Penalized Regression

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Penalized regression

- Another potential remedy for collinearity
- Decreases variability of estimated coefficients at the cost of introducing bias
- Also known as regularization
- Important beyond the collinearity context
  - Certain types of penalties can be used for variable selection in a natural way
  - Penalized regression provides solutions in ill-posed (rank-deficient) problems
  - Familiar examples of such models are ANOVA models with all dummy variables
  - A more realistic situation is models with $p > n$ (more covariates than observations)

Penalized likelihood and Bayesian interpretation

- We have already seen an example of penalized regression: smoothing splines
- Given data $\{(x_i, y_i) : x_i \in [a, b]\}$, goal is to find f that minimizes (given $\lambda > 0$)

$$\sum_i (y_i - f(x_i))^2 + \lambda \int_a^b (f''(t))^2 dt$$

- The solution is a natural cubic spline
- Here f is the parameter of interest
- The (ill-posed) least squares problem is regularized by adding a penalty for "undesirable" (wiggly) solutions
- The same idea can be applied for usual (finite-dimensional) parameters as well
- Penalized regression is a special case of the more general penalized likelihood approach
- This is easiest to motivate using a Bayesian argument
- Consider unknown parameter θ and observed data y with

$$\begin{aligned} \theta &\sim p(\theta) \qquad \text{(prior)} \\ y|\theta &\sim p(y|\theta) \end{aligned}$$

- Bayesian inference is based on the posterior distribution of θ, given by

$$p(\theta|y) = \frac{p(\theta, y)}{p(y)} = \frac{p(\theta)\, p(y|\theta)}{p(y)}$$

- Here $p(y)$ is the marginal density of y given by

$$p(y) = \int p(\theta)\, p(y|\theta)\, d\theta$$

- How does posterior $p(\theta|y)$ lead to inference on θ?
- We could look at $E(\theta|y)$, $V(\theta|y)$, etc.
- We could also look at the maximum-a-posteriori (MAP) estimator

$$\hat{\theta} = \arg\max_{\theta} p(\theta|y)$$

- This is analagous to MLE in the classical frequentist setup
- Unfortunately, $p(y)$ is in general difficult to compute
- This has led to methods to simulate from $p(\theta|y)$ without knowing $p(y)$ (MCMC)
- Fortunately, MAP estimation does *not* require $p(y)$, which does not depend on θ
- $\hat{\theta}$ is given by

$$\begin{aligned}
\hat{\theta} &= \arg\max_{\theta}\ p(\theta|y) \\
&= \arg\max_{\theta}\ \frac{p(\theta)\, p(y|\theta)}{p(y)} \\
&= \arg\max_{\theta}\ p(y|\theta)\, p(\theta) \\
&= \arg\max_{\theta}\ [\log p(y|\theta) + \log p(\theta)]
\end{aligned}$$

- The first term is precisely the usual log-likelihood
- The second term can be viewed as a "regularization penalty" for "undesirable" θ

Penalized regression: normal linear model with normal prior

- Assume the usual normal linear model

$$\mathbf{y}|\mathbf{X}, \beta \sim N(\mathbf{X}\beta, \sigma^2\mathbf{I})$$

- Addidionally, assume an i.i.d. mean-zero normal prior for each β_j

$$\beta \sim N(\mathbf{0}, \tau^2\mathbf{I})$$

- Then it is easy to see that if L is the penalized log-likelihood, then

$$-2L(\beta) = C(\sigma^2, \tau^2) + \frac{1}{\sigma^2}\sum_{i=1}^{n}(y_i - \mathbf{x}_i^T\beta)^2 + \frac{1}{\tau^2}\sum_{j=1}^{p}\beta_j^2$$

- Thus, the MAP estimate of β is (as a function of the unknown σ^2 and "prior parameter" τ^2)

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n}(y_i - \mathbf{x}_i^T\beta)^2 + \frac{\sigma^2}{\tau^2}\sum_{j=1}^{p}\beta_j^2$$

Ridge regression

- This is known as Ridge regression, with the problem defined in terms of the "tuning parameter" λ

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - \mathbf{x}_i^T \beta)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

- As discussed earlier, this approach does not really make sense unless columns of $\mathbf{X}$ are standardized
- It is also not meaningful to penalize the intercept
- For these reasons, in what follows, we assume without loss of generality that
  - Columns of $\mathbf{X}$ have been centered and scaled to have mean 0 and variance 1
  - $\mathbf{y}$ has been centered to have mean 0
  - The model is fit without an intercept (which is separately estimated as $\bar{y}$)
- In practice, these issues are usually handled by model fitting software in the background

Ridge regression: solution

- It is easy to see that the objective function to be minimized is

$$\mathbf{y}^T\mathbf{y} + \beta^T\mathbf{X}^T\mathbf{X}\beta - 2\mathbf{y}^T\mathbf{X}\beta + \lambda\beta^T\beta = \mathbf{y}^T\mathbf{y} + \beta^T(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\beta - 2\mathbf{y}^T\mathbf{X}\beta$$

- The corresponding normal equations are

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})\beta = \mathbf{X}^T\mathbf{y}$$

- This gives the Ridge estimator

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

- Note that $\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}$ is *always* invertible
- To prove this, use the singular value decomposition of $\mathbf{X}^T\mathbf{X} = \mathbf{A}\mathbf{\Lambda}\mathbf{A}^T$

$$\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I} = \mathbf{A}(\mathbf{\Lambda} + \lambda\mathbf{I})\mathbf{A}^T$$

- Even if $\mathbf{\Lambda}$ has some zero diagonal entries, all diagonal entries of $\mathbf{\Lambda} + \lambda\mathbf{I}$ are at least λ
- As $\lambda \to 0$, $\hat{\beta}_{ridge} \to \hat{\beta}_{OLS}$
- As $\lambda \to \infty$, $\hat{\beta}_{ridge} \to \mathbf{0}$
- In the special case where columns of $\mathbf{X}$ are orthogonal ($\mathbf{A} = \mathbf{I}$)

$$\hat{\beta}_{ridge} = \frac{1}{1+\lambda}\hat{\beta}_{OLS}$$

- This illustates the essential feature of ridge regression: shrinkage towards 0 (the prior mean of β)
- The ridge penalty introduces bias by shrinkage but reduces variance

Ridge regression in the presence of collinearity

- Recall our experiment with simulated collinearity

```
simCollinear <- function(n = 100)
{
    z1 <- rnorm(n)
    z2 <- rnorm(n)
    x1 <- z1 + z2 + 0.1 * rnorm(n)
    x2 <- z1 - 2 * z2 + 0.1 * rnorm(n)
    x3 <- 2 * z1 - z2 + 0.1 * rnorm(n)
    y <- x1 + 2 * x2 + 2 * rnorm(n) # x3 has coefficient 0
    data.frame(y, x1, x2, x3)
}
d3 <- simCollinear()
lm(y ~ . , data = d3)
```

```

Call:
lm(formula = y ~ ., data = d3)

Coefficients:
(Intercept)           x1           x2           x3
    -0.3256       0.7419       1.8612       0.1909
```

```
library(MASS) # for lm.ridge()
lm.ridge(y ~ . , data = d3, lambda = 1)
```

```
                   x1         x2         x3
-0.3339996  0.1511181  1.2421567  0.7907122
```

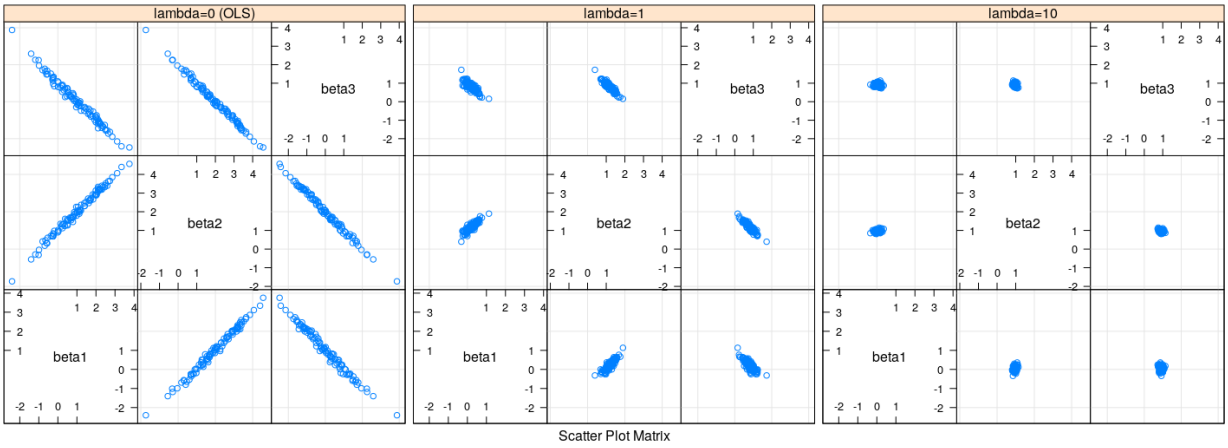
```
lm.ridge(y ~ . , data = d3, lambda = 10)
```

```
                     x1          x2          x3
-0.34263086  0.01199235  1.03851408  0.89352016
```

```
## Replicate this several times
sim.results <-
    replicate(100,
    {
        d3 <- simCollinear()
        beta.ols <- coef(lm(y ~ . , data = d3))[-1]
        beta.ridge.1 <- coef(lm.ridge(y ~ . , data = d3, lambda = 1))[-1]
        beta.ridge.10 <- coef(lm.ridge(y ~ . , data = d3, lambda = 10))[-1]
        data.frame(beta1 = c(beta.ols[1], beta.ridge.1[1], beta.ridge.10[1]),
                   beta2 = c(beta.ols[2], beta.ridge.1[2], beta.ridge.10[2]),
                   beta3 = c(beta.ols[3], beta.ridge.1[3], beta.ridge.10[3]),
                   which = c("lambda=0 (OLS)", "lambda=1", "lambda=10"))
    }, simplify = FALSE)
sim.df <- do.call(rbind, sim.results)
```

Ridge regression in the presence of collinearity

```
splom(~ data.frame(beta1, beta2, beta3) | which, data = sim.df, grid = TRUE)
```



Bias and variance of Ridge regression

- Recall that true $\beta = (1, 2, 0)$

```
with(sim.df, rbind(tapply(beta1, which, mean),
                   tapply(beta2, which, mean),
                   tapply(beta3, which, mean)))
```

```
     lambda=0 (OLS)  lambda=1  lambda=10
[1,]    1.024926051 0.2217080 0.04698428
[2,]    1.997629453 1.1864466 0.96557666
[3,]   -0.005341892 0.7949516 0.92124664
```

```
with(sim.df, rbind(tapply(beta1, which, sd),
                   tapply(beta2, which, sd),
                   tapply(beta3, which, sd)))
```

```
     lambda=0 (OLS)  lambda=1  lambda=10
[1,]       1.163054 0.2630750 0.11957701
[2,]       1.174441 0.2519598 0.07013490
[3,]       1.171263 0.2512505 0.08062144
```

- The variance of the ridge estimator is

$$V(\hat{\beta}) = \sigma^2 \mathbf{W}\mathbf{X}^T\mathbf{X}\mathbf{W} \quad \text{where} \quad \mathbf{W} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}$$

- The expectation of the ridge estimator is

$$E(\hat{\beta}) = \mathbf{W}\mathbf{X}^T\mathbf{X}\beta$$

- The bias of the ridge estimator is

$$\text{bias}(\hat{\beta}) = (\mathbf{W}\mathbf{X}^T\mathbf{X} - \mathbf{I})\beta = -\lambda\mathbf{W}\beta$$

- This follows because

$$\mathbf{W}(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}) = \mathbf{I} \implies \mathbf{W}\mathbf{X}^T\mathbf{X} - \mathbf{I} = \lambda\mathbf{W}$$

- It can be shown that
  - the total variance $\sum_j V(\hat{\beta}_j)$ is monotone decreasing w.r.t. λ
  - the total squared bias $\sum_j \text{bias}^2(\hat{\beta}_j)$ is monotone increasing w.r.t. λ
- It can also be shown that there exists some λ for which the total MSE of $\hat{\beta}$ is less than the MSE of $\hat{\beta}_{OLS}$
- This is a surprising result that is an instance of a more general phenomenon in decision theory
- Note however that the total MSE has no useful interpretation for the overall fit
- We still need to address the problem of choosing λ
- Before doing so, let us consider a related (but much more interesting) estimator called LASSO

LASSO

- LASSO stands for "Least Absolute Shrinkage and Selection Operator"
- The LASSO estimator is given by solving a penalized regression with a L_1 penalty (rather than L_2)

$$\hat{\beta} = \arg\min_{\beta} \quad \frac{1}{2}\sum_{i=1}^{n}(y_i - \mathbf{x}_i^T\beta)^2 + \lambda\sum_{j=1}^{p}|\beta_j|$$

- This corresponds to an i.i.d. double exponential prior on each β_j
- Even though the change seems subtle, the behaviour of the estimator changes dramatically
- The problem is much more difficult to solve numerically (except when $\mathbf{X}$ is orthogonal — exercise)
- It is an area of active research, and implementations have improved considerably over the last few decades
- We will not go into further theoretical details, but only look at some practical aspects

LASSO in the presence of collinearity

```
library(glmnet) # usage: glmnet(X, y, alpha, ...)
coef(with(d3, glmnet(cbind(x1, x2, x3), y, alpha = 1, lambda = 1)))
```

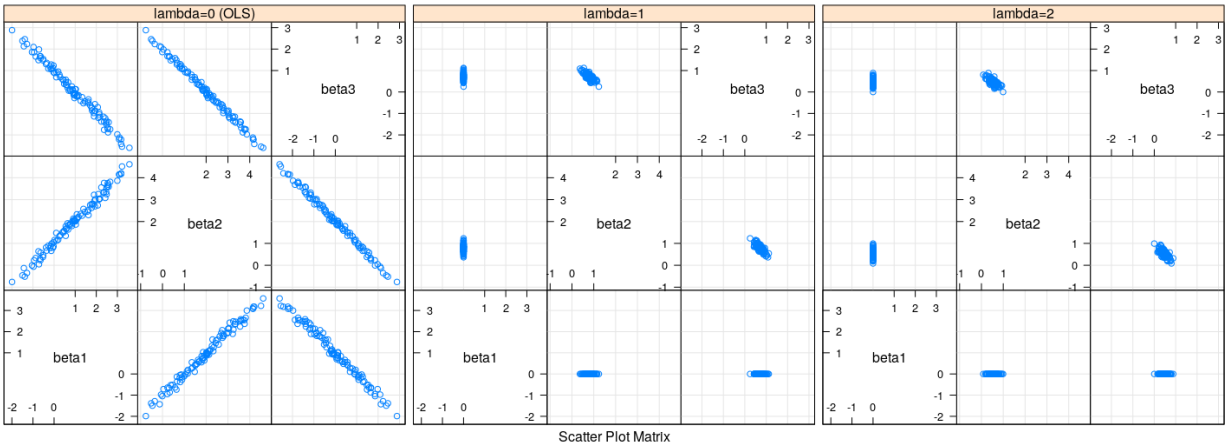
```
4 x 1 sparse Matrix of class "dgCMatrix"
                    s0
(Intercept) -0.3733872
x1           .
x2           0.8227224
x3           0.6775433
```

```
## Replicate this several times
sim.results.lasso <-
    replicate(100,
    {
        d3 <- simCollinear()
        beta.ols <- coef(lm(y ~ . , data = d3))[-1]
        fm.lasso <- with(d3, glmnet(cbind(x1, x2, x3), y, alpha = 1, lambda = c(2, 1)))
```

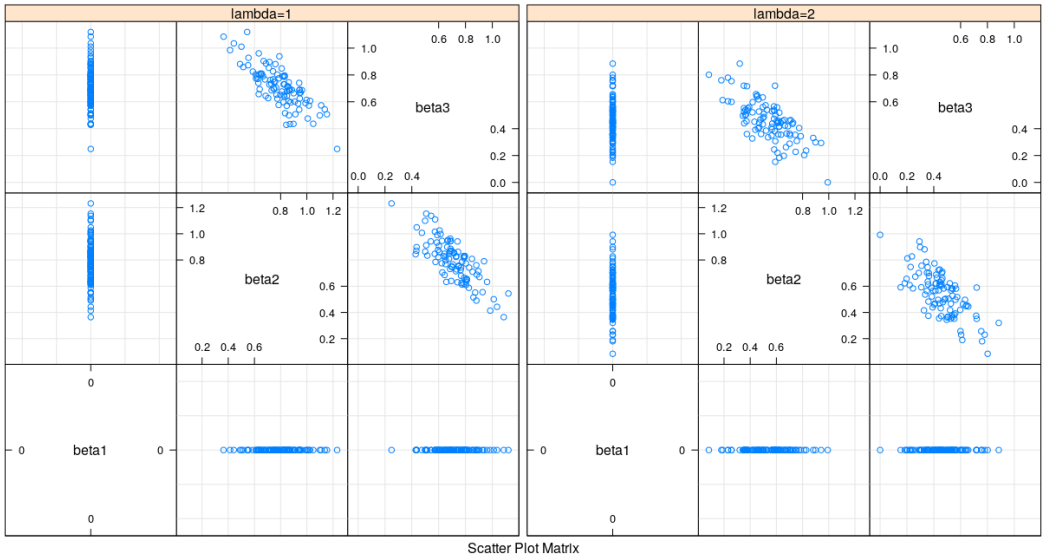
```
        beta.lasso <- as.matrix(coef(fm.lasso))[-1, ]
        data.frame(beta1 = c(beta.ols[1], beta.lasso[1,2], beta.lasso[1,1]),
                   beta2 = c(beta.ols[2], beta.lasso[2,2], beta.lasso[2,1]),
                   beta3 = c(beta.ols[3], beta.lasso[3,2], beta.lasso[3,1]),
                   which = c("lambda=0 (OLS)", "lambda=1", "lambda=2"))
    }, simplify = FALSE)
sim.df.lasso <- do.call(rbind, sim.results.lasso)
```

LASSO in the presence of collinearity

```
splom(~ data.frame(beta1, beta2, beta3) | which, data = sim.df.lasso, grid = TRUE)
```




```
splom(~ data.frame(beta1, beta2, beta3) | which, data = sim.df.lasso, grid = TRUE, subset = which != "la
```



Bias and variance of LASSO

- Recall that true $\beta = (1, 2, 0)$

```
with(sim.df.lasso, rbind(tapply(beta1, which, mean),
                         tapply(beta2, which, mean),
                         tapply(beta3, which, mean)))
```

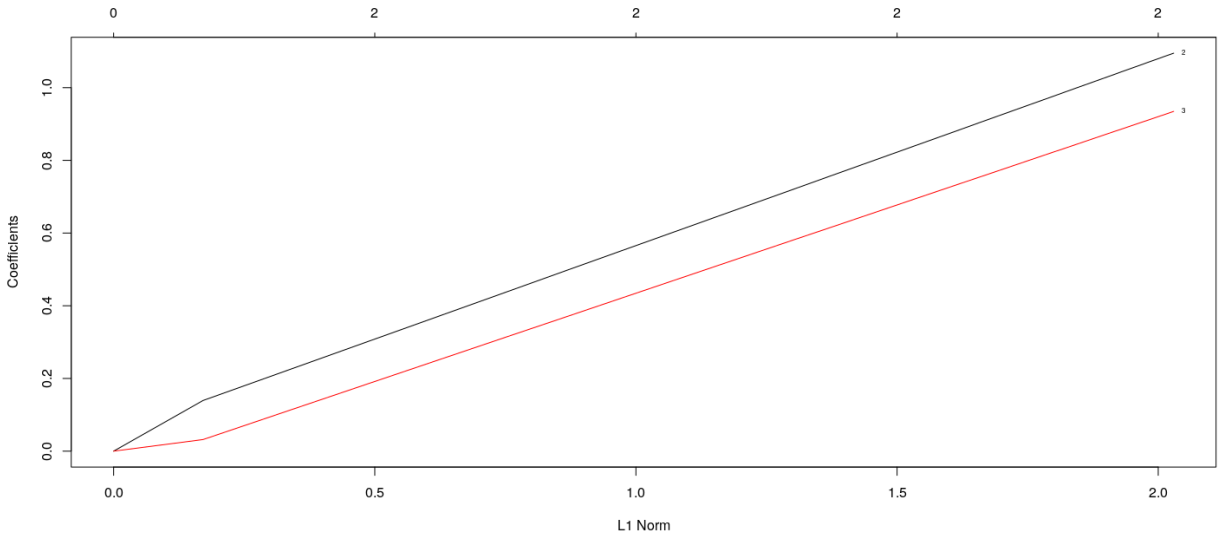
```
     lambda=0 (OLS)  lambda=1  lambda=2
[1,]    0.972813560 0.0000000 0.0000000
[2,]    2.008541811 0.7920059 0.5423446
[3,]   -0.002656804 0.7109653 0.4587019
```

```
with(sim.df.lasso, rbind(tapply(beta1, which, sd),
                         tapply(beta2, which, sd),
                         tapply(beta3, which, sd)))
```

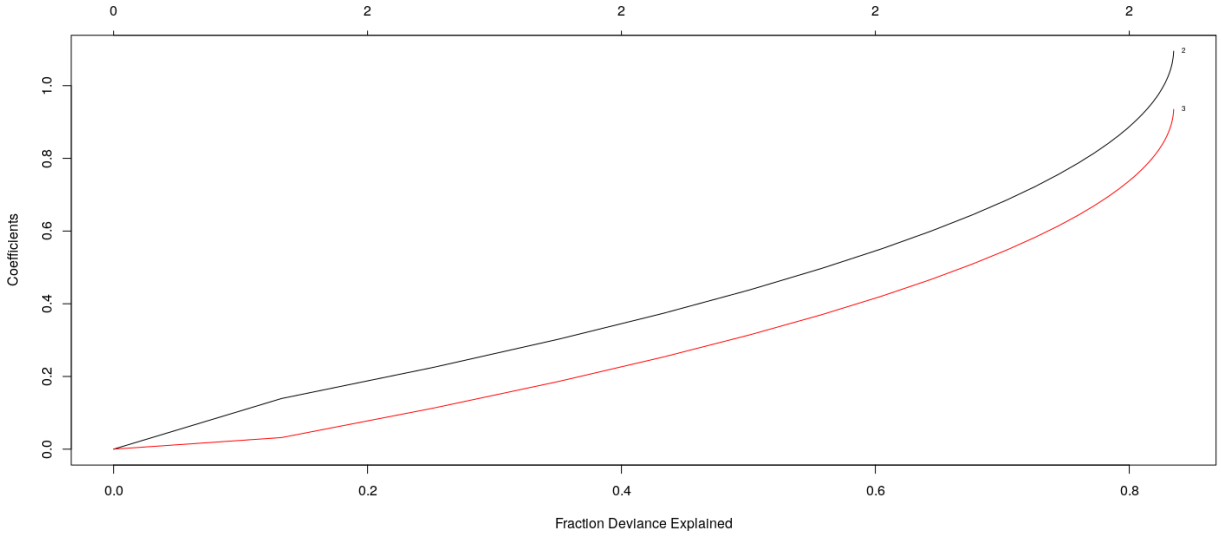
```
     lambda=0 (OLS)  lambda=1  lambda=2
[1,]       1.282199 0.0000000 0.0000000
[2,]       1.274482 0.1630202 0.1698728
[3,]       1.281313 0.1495002 0.1506298
```

Coefficients as a function of λ : LASSO

```
fm.lasso <- with(d3, glmnet(cbind(x1, x2, x3), y, alpha = 1))
plot(fm.lasso, xvar = "norm", label = TRUE)
```

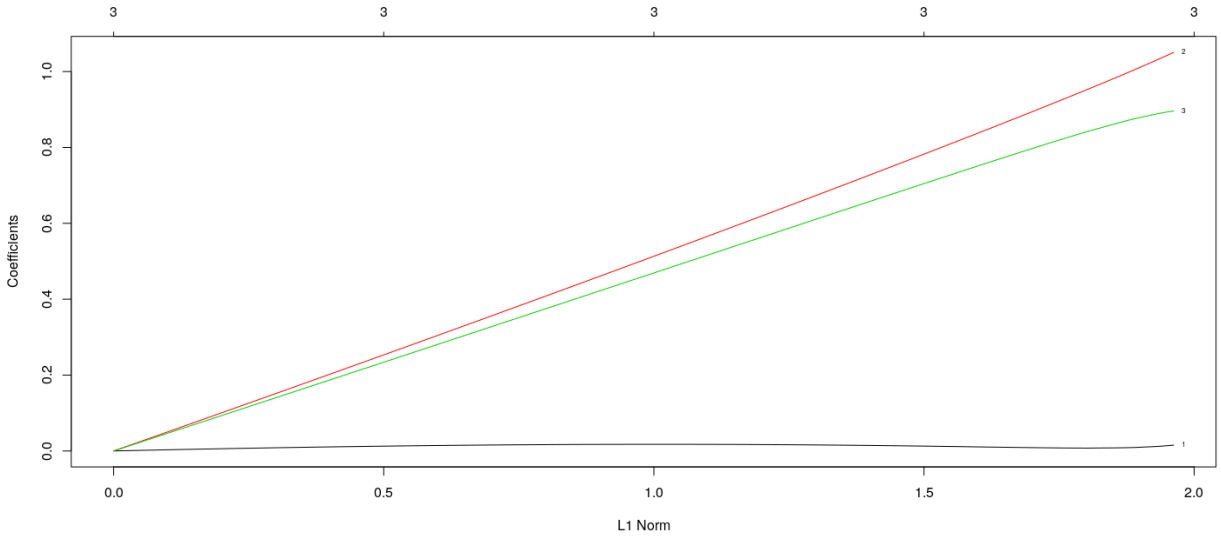



```
fm.lasso <- with(d3, glmnet(cbind(x1, x2, x3), y, alpha = 1))
plot(fm.lasso, xvar = "dev", label = TRUE)
```

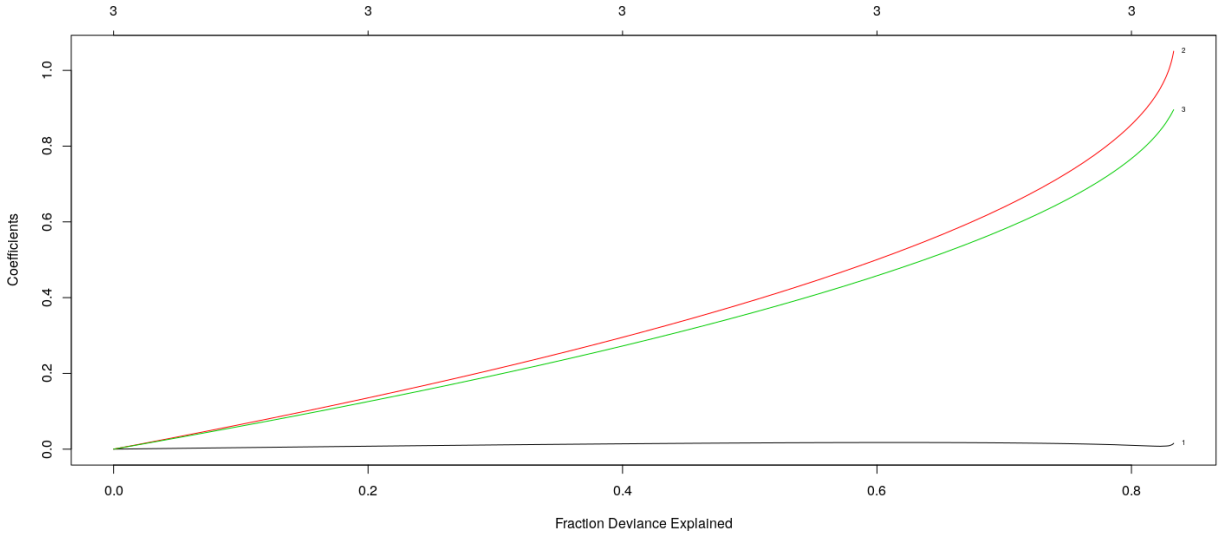


Coefficients as a function of λ : Ridge

```
fm.ridge <- with(d3, glmnet(cbind(x1, x2, x3), y, alpha = 0))
plot(fm.ridge, xvar = "norm", label = TRUE)
```




```
fm.ridge <- with(d3, glmnet(cbind(x1, x2, x3), y, alpha = 0))
plot(fm.ridge, xvar = "dev", label = TRUE)
```



Example: Salary of hitters in Major League Baseball (1987)

```
data(Hitters, package = "ISLR")
str(Hitters)
```

```
'data.frame':   322 obs. of  20 variables:
 $ AtBat    : int  293 315 479 496 321 594 185 298 323 401 ...
 $ Hits     : int  66 81 130 141 87 169 37 73 81 92 ...
 $ HmRun    : int  1 7 18 20 10 4 1 0 6 17 ...
 $ Runs     : int  30 24 66 65 39 74 23 24 26 49 ...
 $ RBI      : int  29 38 72 78 42 51 8 24 32 66 ...
 $ Walks    : int  14 39 76 37 30 35 21 7 8 65 ...
 $ Years    : int  1 14 3 11 2 11 2 3 2 13 ...
 $ CAtBat   : int  293 3449 1624 5628 396 4408 214 509 341 5206 ...
 $ CHits    : int  66 835 457 1575 101 1133 42 108 86 1332 ...
 $ CHmRun   : int  1 69 63 225 12 19 1 0 6 253 ...
 $ CRuns    : int  30 321 224 828 48 501 30 41 32 784 ...
 $ CRBI     : int  29 414 266 838 46 336 9 37 34 890 ...
 $ CWalks   : int  14 375 263 354 33 194 24 12 8 866 ...
 $ League   : Factor w/ 2 levels "A","N": 1 2 1 2 2 1 2 1 2 1 ...
 $ Division : Factor w/ 2 levels "E","W": 1 2 2 1 1 2 1 2 2 1 ...
 $ PutOuts  : int  446 632 880 200 805 282 76 121 143 0 ...
 $ Assists  : int  33 43 82 11 40 421 127 283 290 0 ...
 $ Errors   : int  20 10 14 3 4 25 7 9 19 0 ...
 $ Salary   : num  NA 475 480 500 91.5 750 70 100 75 1100 ...
 $ NewLeague: Factor w/ 2 levels "A","N": 1 2 1 2 2 1 1 1 2 1 ...
```

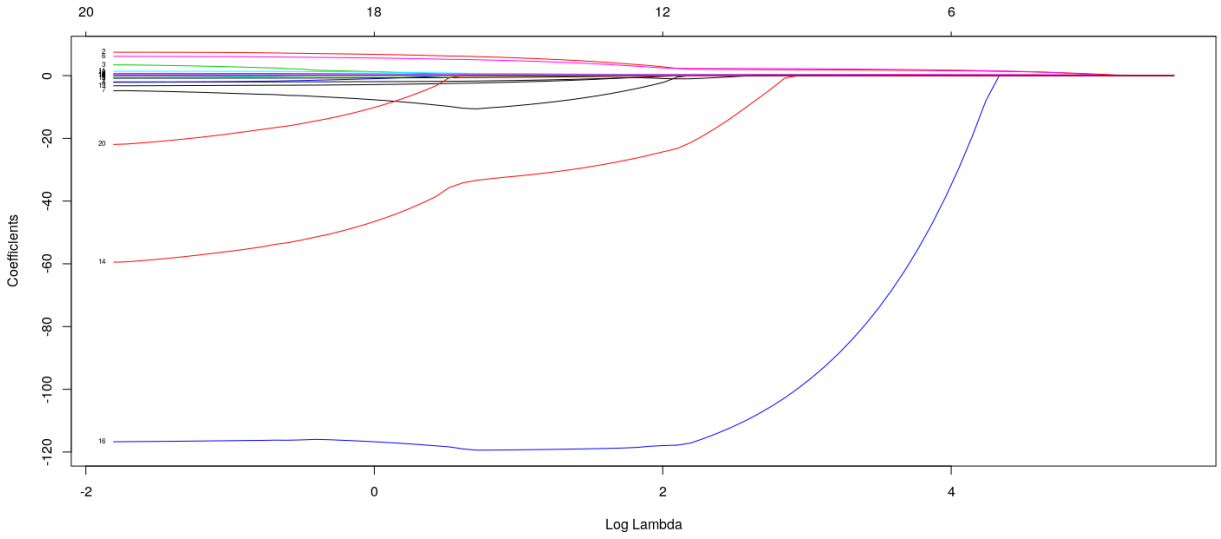
```
Hitters <- na.omit(Hitters)
dim(Hitters)
```

```
[1] 263  20
```

```
y <- Hitters$Salary
X <- model.matrix( ~ . - Salary - 1, Hitters) # converts factors into dummy variables
```

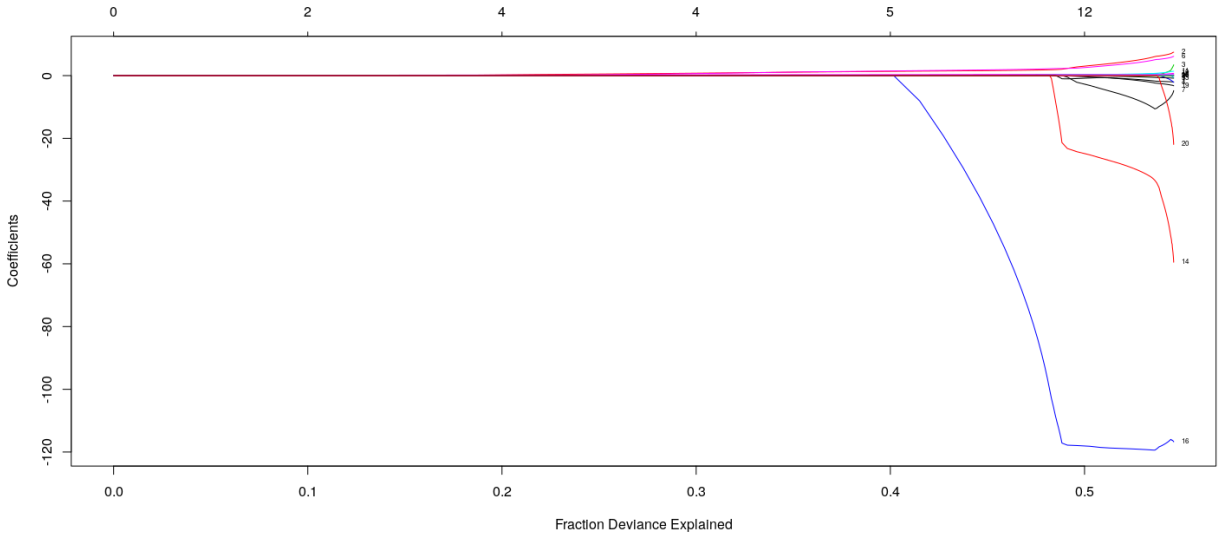
```
fm.lasso <- glmnet(X, y, alpha = 1)
fm.ridge <- glmnet(X, y, alpha = 0)

## top axis labels indicate number of nonzero coefficients
plot(fm.lasso, xvar = "lambda", label = TRUE)
```



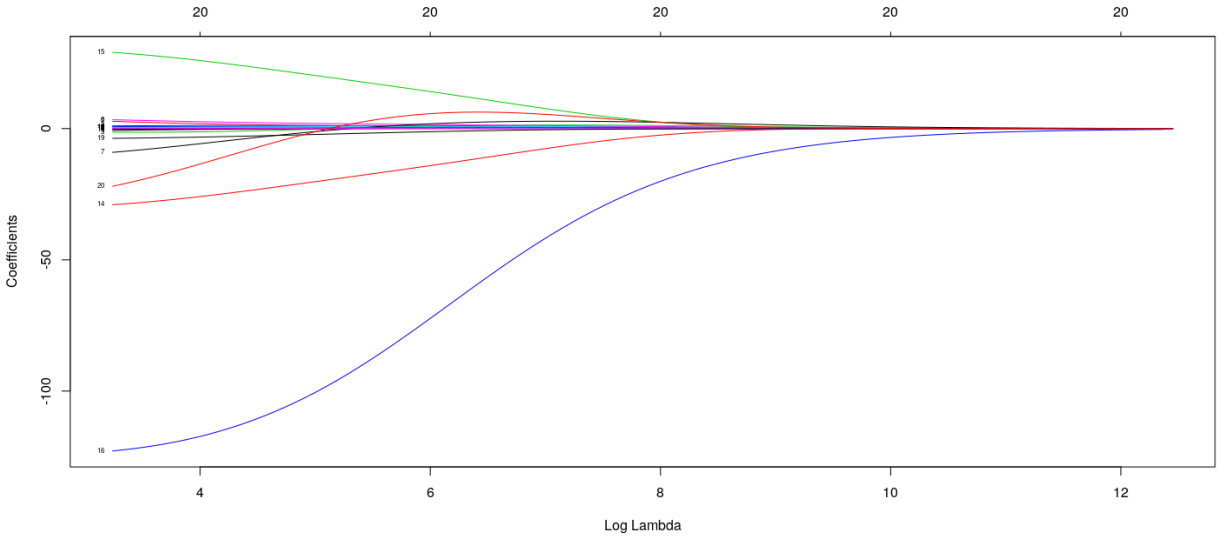
Example: Salary of hitters in Major League Baseball (1987)

```
## top axis labels indicate number of nonzero coefficients
plot(fm.lasso, xvar = "dev", label = TRUE)
```



Example: Salary of hitters in Major League Baseball (1987)

```
## top axis labels indicate number of nonzero coefficients (not useful for Ridge)
plot(fm.ridge, xvar = "lambda", label = TRUE)
```

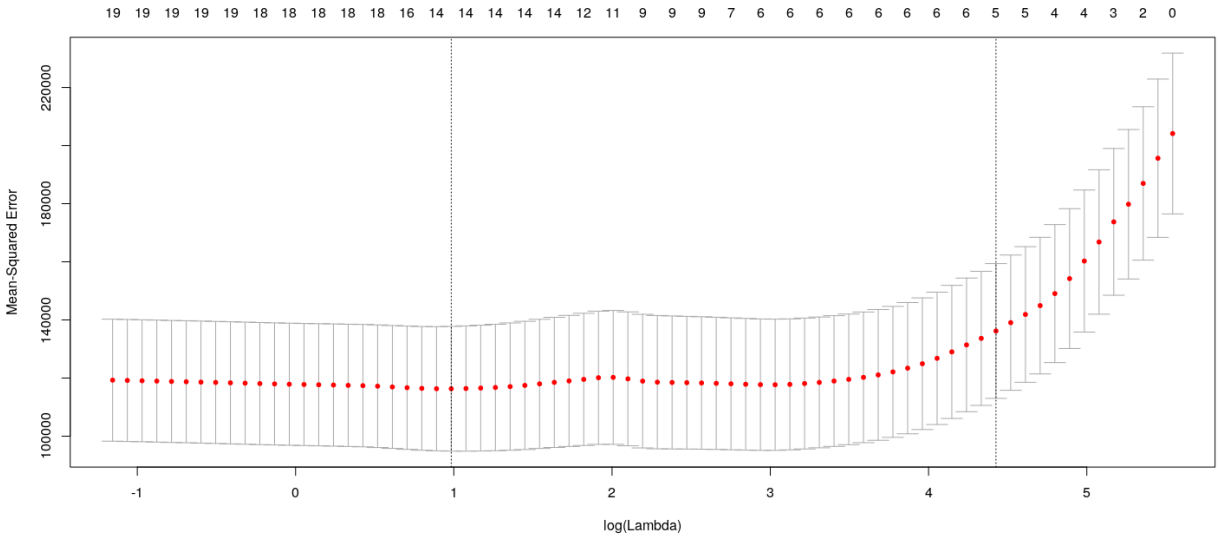


Choosing λ

- Usual model selection criteria can be used (AIC, BIC, etc.)
- Using cross-validation is more common
- Note that there is no closed form expression for $e_{i(-i)}$ in general
- Leave-one-out (n-fold) cross-validation is computationally intensive for large data sets
- The `cv.glmnet()` function performs k-fold cross-validation ($k = 10$ by default)
  - Divides dataset randomly into k (roughly) equal parts
  - Predicts on each part using model fit with remaining $(k-1)$ parts
  - Computes overall prediction error

```
cv.lasso <- cv.glmnet(X, y, alpha = 1, nfolds = 50)
cv.ridge <- cv.glmnet(X, y, alpha = 0, nfolds = 50)

plot(cv.lasso)
```



The two lines on the plot correspond to

- λ that minimizes cross-validation error
- largest value of λ such that error is within 1 standard error of the minimum

```
c(lambda.min = cv.lasso$lambda.min,
  lambda.1se = cv.lasso$lambda.1se)
```

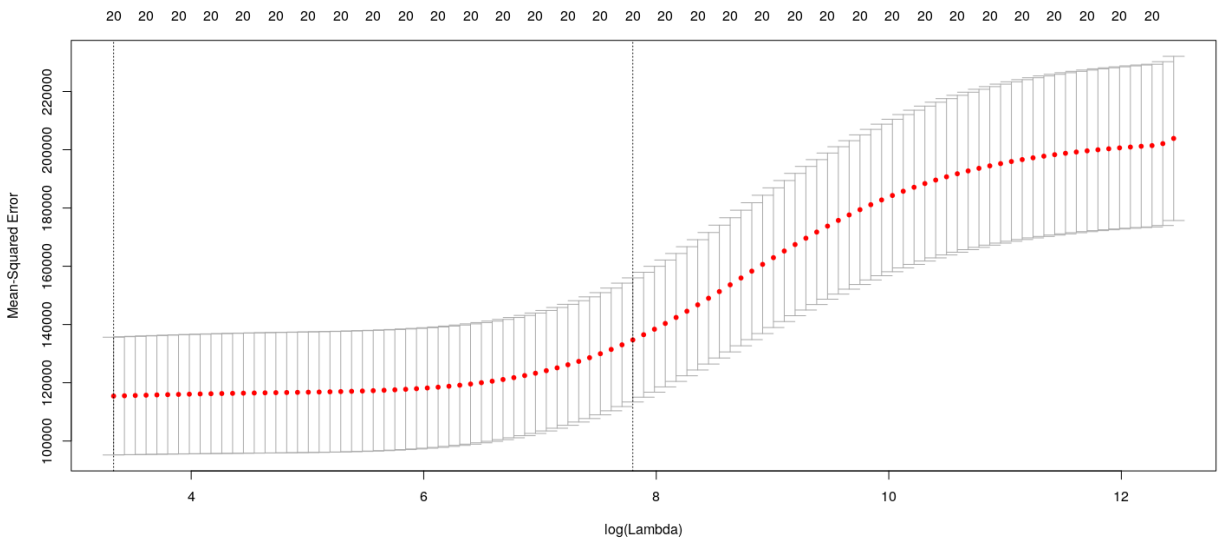
```
lambda.min lambda.1se
  2.674375  83.593378
```

```
s.cv <- c(lambda.min = cv.lasso$lambda.min, lambda.1se = cv.lasso$lambda.1se)
round(coef(cv.lasso, s = s.cv), 3) # corresponding coefficients
```

```
21 x 2 sparse Matrix of class "dgCMatrix"
                    1       2
(Intercept)  155.817 167.912
AtBat         -1.547   .
Hits           5.661   1.293
HmRun          .       .
Runs           .       .
RBI            .       .
Walks          4.730   1.398
Years         -9.596   .
CAtBat         .       .
CHits          .       .
CHmRun         0.511   .
CRuns          0.659   0.142
CRBI           0.393   0.322
CWalks        -0.529   .
LeagueA      -32.065   .
LeagueN        0.000   .
DivisionW   -119.299   .
PutOuts        0.272   0.047
Assists        0.173   .
Errors        -2.059   .
```

```
NewLeagueN      .         .
```

```
plot(cv.ridge)
```



How well does LASSO work for variable selection?

- We repeat our earlier simulation example
- Let us look at number of variables selected when none are related to the response

```
## Replicate this experiment
num.nonzero.coefs <-
    replicate(100,
    {
        d <- matrix(rnorm(100 * 21), 100, 21)
        cv.lasso <- cv.glmnet(x = d[,-1], y = d[,1])
        lambda.cv <- cv.lasso$lambda.1se
        sum(coef(cv.lasso, s = lambda.cv)[-1] != 0) # exclude intercept
    })
table(num.nonzero.coefs)
```

```
num.nonzero.coefs
 0  2
99  1
```

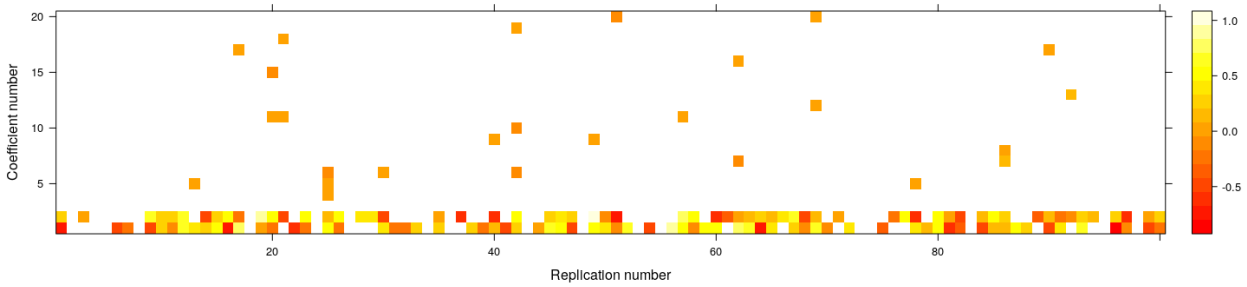
- So Type-I error probability is much lower for LASSO compared to stepwise regression

How well does LASSO work for variable selection?

- How about power to detect effects that are present? Choose $\beta_1, \beta_2 \sim U(-1, 1)$, other $\beta_j = 0$

```
coefs <- replicate(100,
{
    X <- matrix(rnorm(100 * 20), 100, 20)
    y <- X[,1:2] %*% runif(2, -1, 1) + rnorm(100)
```

```
    cv.lasso <- cv.glmnet(X, y)
    lambda.cv <- cv.lasso$lambda.1se
    coef(cv.lasso, s = lambda.cv)[-1] # exclude intercept
})
coefs[coefs == 0] <- NA
levelplot(t(coefs), col.regions = heat.colors, xlab = "Replication number", ylab = "Coefficient number"
```



Why does LASSO lead to exact 0 coefficients?

- Alternative formulation of Ridge regression: consider problem of minimizing

$$\sum_{i=1}^{n}(y_i - \mathbf{x}_i^T\beta)^2 \quad \text{subject to} \quad \|\beta\|^2 = \sum \beta_j^2 \leq t$$

- Claim: The solution $\hat{\beta}$ is the usual Ridge estimate for some λ
- Case 1 : $\|\hat{\beta}_{OLS}\|^2 \leq t \implies \hat{\beta} = \hat{\beta}_{OLS}, \lambda = 0$
- Case 2 : $\|\hat{\beta}_{OLS}\|^2 > t$
  - Then must have $\|\hat{\beta}\|^2 = t$ (otherwise can move closer to $\hat{\beta}_{OLS}$)
  - The Lagrangian is $\|\mathbf{y} - \mathbf{X}\beta\|^2 + \lambda\|\hat{\beta}\|^2 - \lambda t$
  - This is the same optimization problem as before
  - λ is defined implicitly as a function of t, to ensure $\|\hat{\beta}\|^2 = t$
- The LASSO problem can be similarly formulated as: minimize $\|\mathbf{y} - \mathbf{X}\beta\|^2$ subject to $\sum|\beta_j| \leq t$
- This interpretation gives a useful geometric justification for the variable selection behaviour of LASSO

Comparative geometry of Ridge and LASSO optimization

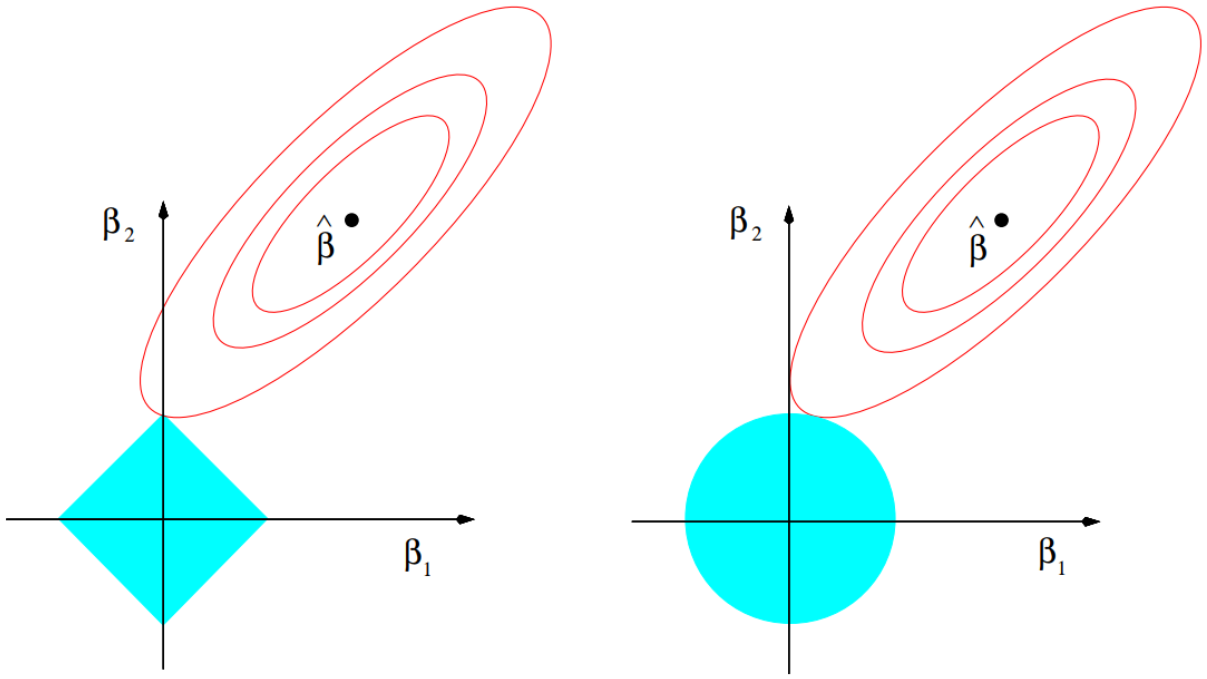


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

(From Elements of Statistical Learning, page 71)