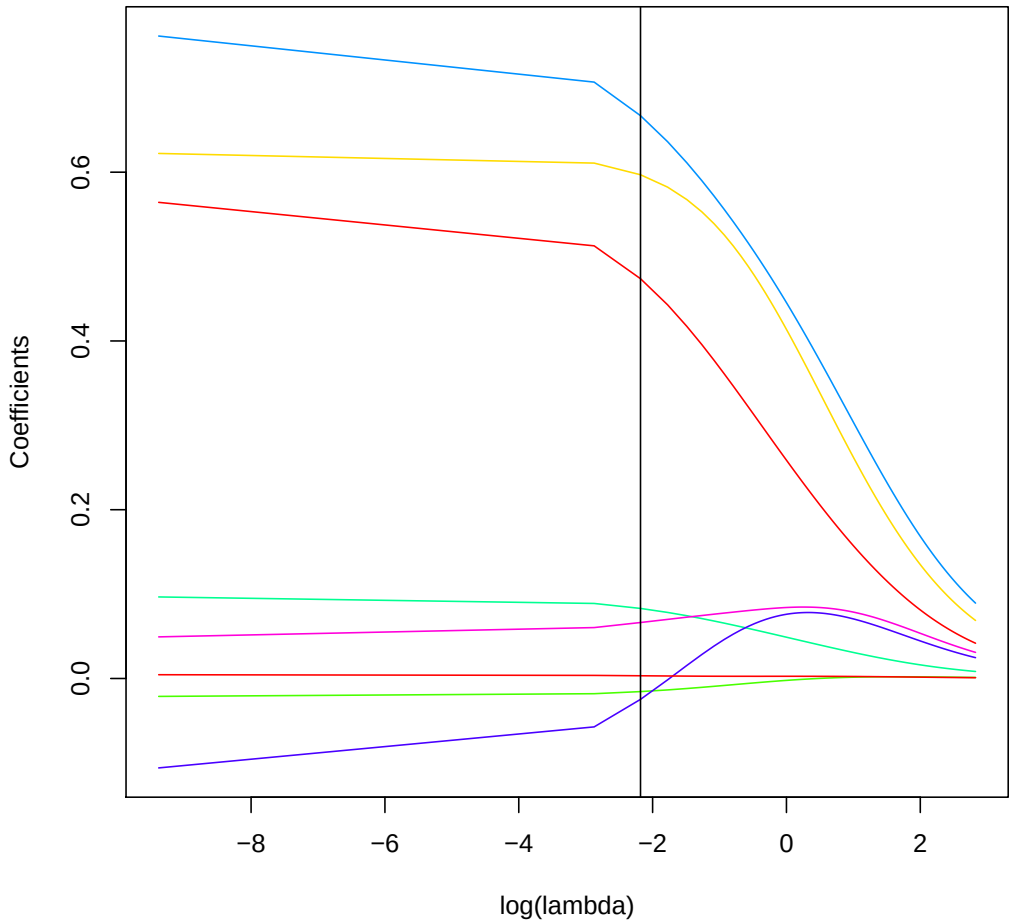
```
> print(ridge.svd[1:3])
[1]  0.55869858  0.60999902 -0.01933688

> print(coef(ridge.lm)[1:3])
[1]  0.55869858    0.60999902   -0.01933688

> print(coef(ridge.glmnet,s=lam/n)[1:4])
[1]  0.00000000  0.55911894  0.61313693 -0.01950889
```

Ridge Regression: CV plot

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

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



Ridge regression path



Important: Ridge doesn't set any coefficients to zero for any λ

Ridge Regression: Using glmnet

Suppose we have training data X and Y loaded into R

Suppose we also have test data Xtest loaded into R

```
out.glmnet = cv.glmnet(x=X,y=Y,alpha=0)
betaHat    = coef(out.glmnet,s='lambda.min')
Yhat       = predict(out.glmnet,type='link',
                     s='lambda.min',newx=Xtest)
#Alternatively
Yhat       = Xtest %*% betaHat
```

Ridge Regression: Using glmnet

The input to glmnet must be a matrix!

```
> Xdf = data.frame('x1'=rnorm(50),
+                  'x2'=sample(c('yes','no'),replace=TRUE,size=50))
> head(Xdf)
          x1  x2
1 -0.6264538  no
2  0.1836433 yes
3 -0.8356286 yes
4  1.5952808  no
>  X = model.matrix(~.-1,Xdf)
> head(X)
          x1 x2no x2yes
1 -0.6264538    1     0
2  0.1836433    0     1
3 -0.8356286    0     1
4  1.5952808    1     0
```

(Don't include an intercept in glmnet if doing this)

```
out.glmnet = cv.glmnet(x=X,y=Y,alpha=0,intercept=FALSE)
```

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)
- 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 β)

An intuitive idea

Ridge regression $\min ||\mathbb{Y} - \mathbb{X}\beta||_2^2$ subject to $||\beta||_2^2 \leq t$

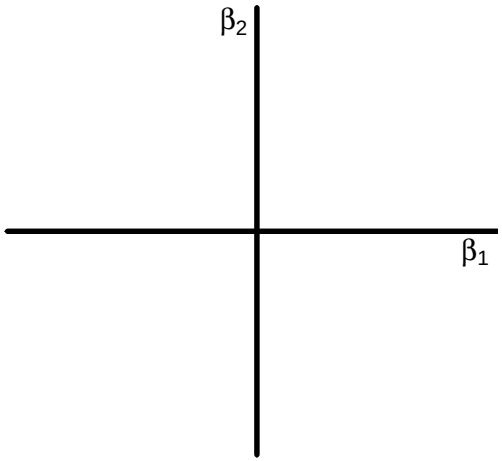
Best linear regression model $\min ||\mathbb{Y} - \mathbb{X}\beta||_2^2$ subject to $||\beta||_0 \leq t$

($||\beta||_0 =$ the number of nonzero elements in β)

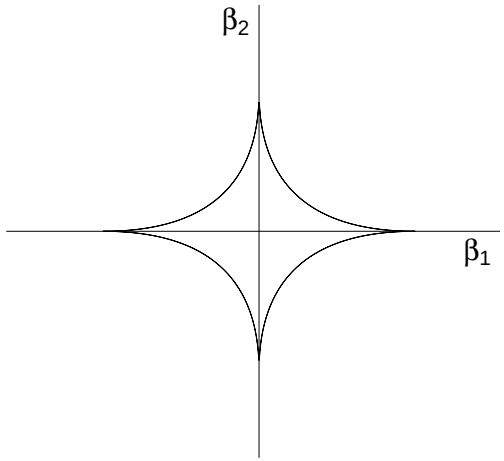
	Best linear regression model	Ridge regression
Computationally Feasible?	No	Yes
Does Model Selection?	Yes	No

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

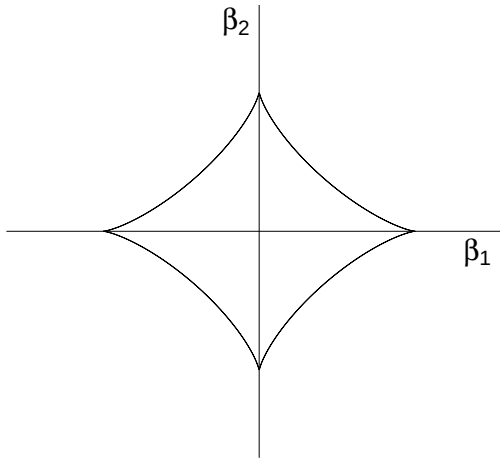
Geometry of regularization in $\mathbb{R}^2$: Convexity



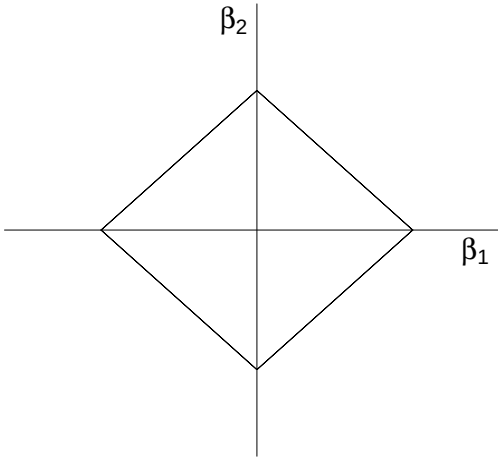
$||\beta||_0 \leq t$



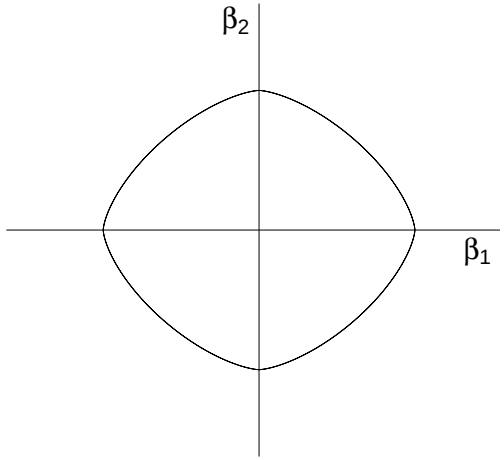
$||\beta||_{\frac{1}{2}} \leq t$



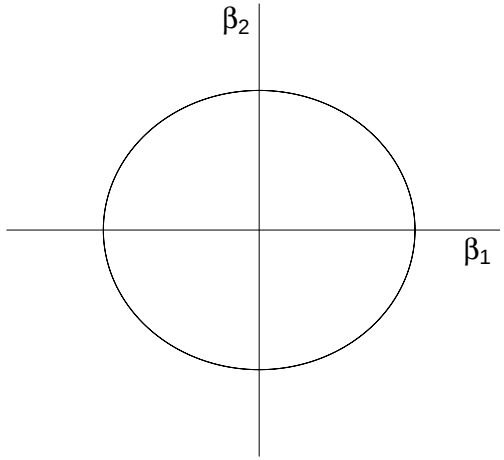
$||\beta||_{\frac{3}{4}} \leq t$



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

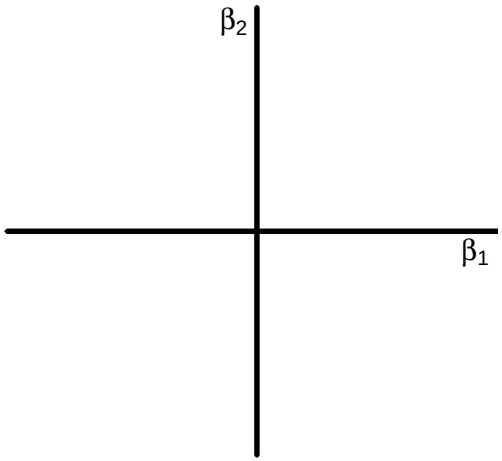


$||\beta||_{\frac{3}{2}} \leq t$

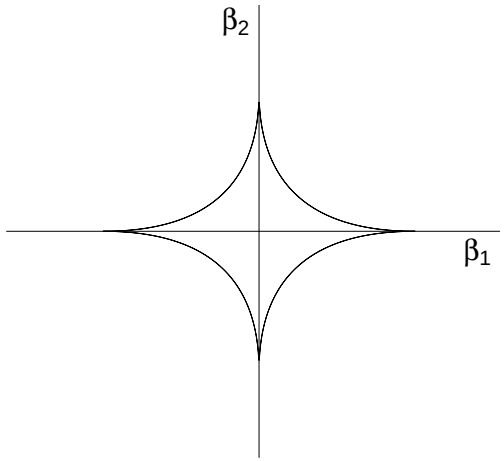


$||\beta||_2 \leq t$

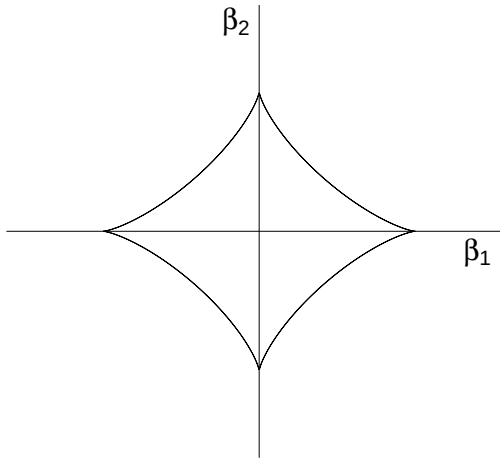
Geometry of regularization in $\mathbb{R}^2$: Convexity



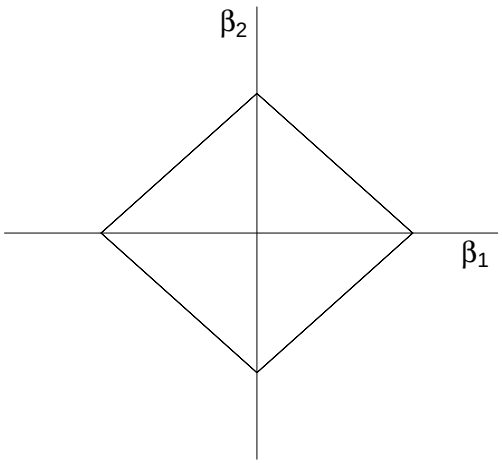
$||\beta||_0 \leq t$



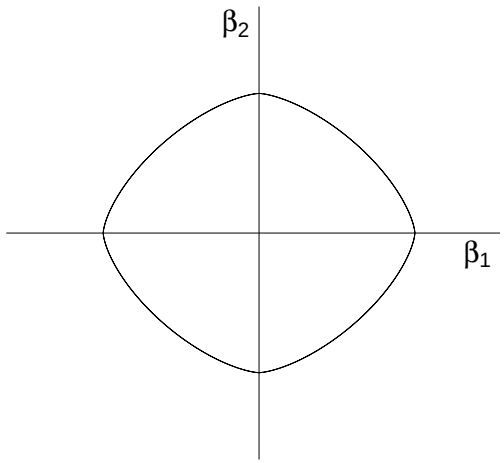
$||\beta||_{\frac{1}{2}} \leq t$



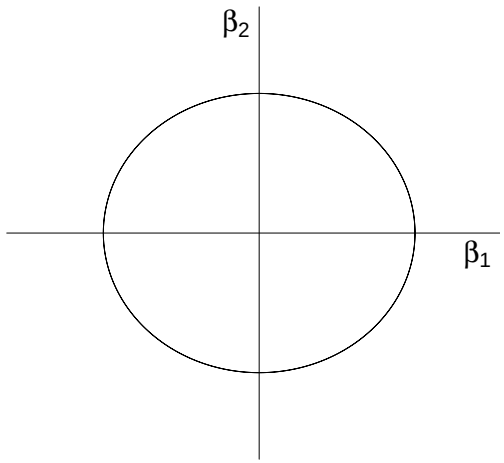
$||\beta||_{\frac{3}{4}} \leq t$



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

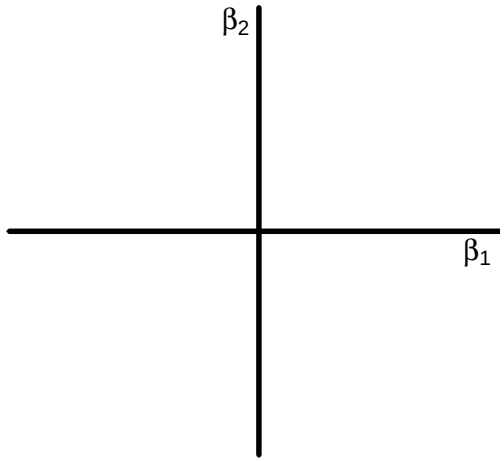


$||\beta||_{\frac{3}{2}} \leq t$

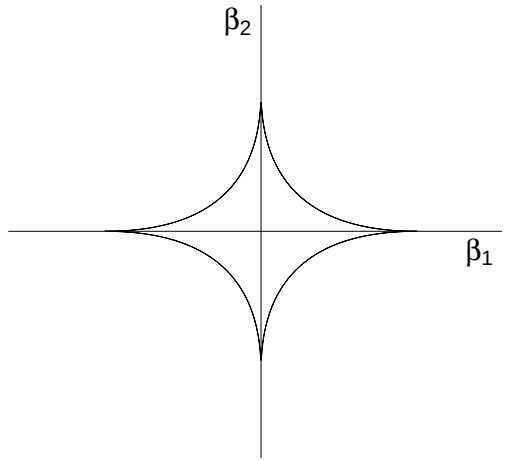


$||\beta||_2 \leq t$

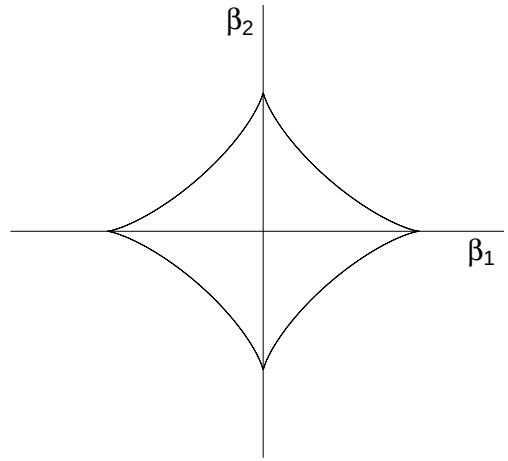
Geometry of regularization in $\mathbb{R}^2$: Convexity



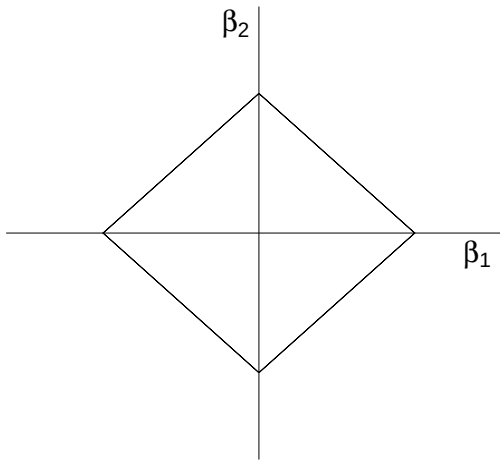
$||\beta||_0 \leq t$



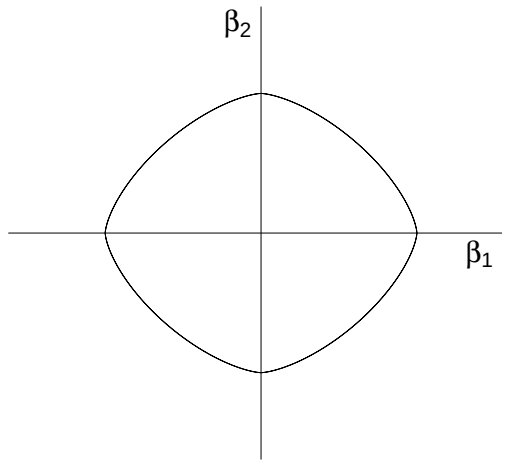
$||\beta||_{\frac{1}{2}} \leq t$



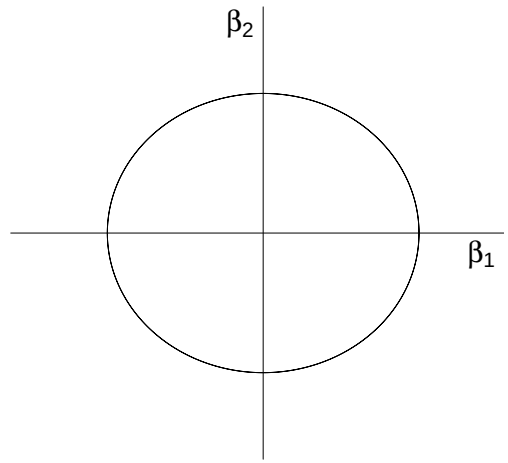
$||\beta||_{\frac{3}{4}} \leq t$



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

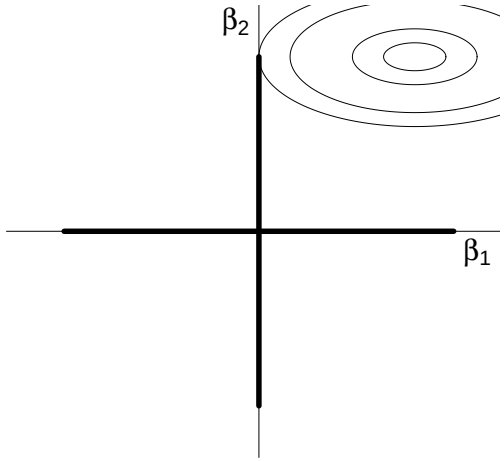


$||\beta||_{\frac{3}{2}} \leq t$

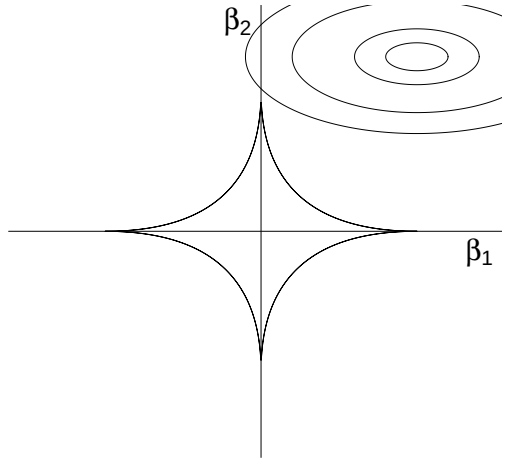


$||\beta||_2 \leq t$

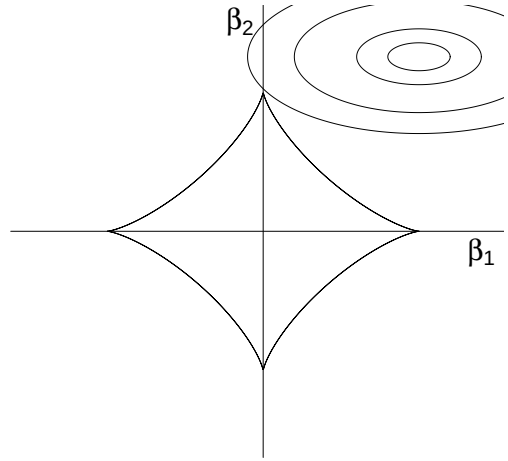
Geometry of regularization in $\mathbb{R}^2$: Model selection



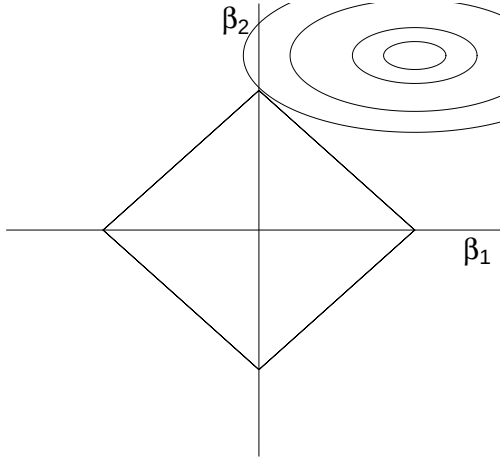
$||\beta||_0 \leq t$



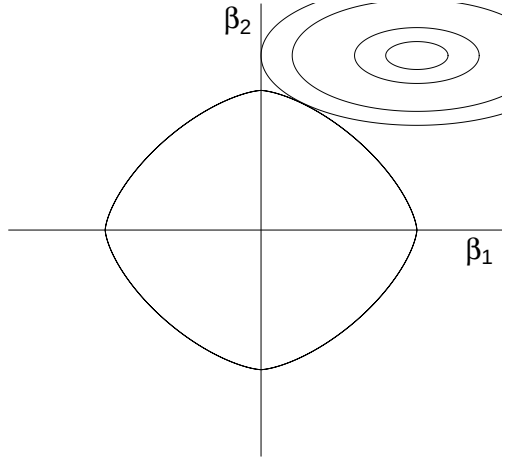
$||\beta||_{\frac{1}{2}} \leq t$



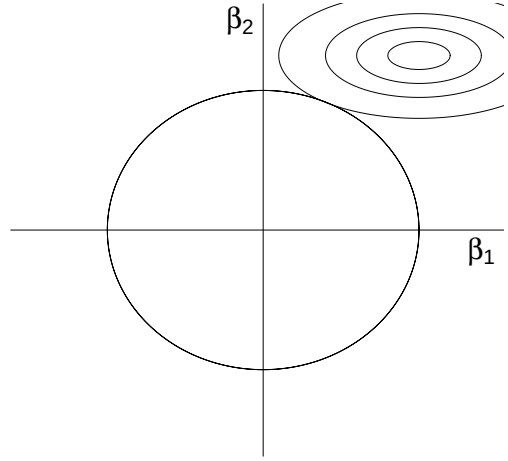
$||\beta||_{\frac{3}{4}} \leq t$



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

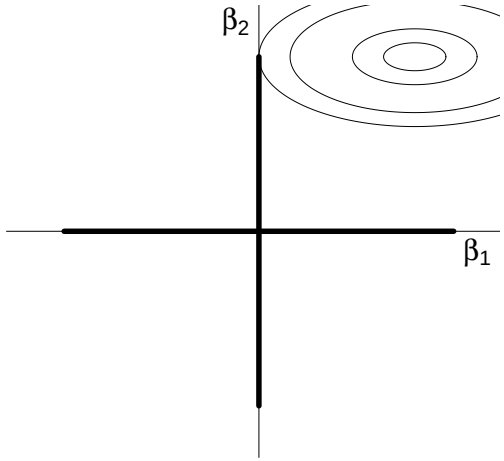


$||\beta||_{\frac{3}{2}} \leq t$

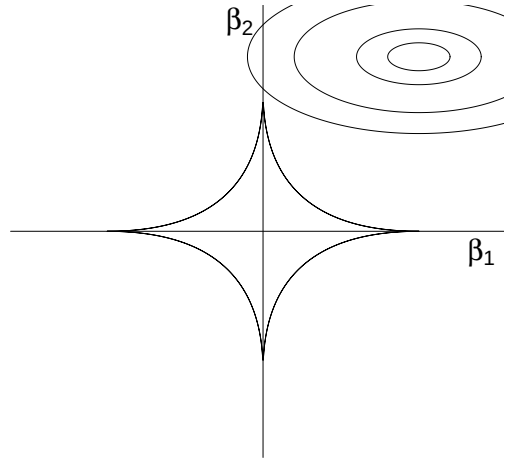


$||\beta||_2 \leq t$

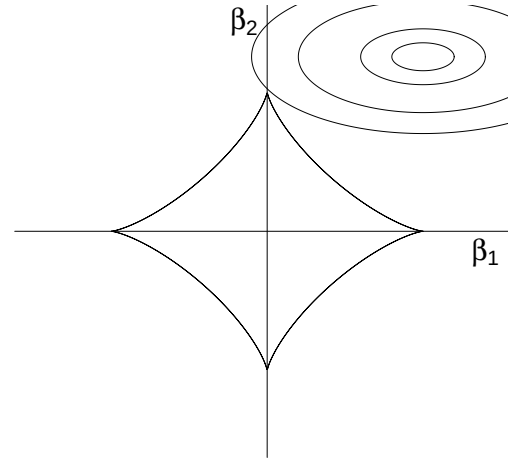
Geometry of regularization in $\mathbb{R}^2$: Model selection



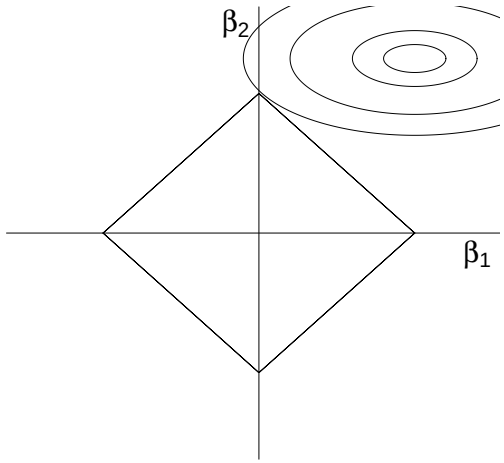
$||\beta||_0 \leq t$



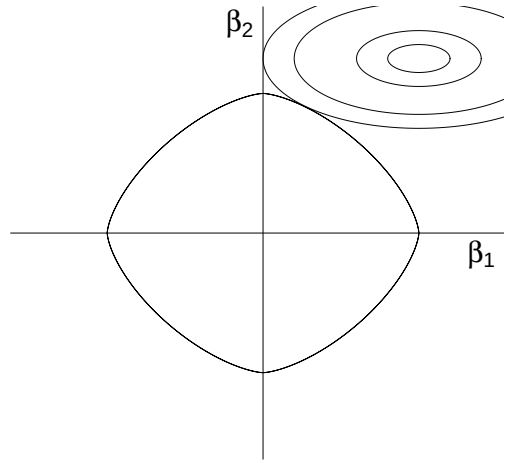
$||\beta||_{\frac{1}{2}} \leq t$



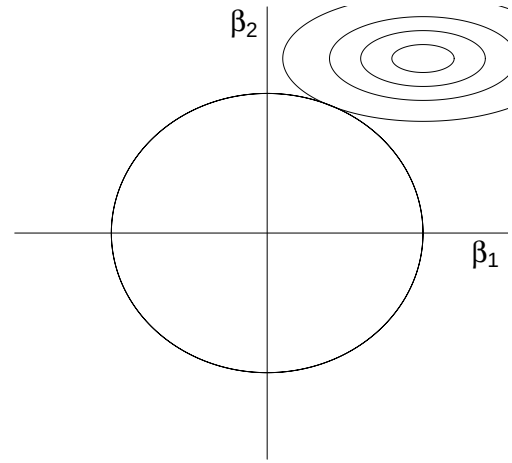
$||\beta||_{\frac{3}{4}} \leq t$



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

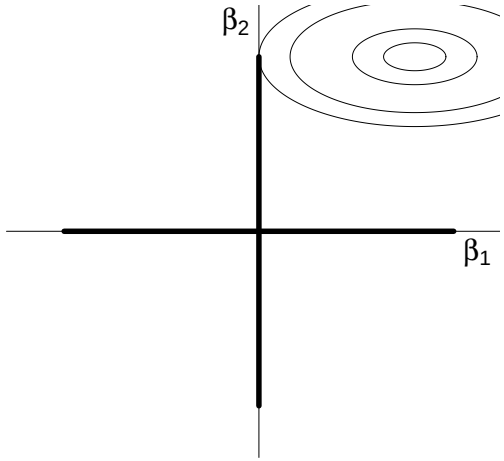


$||\beta||_{\frac{3}{2}} \leq t$

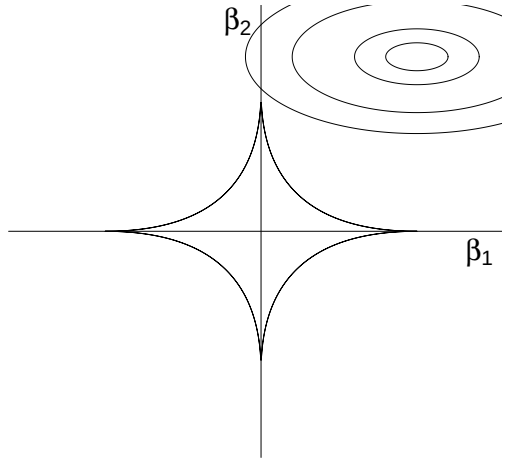


$||\beta||_2 \leq t$

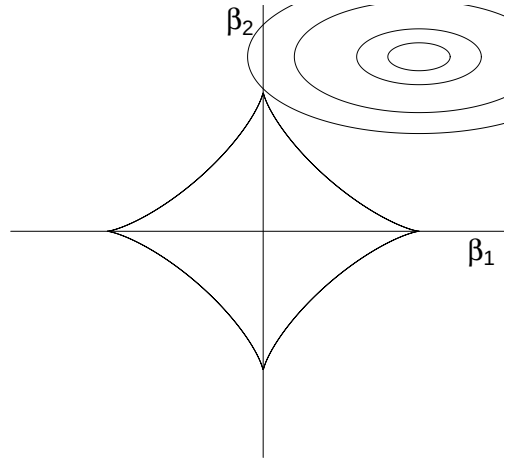
Geometry of regularization in $\mathbb{R}^2$: Model selection



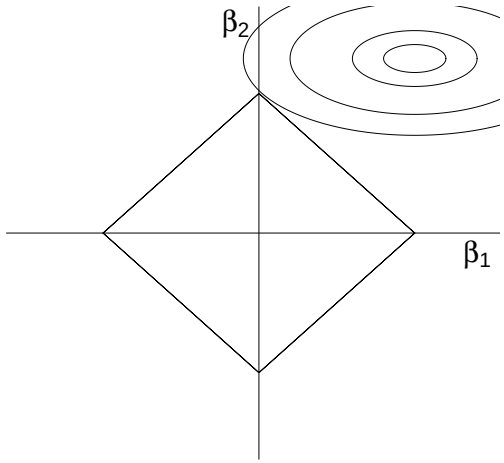
$||\beta||_0 \leq t$



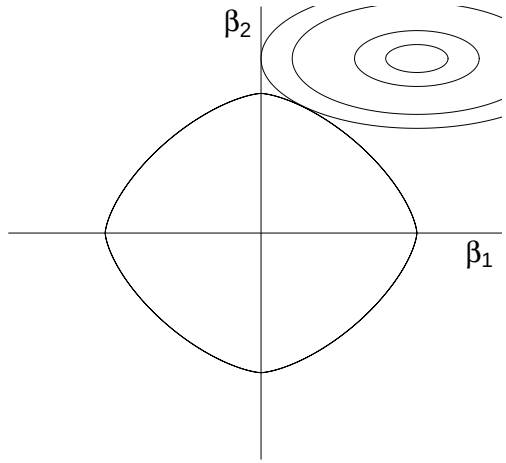
$||\beta||_{\frac{1}{2}} \leq t$



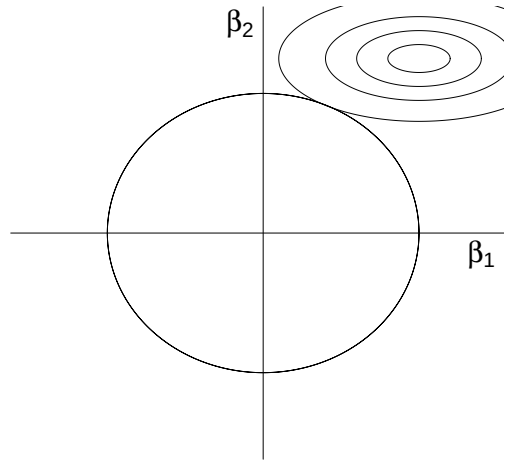
$||\beta||_{\frac{3}{4}} \leq t$



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

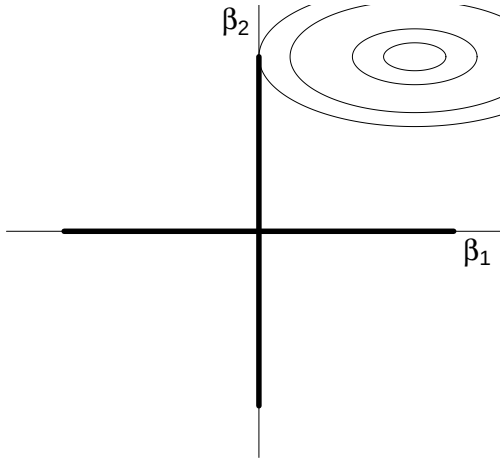


$||\beta||_{\frac{3}{2}} \leq t$

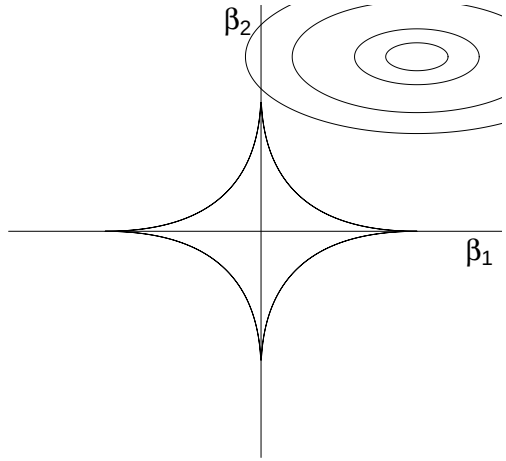


$||\beta||_2 \leq t$

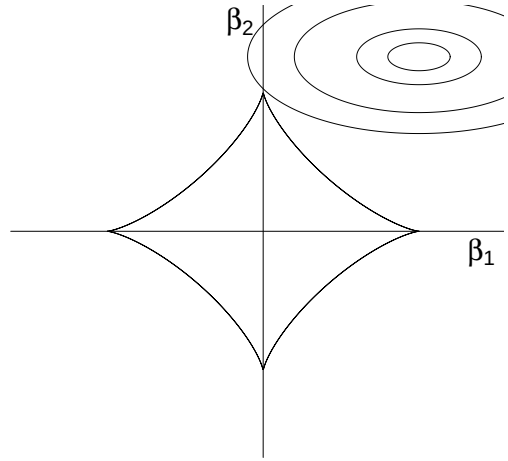
Geometry of regularization in $\mathbb{R}^2$: Both



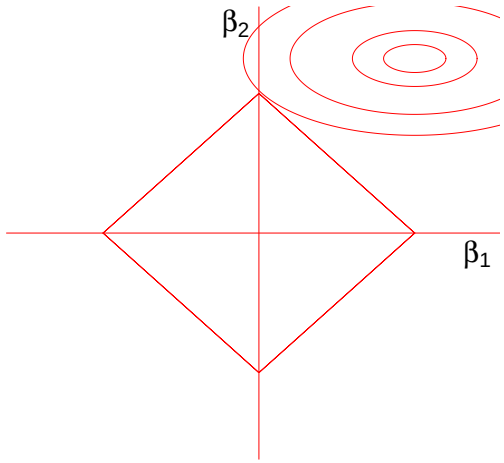
$||\beta||_0 \leq t$



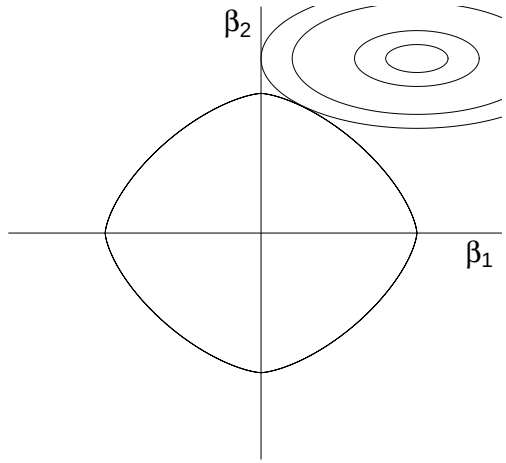
$||\beta||_{\frac{1}{2}} \leq t$



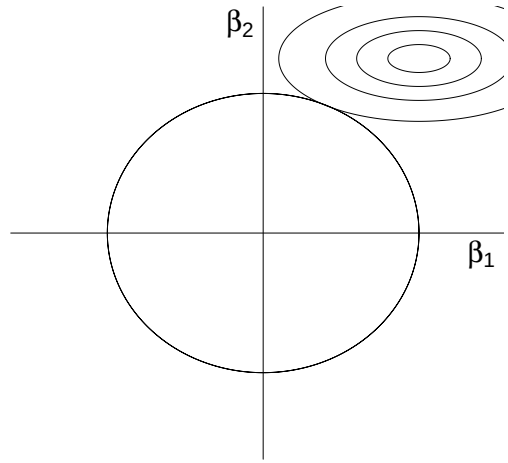
$||\beta||_{\frac{3}{4}} \leq t$



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



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

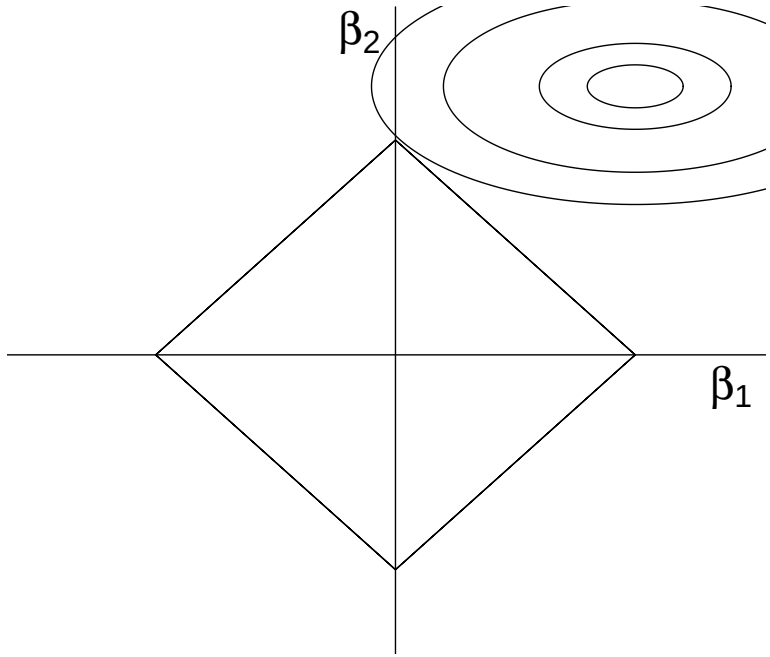


$||\beta||_2 \leq t$

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

Lasso

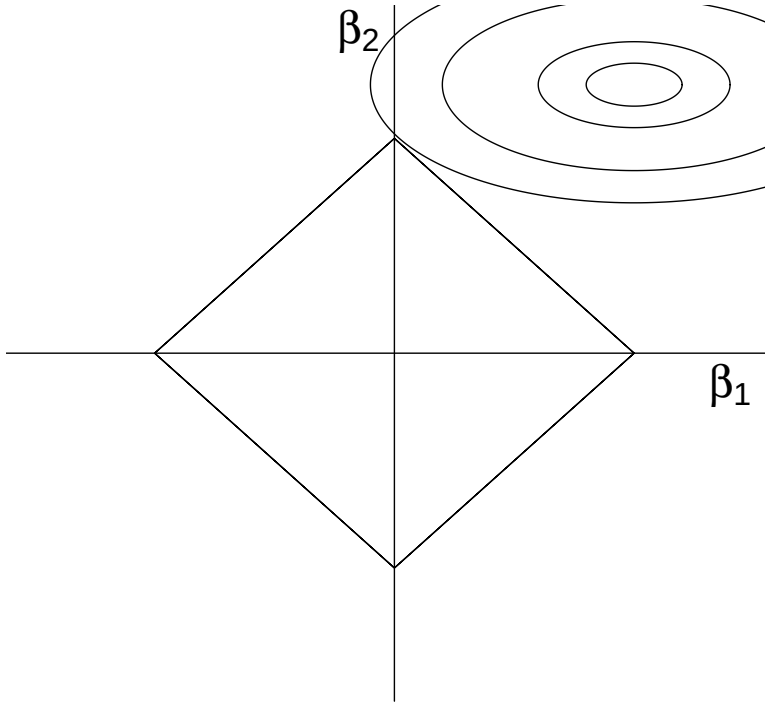
The estimator satisfies

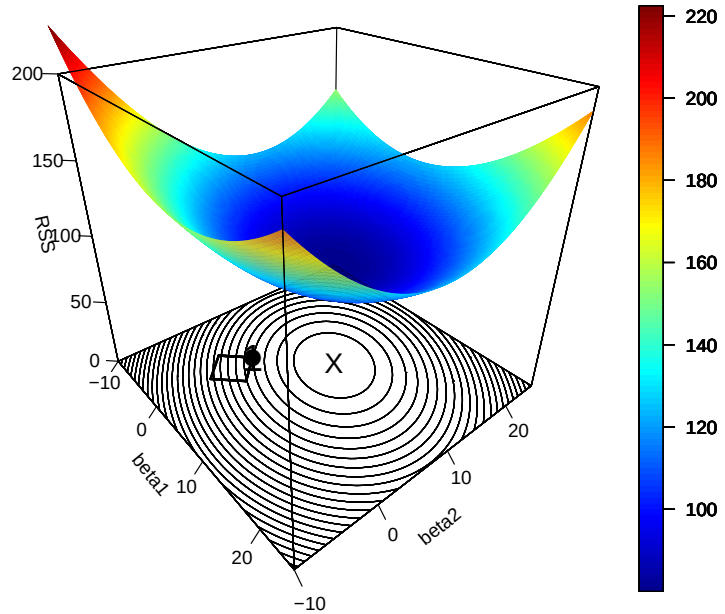
$$\hat{\beta}_{\text{lasso}}(t) = \underset{||\beta||_1 \leq t}{\text{argmin}} ||\mathbb{Y} - \mathbb{X}\beta||_2^2$$

In its corresponding Lagrangian dual form:

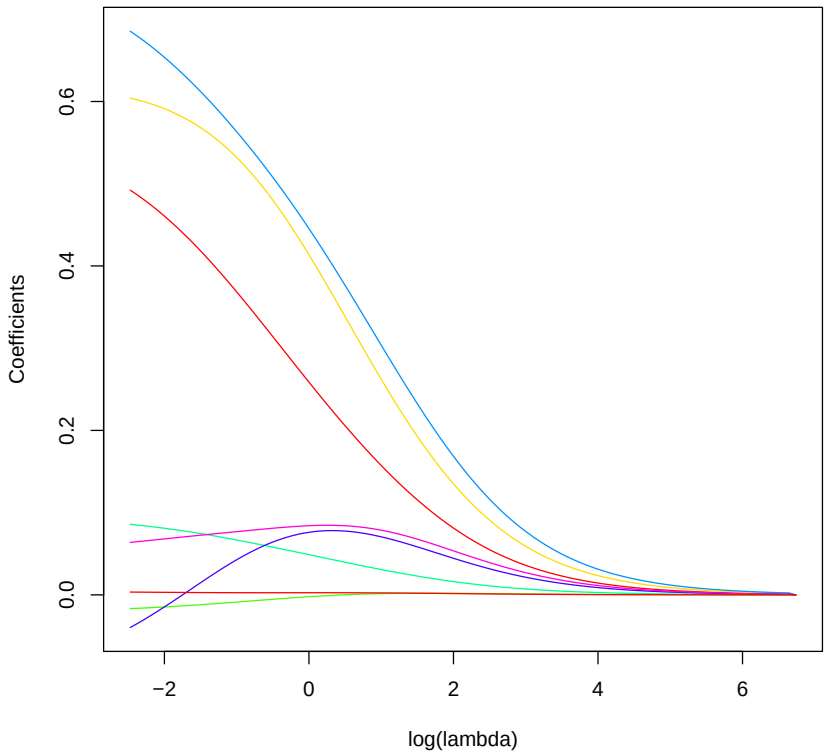
$$\hat{\beta}_{\text{lasso}}(\lambda) = \underset{\beta}{\text{argmin}} ||\mathbb{Y} - \mathbb{X}\beta||_2^2 + \lambda||\beta||_1$$

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

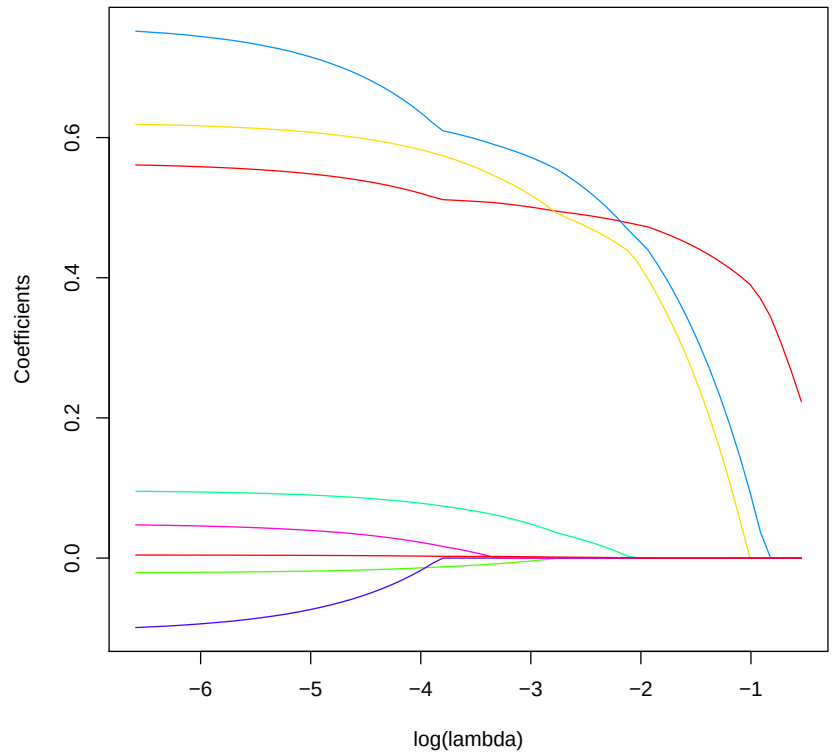




Lasso regression path



Ridge



Lasso

The lasso in R: glmnet

Luckily, we already know how to lasso

Just change the 'alpha =0' to 'alpha =1', and you're lassoing

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

glmnet uses an iterative scheme for finding the lasso solution over a grid of λ values

(Technically, it uses coordinate descent, which is related to gradient descent)

It can...

- handle other likelihoods than Gaussian
- supports/exploits sparse matrices (e.g. for text processing)
- use warm restarts for the grid of λ to produce more stable fits/faster computations

Optimality conditions: Review

$$\text{minimize } F(x) \tag{3}$$
$$\text{subject to } x \in \mathbb{R}^p \tag{4}$$

$$\text{Search for } x_* \text{ such that } \nabla F|_{x_*} = 0$$

- Turns a geometric problem into an algebraic problem: solve for the point where the gradient vanishes
- Is necessary for optimality of x_*. Is sufficient if F is convex and smooth.

Gradient descent: Intuition

A summary:

1. Start with some initial x^0
2. Propose x to reduce $F(x)$
3. Alternate between 1. and 2. until the objective function doesn't change (much).

Algorithmically, the implementations tend to look like

$$x[k+1] \leftarrow x[k] + \alpha[k]v[k],$$

where

- $x[k]$ is the current value of the minimizing parameter
- $v[k]$ is a direction that (hopefully) reduces F
- $\alpha[k]$ is a relaxation term.

Gradient descent

Define $\nabla F|_x \in \mathbb{R}^p$ to be the vector of partial derivatives

Recall the general form $x[k+1] \leftarrow x[k] + \alpha[k]v[k]$

Gradient descent follows the path of steepest descent

$$x[k+1] \leftarrow x[k] - \alpha[k]\nabla F|_{x[k]}$$

If F is a nice enough function, gradient descent is guaranteed to converge to a minimizer

Gradient descent example

If we look at multiple regression via least squares we get:

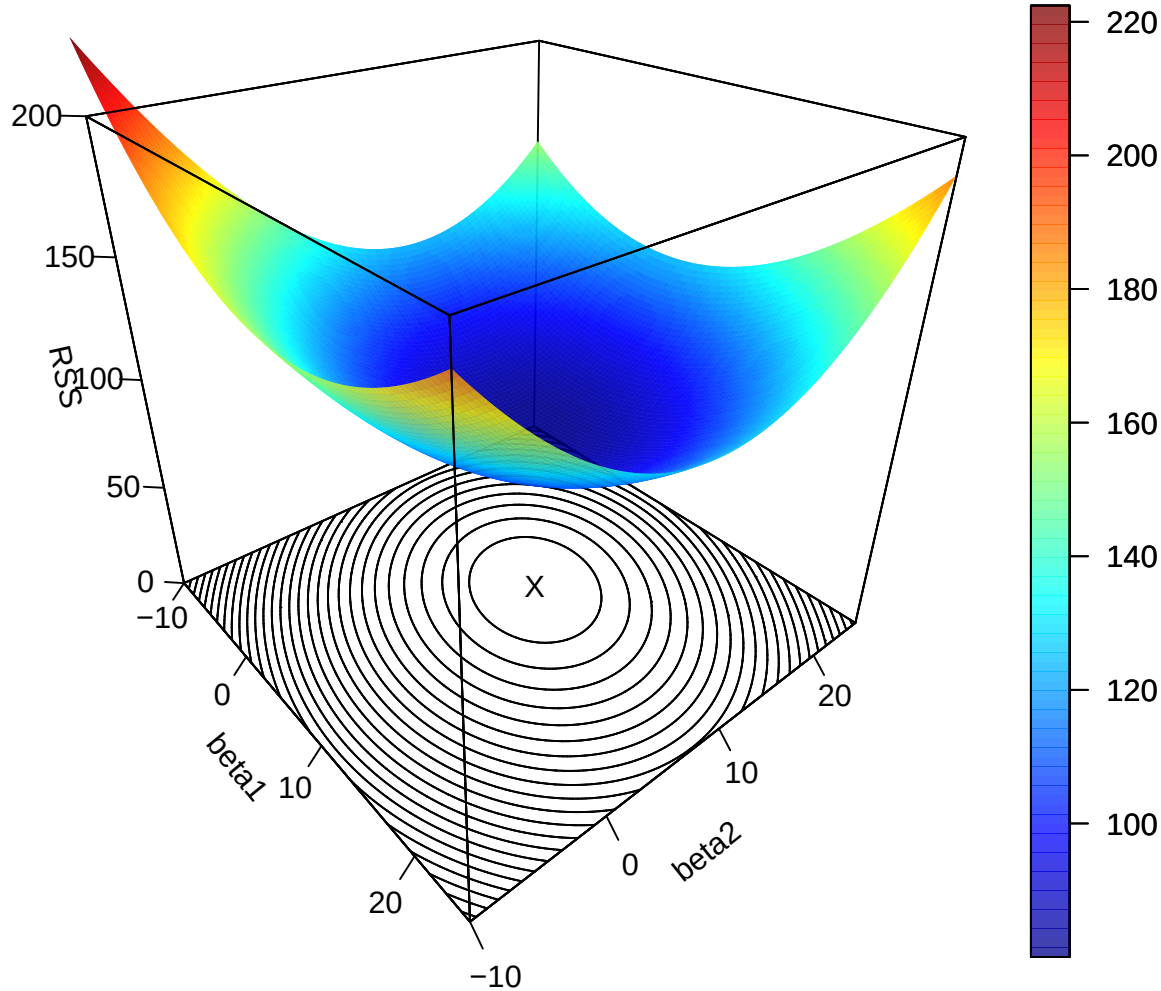
$$x \leftrightarrow \beta \qquad F(x) \leftrightarrow ||Y - \mathbb{X}\beta||_2^2$$

$$\begin{aligned}
\min_{\beta} ||Y - \mathbb{X}\beta||_2^2 \Rightarrow \frac{\partial}{\partial \beta_j} ||Y - \mathbb{X}\beta||_2^2 \\
&= \frac{\partial}{\partial \beta_j} \sum_{i=1}^{n} (Y_i - X_i^\top \beta)^2 \\
&= 2 \sum_{i=1}^{n} (Y_i - X_i^\top \beta) X_{ij}
\end{aligned}$$

For each $k = 1, 2, 3, ...,$ we cycle over j and make the update:

$$\hat{\beta}_j[k+1] = \hat{\beta}_j[k] - \alpha[k] \sum_{i=1}^{n} (Y_i - X_i^\top \hat{\beta}[k]) X_{ij}$$

Gradient descent example



With $RSS = ||Y - \mathbb{X}\beta||_2^2$ for $p = 2$

Stochastic gradient descent

The gradient descent update again:

$$\hat{\beta}_j[k+1] = \hat{\beta}_j[k] - \alpha[k] \sum_{i=1}^{n} (Y_i - X_i^\top \hat{\beta}[k]) X_{ij}$$

(We call this batch gradient descent)

Notice that it depends on all of the data $\rightarrow$ expensive to compute

Instead, we can randomly sample i from $\{1, 2, \ldots, n\}$ and use:

$$\hat{\beta}_j[k+1] = \hat{\beta}_j[k] - \alpha[k] (Y_i - X_i^\top \hat{\beta}[k]) X_{ij}$$

(We call this stochastic gradient descent)

Gradient descent: Relaxation term

The gradient descent update again:

$$\hat{\beta}_j[k+1] = \hat{\beta}_j[k] - \alpha[k] \sum_{i=1}^{n} (Y_i - X_i^\top \hat{\beta}[k]) X_{ij}$$

For either batch or stochastic gradient descent $\rightarrow$ choose $\alpha[k]$

Two common choices:

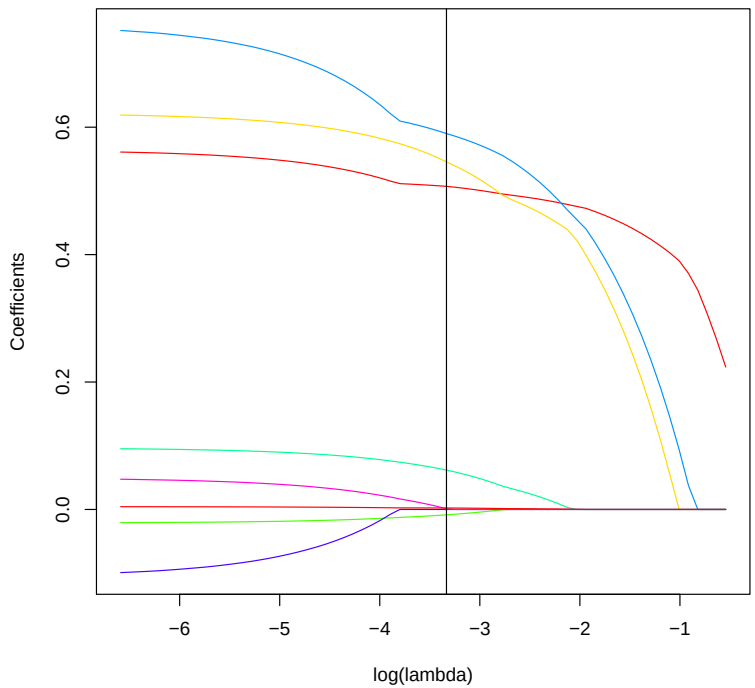
- Set $\alpha[k] = \alpha$ to some constant
  (Choose this constant very small)
- Set $\alpha[k] = \alpha/k$ for a large(ish) α

In both cases, check how fast $||\nabla F|_x||_2$ is decreasing. If too slow, increase α

The lasso in R: LARS

Alternatively, the lars package exploits the fact that the coefficient profiles are piecewise linear, which leads to an algorithm with the same computational cost as the full least-squares fit on the data

(Efron et al. (2004) for the LARS algorithm)



Choosing the tuning parameter for lasso

Note that for the grid λ, we need only look over the interval

$$\left[0, ||\mathbb{X}^\top Y||_\infty\right) = \left[0, \max_{1 \le j \le p} |x_j^\top Y|\right)$$

A grid of t has a similar restriction $[0, t_0)$, where

$$t_0 = \min_{\{b : \mathbb{X}b = 0\}} ||\hat{\beta}_{\text{LS}} + b||_1$$

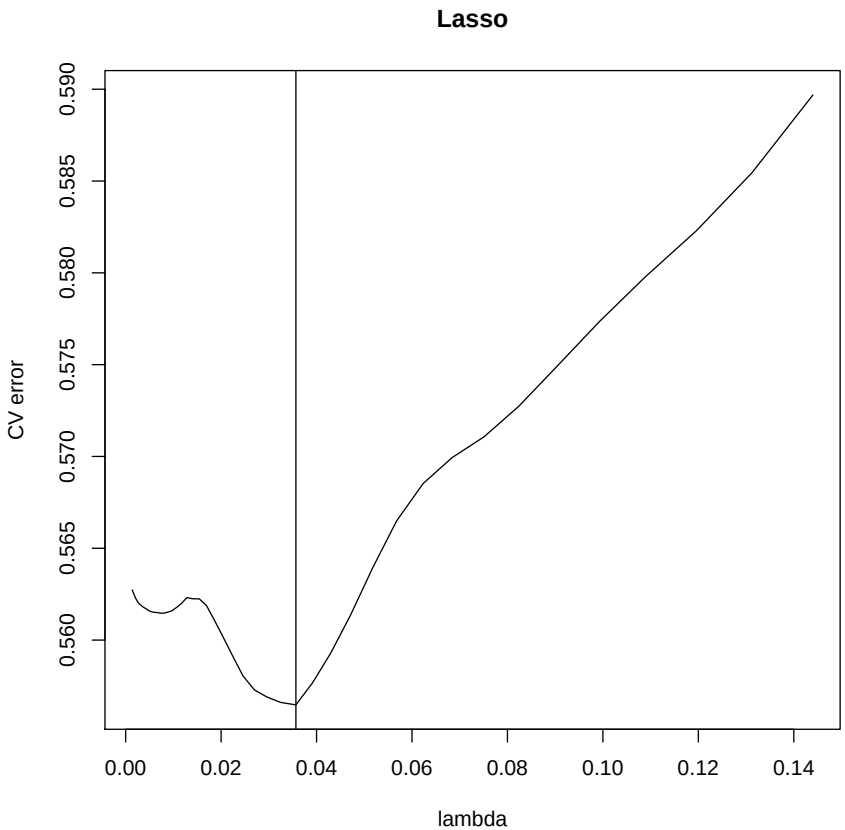
For cross-validation, the heavy lifting has been done for us

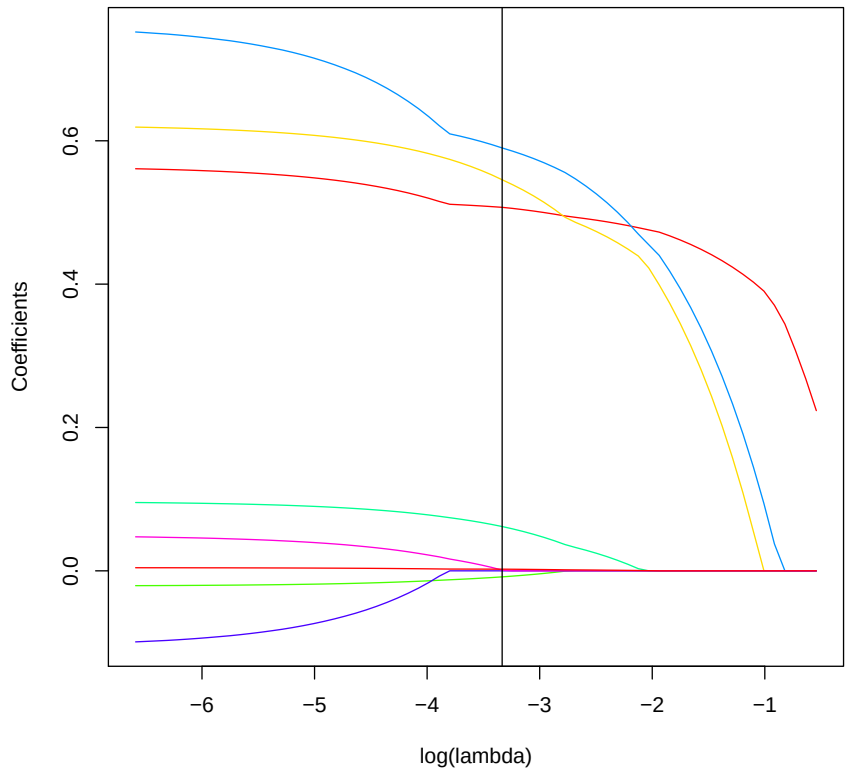
```
cv.glmnet(x=X,y=Y,alpha=1)
```

Alternatively, we can use GIC with:

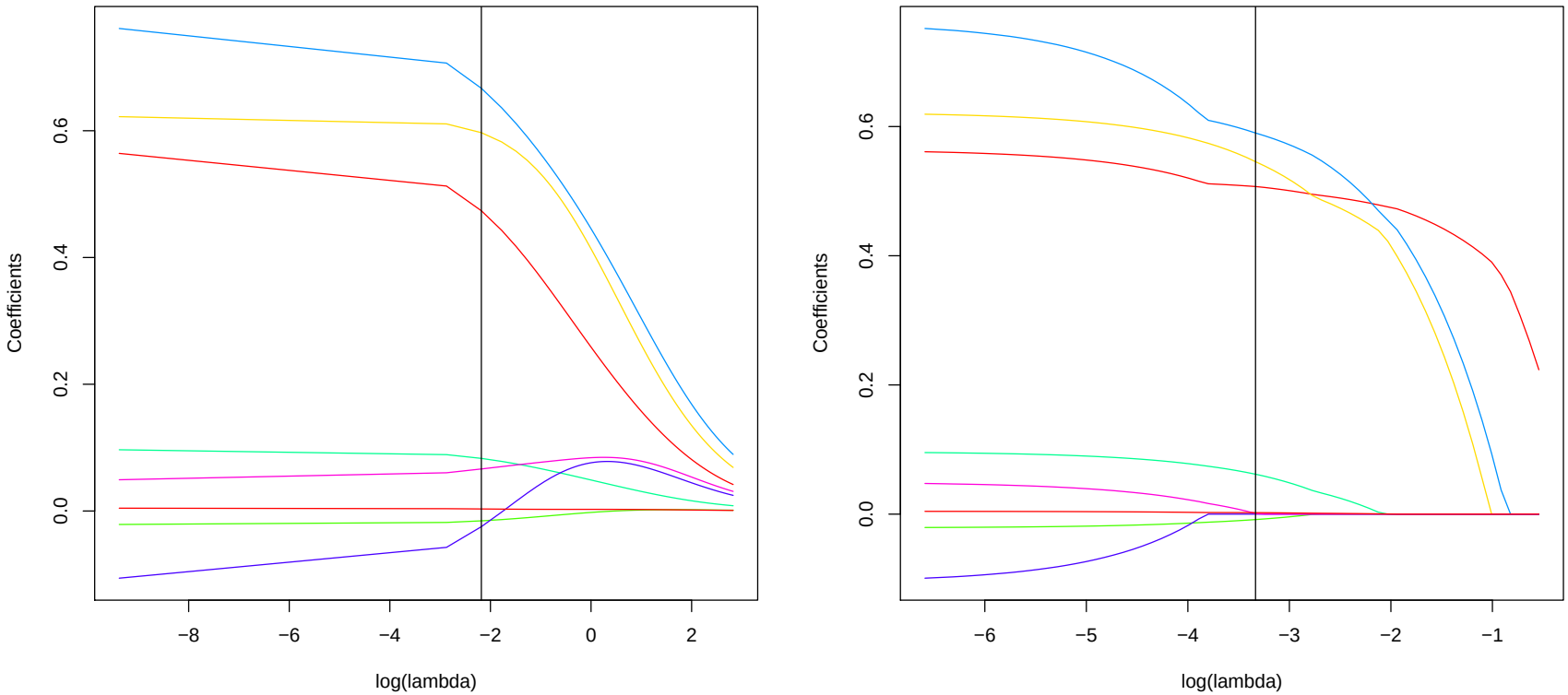
$$\hat{\text{df}}(\lambda) = \ \# \text{ of nonzero entries in } \hat{\beta}_{\text{lasso}}(\lambda)$$

The lasso coefficient path





Comparison: Regression path



Vertical line at minimum CV tuning parameter

Comparison of lars and glmnet

There are two main problems with glmnet

- 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 iterative nature sometimes results in bad coefficient vectors

  (such as having more than $\min\{n, p\}$ nonzero coefficients, which shouldn't happen)

There are two main problems with lars

- It is slow(er)
- It doesn't support other tasks like classification

Lasso: Using glmnet

```
> head(X)
          x1 x2no x2yes
1 -0.6264538    1     0
2  0.1836433    0     1
3 -0.8356286    0     1
4  1.5952808    1     0

Y = rnorm(50) + X %*% c(2,1,0)
XtestDf = data.frame('x1'=rnorm(50),
                     'x2'=sample(c('yes','no'),replace=T,size=50))
Xtest = model.matrix(~.-1,XtestDf)
Ytest    = rnorm(50) + Xtest %*% c(2,1,0)
```

How we procede depends on the scaling used

Lasso: Using glmnet

Have glmnet scale the matrix

```
out.glmnet = cv.glmnet(x=X,y=Y,alpha=1,intercept=FALSE)
> out.glmnet$glmnet.fit$beta[,1:5]
3 x 5 sparse Matrix of class "dgCMatrix"
      s0          s1        s2        s3        s4
x1     . 0.17933060 0.3315882 0.4703213 0.5967298
x2no   . 0.04758533 0.1432868 0.2304860 0.3099386
x2yes  . .          .         .         .
> coef(out.glmnet,s='lambda.min')
4 x 1 sparse Matrix of class "dgCMatrix"
                      1
(Intercept)  .
x1           1.85359875
x2no         1.10466792
x2yes       -0.07347329
Yhat       = predict(out.glmnet,type='link',
                     s='lambda.min',newx=Xtest)
> print(mean((Yhat-Ytest)**2))
[1] 1.303287
```

Lasso: Using glmnet

If we don't want glmnet to scale the entire matrix

```
qualFeature = c(FALSE,TRUE,TRUE)
scalings    = scale(X)
Xbar        = attributes(scalings)$'scaled:center'
> Xbar
       x1       x2no      x2yes
0.1004483 0.5200000 0.4800000
Xsd  = attributes(scalings)$'scaled:scale'
Xbar[qualFeature] = 0
Xsd[qualFeature]  = 1

XScale = scale(X,center=Xbar,scale=Xsd)
> head(XScale)
           x1 x2no x2yes
1 -0.8743173    1     0
2  0.1000669    0     1
3 -1.1259126    0     1
4  1.7979834    1     0
```

Lasso: Using glmnet

If we don't want glmnet to scale the entire matrix

```
out.glmnet = cv.glmnet(x=XScale,y=Y,alpha=1,
                       intercept=FALSE,standardize=FALSE)
> coef(out.glmnet,s='lambda.min')
4 x 1 sparse Matrix of class "dgCMatrix"
                    1
(Intercept) .
x1          1.494099
x2no        1.182825
x2yes       .

XtestScale = scale(Xtest,center=Xbar,scale=Xsd)
Yhat          = predict(out.glmnet,type='link',
                        s='lambda.min',newx=XtestScale)
> print(mean((Yhat-Ytest)**2))
[1] 1.330784
```

Lasso: Using lars

```
> out.lars = lars(X,Y,type='lasso',intercept=FALSE)
> summary(out.lars)
LARS/LASSO
Call: lars(x = X, y = Y, type = "lasso", intercept = FALSE)
  Df     Rss       Cp
0  0 225.359 247.2196
1  1  55.694  25.4540
2  2  39.777   6.4612
3  3  35.636   3.0000
> out.lars$Cp
         0          1          2          3
247.219562  25.454022   6.461221   3.000000
attr(,"sigma2")
        3
0.7582225
attr(,"n")
[1] 50
```

Postamble:

- All subsets and its stepwise approximations involve trading of between global & slow and local & fast
- Instead, we approach this problem via convex relaxation, which means solving a nearby problem in a global & fast way.
  (This can be seen by relaxing the non-convex constraint set to a convex set)
- Different relaxations result in different procedures
  (Choosing a 'circle' constraint set leads to ridge regression while choosing a 'diamond' constraint set leads to the lasso)