Ridge Regression in R

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Math 243: Stat Learning

October 15th, 2021

Outline

In today's class, we will...

- Discuss LASSO as a method of penalized regression AND variable selection

Section 1

The LASSO

Metrics on R^p

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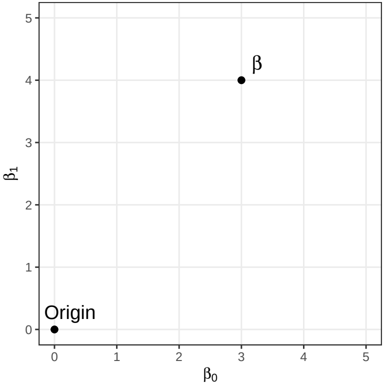
- Sometimes, its useful to consider the ℓ_0 "norm" and ℓ_∞ norm

$$\|x\|_0 = \#(x_i \neq 0) \qquad \|x\|_\infty = \max |\beta_i|$$

Geometric Perspective



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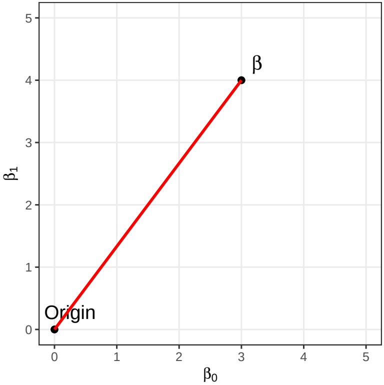

- $\|\beta\|_2 = \sqrt{3^2 + 4^2} = 5$

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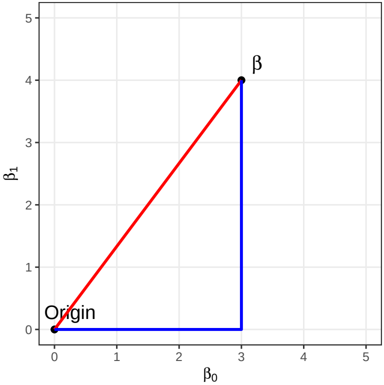

- $\|\beta\|_2 = \sqrt{3^2 + 4^2} = 5$
- $\|\beta\|_1 = 3 + 4 = 7$

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- What does a circle of radius r look like in the ℓ_2 norm?

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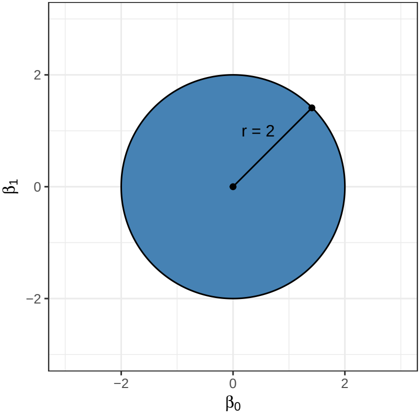
$$\sqrt{\beta_0^2 + \beta_1^2} = \|\beta\|_2 \leq r$$



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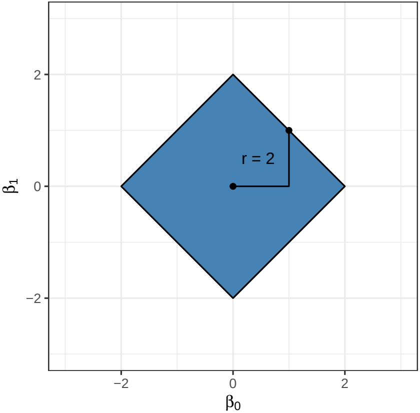

LASSO

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- In addition to shrinking coefficients, it also happens to perform variable selection!

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Suppose q is 0, 1, or 2. For each $\lambda \geq 0$, there is exactly one $s \geq 0$ so that if β minimizes

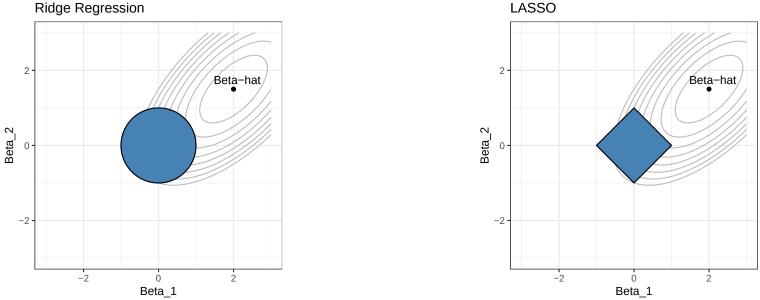
$$\mathrm{RSS} + \lambda\|\beta\|_q$$

then β minimizes

$$\mathrm{RSS} \qquad \text{subject to } \|\beta\|_q \leq s$$

Variable Selection with LASSO

For LASSO, the solution to the optimization problem often lies on a vertex of the domain, which corresponds to a subspace where one or more parameters are 0.



- Contours denote lines of constant RSS.

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  - In general, LASSO tends to outperform Ridge Regression in cases where some of the coefficients are nearly or truly 0.
  - Ridge Regression outperforms LASSO when all coefficients are significant (but variance is still a liability for MSE)

Section 2

LASSO in R

Solubility, once more

The `solubility` data set from the `AppliedPredictiveModeling` package contains solubility and chemical structure for a sample of 1,267 different compounds.

- But suppose we only have a fraction of the data to work with. . .

```
set.seed(1013)
library(AppliedPredictiveModeling)
data(solubility)
solTest <- data.frame(solTestX, Solubility = solTestY) %>% sample_frac(.3)
solTrain <- data.frame(solTrainX, Solubility =  solTrainY) %>% sample_frac(.3)
solTest <- solTest %>% dplyr::select(!starts_with("FP"))
solTrain <- solTrain %>%  dplyr::select(!starts_with("FP"))
```

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```
library(glmnet)
grid = 10^(seq( -5, 5, length = 100))
x<-model.matrix(Solubility ~., data = solTrain)[,-1]
y<-solTrain$Solubility
lasso_mod <- glmnet(x, y, alpha = 1, lambda = grid)
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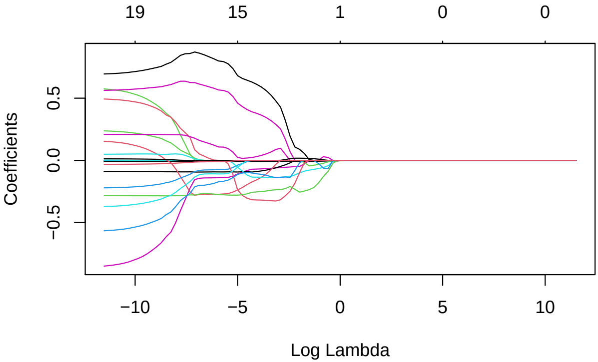
- But note what happens to coefficients:

```
coef(lasso_mod)[1:5,c(1:3,98:100)]
```

```
## 5 x 6 sparse Matrix of class "dgCMatrix"
##                    s0        s1        s2           s97           s98
## (Intercept)  -2.775404 -2.775404 -2.775404  6.393845e-01  6.413927e-01
## MolWeight     .         .         .        -8.100227e-03 -8.100687e-03
## NumAtoms      .         .         .        -5.785492e-04 -6.844627e-04
## NumNonHAtoms  .         .         .         2.340836e-01  2.358484e-01
## NumBonds      .         .         .        -1.342641e-05 -1.501692e-05
##                       s99
## (Intercept)   6.430179e-01
## MolWeight    -8.101076e-03
## NumAtoms     -7.733290e-04
## NumNonHAtoms  2.372857e-01
## NumBonds     -2.094374e-05
```

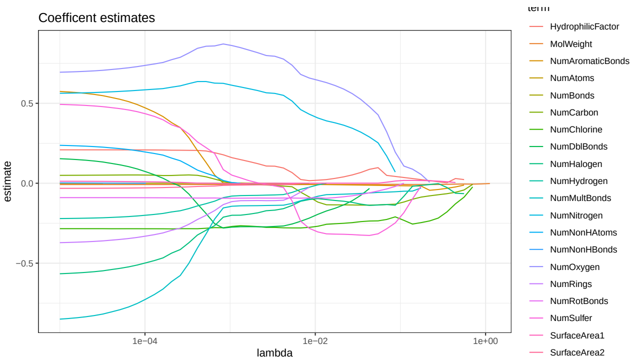
Coefficient Paths

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



Coefficient Paths

```
library(broom)
tidied <- tidy(lasso_mod) %>% filter(term != "(Intercept)")
ggplot(tidied, aes(lambda, estimate, group = term, color = term)) +
    geom_line() + scale_x_log10()+ theme_bw()+labs(title = "Coeffcent estimates")
```



Cross-Validation

- To find the optimal penalty, we use `cv.glmnet`:

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```
set.seed(1010)
my_cv<-cv.glmnet(x, y, alpha = 1, lambda = grid, nfolds = 10)

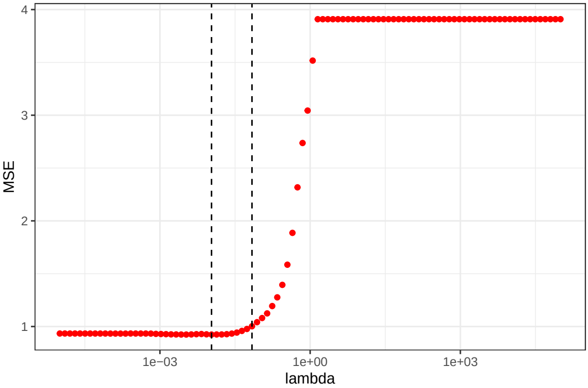
best_L <- my_cv$lambda.min
reg_L <- my_cv$lambda.1se

data.frame(best_L, reg_L)
```

```
##   best_L  reg_L
## 1 0.0107 0.0689
```

Cross-validation plot

```
tidied <- tidy(my_cv)
ggplot(tidied, aes(x = lambda, y = estimate))+geom_point( color = "red")+
  scale_x_log10()+theme_bw()+labs(y = "MSE")+
  geom_vline(xintercept = best_L, linetype = "dashed" )+
  geom_vline(xintercept = reg_L, linetype = "dashed")
```



Feature Selection

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```
s <- which(lasso_mod$lambda==best_L)
s
```

```
## [1] 70
```

```
coef(lasso_mod)[,s]
```

```
##       (Intercept)         MolWeight          NumAtoms      NumNonHAtoms
##           0.03232          -0.00806           0.00000           0.00000
##          NumBonds       NumNonHBonds      NumMultBonds       NumRotBonds
##           0.00000           0.00000          -0.08122          -0.09071
##       NumDblBonds  NumAromaticBonds       NumHydrogen         NumCarbon
##          -0.19428           0.00000          -0.01010          -0.11791
##       NumNitrogen         NumOxygen         NumSulfer       NumChlorine
##           0.40824           0.64413          -0.30461          -0.26894
##        NumHalogen          NumRings HydrophilicFactor      SurfaceArea1
##          -0.09626           0.00000           0.01904           0.00000
##      SurfaceArea2
##           0.00000
```

```
sum(coef(lasso_mod)[,s] !=0 )
```

```
## [1] 13
```

Overall Performance

- Recall that glmnet already fits a model, so we just need to use predict to get predictions:

```
x_tst <- model.matrix(Solubility ~., data = solTest)[,-1]
lasso_preds <- predict(lasso_mod, s = best_L, newx = x_tst)
mse <- mean( (solTest$Solubility - lasso_preds)^2)
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```
##    full rr_min lasso_min lasso_1se
## 1 0.753  0.739     0.725     0.734
```

- **LASSO wins!**