Linear Regression Models
P8111

Lecture 16

Jeff Goldsmith
March 24, 2016

THE DEPARTMENT OF BIOSTATISTICS
Columbia University
MAILMAN SCHOOL
OF PUBLIC HEALTH

Today's Lecture

Model Selection

Penalized

- Ridge regression
- Lasso regression

Variable selection

Suppose $Var(\epsilon) = \sigma^2 \boldsymbol{I}$. In Lecture 15 we talked about model selection:

- Given a lot of variables, which should we include in a model?
- Several approaches, but variables were either in or out
- Difficult for large p
- Gives results that are "unbiased" for the truth, but can be high variance

$E(\hat{\beta}_{OLS}) = \beta$

MS focused on Estimation / Testing

Gauss-Markov and MSE

Recall the Gauss-Markov theorem says OLS is BLUE. Maybe "unbiased" is more restrictive than we're interested in.

- Alternatively, we could try to minimize the mean squared error:

$$
\begin{aligned}
MSE(\hat{\beta}) &= E\left[\left(\hat{\beta}-\beta\right)^2\right] \\
&= E\left[\left(\hat{\beta}-E(\hat{\beta})+E(\hat{\beta})-\beta\right)^2\right] \\
&= E\left[\left(\hat{\beta}-E(\hat{\beta})\right)^2\right]+\left(E(\hat{\beta})-\beta\right)^2 \\
&= \text{variance}(\hat{\beta})+\text{bias}^2(\hat{\beta})
\end{aligned}
$$

Penalized regression

- Could try a shrinkage / penalization approach to trade some bias for lower variance and overall MSE
- Rather than a variable selection approach, all parameters stay in the model, but we restrict their effect
- We penalize the size of the coefficients – unimportant variables will have their coefficients forced closer to zero

Ridge regression

OLS is derived by minimizing the RSS:

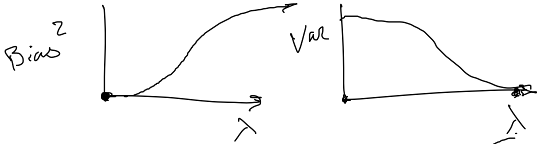
$$\hat{\boldsymbol{\beta}}_{OLS} = \arg\min_{\boldsymbol{\beta}} \left[RSS(\boldsymbol{\beta})\right]$$

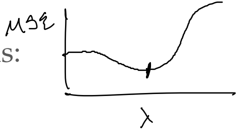
$$= \arg\min_{\boldsymbol{\beta}} \left[\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j}\right)^2\right]$$

$$(y - X\beta)^T (y - X\beta)$$

$$\frac{\partial RSS(\beta)}{\partial \beta} = 0$$

Ridge regression





Ridge regression adds an L_2 penalty to this:

$$\hat{\beta}_R = \arg\min_{\beta} \left[RSS(\beta) + \lambda \, ||\beta||_2 \right]$$

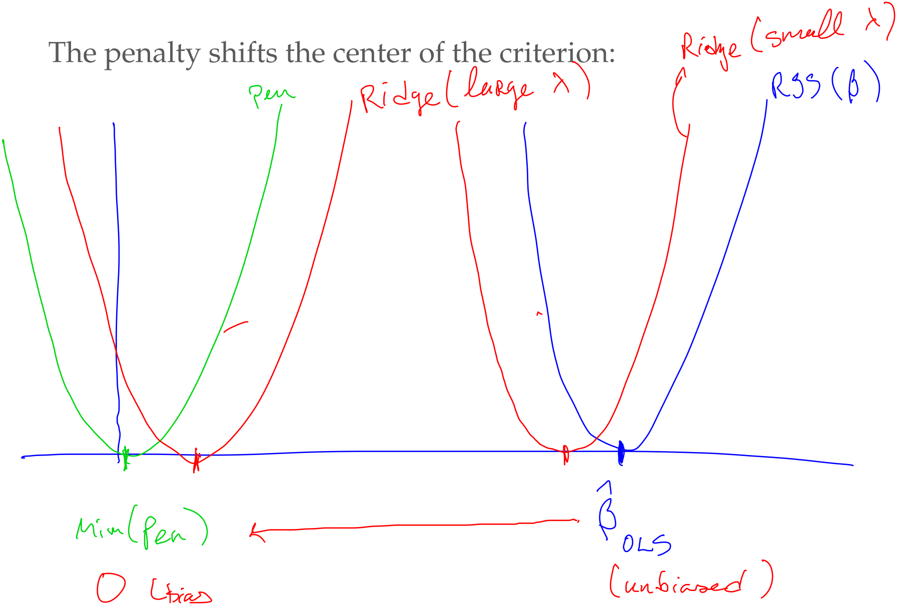
$$= \arg\min_{\beta} \left[\underbrace{\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j} \right)^2}_{RSS(\beta)} + \underbrace{\lambda \sum_{j=1}^{p} \beta_j^2}_{Pen_\lambda(\beta)} \right]$$

$\lambda = 0 \Rightarrow$ OLS

$\lambda \to \infty \Rightarrow \hat{\beta}_R = 0$

Graphical representation

The penalty shifts the center of the criterion:



Ridge regression in matrix notation

In matrix notation, we want to minimize

$$RSS(\boldsymbol{\beta}) + \lambda\,||\boldsymbol{\beta}||_2 = \underbrace{(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})}_{RSS(\beta)} + \lambda\boldsymbol{\beta}^T P\boldsymbol{\beta}$$

where P is the penalty matrix.

$$\lambda \sum_j \beta_j^2$$

$$= \lambda\, \beta^T \beta$$

$$= \lambda\, \beta^T \underline{I}\, \beta$$

Ridge regression in matrix notation

Finding solutions to

$$\min_{\beta} \left(RSS(\boldsymbol{\beta}) + \lambda\,||\boldsymbol{\beta}||_2 \right) = \left((\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) + \boxed{\lambda\boldsymbol{\beta}^T P\boldsymbol{\beta}} \right)$$

Ridge regression estimates

$$\hat{\beta}_{OLS} = (X^T X)^{-1} X^T y$$

The ridge regression estimates are given by

$$\boxed{\hat{\boldsymbol{\beta}}_R} = \left(\boldsymbol{X}^T\boldsymbol{X} + \lambda \cancel{P}\right)^{-1} \boldsymbol{X}^T\boldsymbol{y}$$

λ acts as a tuning parameter

- For "small" values of λ, $\hat{\boldsymbol{\beta}}_R \approx \hat{\boldsymbol{\beta}}_{OLS}$
- For "large" values of λ, $\hat{\boldsymbol{\beta}}_R \approx 0$

Is there an MLE equivalent to this?

Sort of ...

- We'll worry more about this later
- If we assume the β_j's are random (especially Normal) then there's a likelihood function that includes the penalty term

OLS

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

$$\epsilon \sim N(0, \sigma^2 I)$$

$$\Rightarrow \hat{\beta}_{MLE} = (X^TX)^{-1}X^Ty$$

Ridge

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

$$\epsilon \sim N(0, \underline{\sigma^2} I)$$

$$\beta \sim N(0, \sigma_{\beta}^2 P^{-1})$$

$$\Rightarrow \hat{\beta}_{MLE} = (X^TX + \lambda P)^{-1}X^Ty$$

Properties of ridge regression

- Ridge regression estimates are biased:

$$
\begin{aligned}
E(\hat{\boldsymbol{\beta}}_R) &= E\left[\left(\boldsymbol{X}^T\boldsymbol{X} + \lambda P\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}\right] \\
&= \left(\boldsymbol{X}^T\boldsymbol{X} + \lambda P\right)^{-1}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta}
\end{aligned}
$$

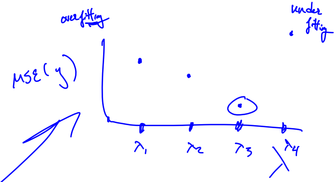
- Tend to have lower variance than OLS
- Often lead to lower MSE's
- Interesting note – penalized estimates may be identifiable even when $p > n$

$(X^TX)^{-1}$ DNE $\qquad (X^TX + \lambda P)^{-1}$ PE!

MSE for predictions

$\min_{\lambda,\beta}\left(MSE(\beta) \right)$

$\hookrightarrow E\left((\hat{\beta}_R - \beta)^2 \right)$



MSE for β can be hard to discuss in practice

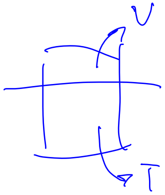
- MSE for predictions can be easier to focus on

$$MSE(\hat{y}_\beta) = E\left[(\hat{y}_\beta - y)^2\right]$$

$(X^T X + \lambda P)^{-1} X^T y$

- Could evaluate this using cross-validation

$X\hat{\beta}_R$



$\lambda_1, \lambda_2, \lambda_3, \lambda_4$

$\hat{\beta}_{R1}, \hat{\beta}_{R2}, \hat{\beta}_{R3}, \hat{\beta}_{R4}$

$\hat{y}_{\hat{\beta}_{R1}}, \hat{y}_{\hat{\beta}_{R2}}, \hat{y}_{\hat{\beta}_{R3}}, \hat{y}_{\hat{\beta}_{R4}}$

y

Tuning parameter selection

The tuning parameter λ is important for overall model fit

- Depending on λ, we may be looking at OLS or $\hat{\beta} = 0$
- "Truth" is usually somewhere in the middle
- It turns out that we've avoided variable selection, but now have to focus on tuning parameter selection
- Cross-validation is a common way of choosing λ

Life expectancy example

Lec 15

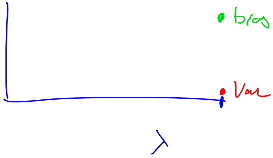
US

- Response: life expectancy
- Predictors: population, capital income, illiteracy rate, murder rate, percentage of high-school graduates, number of days with minimum temperature < 32, land area
- Data for 50 US states
- Time span: 1970-1975

Example

```
> data(state)
> statedata = data.frame(state.x77,row.names=state.abb)
> model.full = lm(Life.Exp ~., data=statedata)
> coef(model.full)
(Intercept) Population      Income Illiteracy      Murder     HS.Grad       Frost        Area
 7.094e+01  5.180e-05 -2.180e-05  3.382e-02 -3.011e-01  4.892e-02 -5.735e-03 -7.383e-08
```

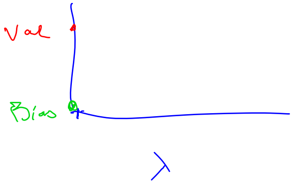
Example



library(MASS)

```
> model.ridge1 = lm.ridge(Life.Exp ~., data=statedata, lambda = 1000000)
> coef(model.ridge1)
(Intercept) Population     Income Illiteracy     Murder    HS.Grad      Frost       Area
  7.087e+01 -1.022e-09  3.716e-08 -6.479e-05 -1.419e-05  4.837e-06  3.383e-07 -8.442e-11
```

Example




```
> model.ridge2 = lm.ridge(Life.Exp ˜., data=statedata, lambda = .0000001)
> coef(model.ridge2)
(Intercept) Population     Income Illiteracy     Murder    HS.Grad      Frost       Area
  7.094e+01  5.180e-05 -2.180e-05  3.382e-02 -3.011e-01  4.892e-02 -5.735e-03 -7.383e-08
```

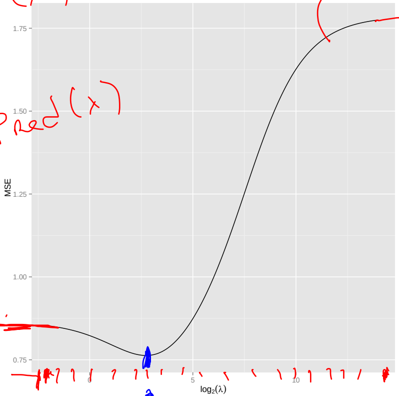
≈ lm

CV Plot

$$\sum_{i \in \text{Valid}} \left(y_i - \text{Pred}_i(\lambda)\right)^2$$

Training → fit(λ)

Valid → Pred(λ)



$\hat{\beta}_R = 0$

high bias

low var

underfitting

OLS

unbiased

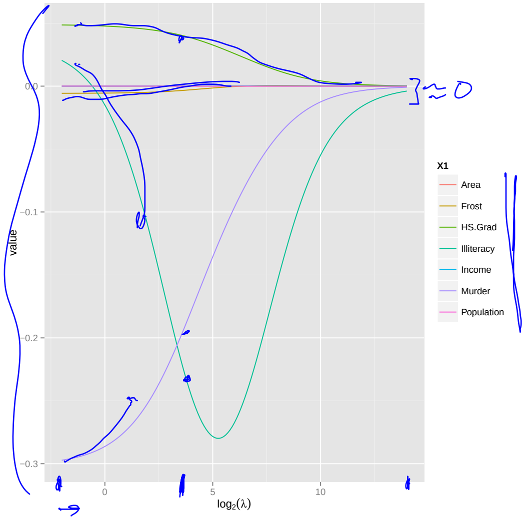
high var

Overfitting

λ ↪ $\hat{\beta}_{R\lambda}$

Coef Plot

OLS

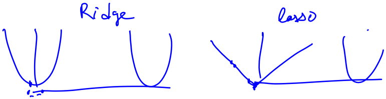


≈ 0

Example

```
> Lam.Final = lam[which(apply(MSE, 2, mean) == min(apply(MSE, 2, mean)))]
> model.ridge2 = lm.ridge(Life.Exp ˜., data=statedata, lambda = Lam.Final)
> round(coef(model.ridge3), 5)
          Population     Income Illiteracy     Murder    HS.Grad      Frost       Area
 70.55067    0.00003    0.00006   -0.16047   -0.22998    0.04334   -0.00438    0.00000
```

Lasso penalization



- Lasso (least absolute shrinkage and selection operator) is a more recent penalized regression estimator
- Basic form is similar to that of ridge regression, but penalty function is different:

$$
\begin{aligned}
\hat{\boldsymbol{\beta}}_L &= \arg\min_{\boldsymbol{\beta}} \left[RSS(\boldsymbol{\beta}) + \lambda \, ||\boldsymbol{\beta}||_1 \right] \\
&= \arg\min_{\boldsymbol{\beta}} \left[\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j} \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right]
\end{aligned}
$$

- Quite popular at the moment – broadly used, many adaptations

Lasso penalization

Some properties of Lasso penalties

- No closed form solution (although there are some computationally useful tricks)
- The different penalty form means Lasso has a tendency to shrink coefficients *all the way* to zero
- Can be useful as an automated variable selection approach
- Still have to choose λ; cross validation is a popular tool for this

Example: Mortality Rate

```
lm(formula = Life.Exp ~ ., data = statedata)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  7.094e+01  1.748e+00  40.586  < 2e-16 ***
Population   5.180e-05  2.919e-05   1.775   0.0832 .
Income      -2.180e-05  2.444e-04  -0.089   0.9293
Illiteracy   3.382e-02  3.663e-01   0.092   0.9269
Murder      -3.011e-01  4.662e-02  -6.459 8.68e-08 ***
HS.Grad      4.893e-02  2.332e-02   2.098   0.0420 *
Frost       -5.735e-03  3.143e-03  -1.825   0.0752 .
Area        -7.383e-08  1.668e-06  -0.044   0.9649
```

Example: Mortality Rate

y ~ X

```
> model.lasso1 = glmnet(X, y, lambda = 0.00001)
> coef(model.lasso1)
8 x 1 sparse Matrix of class "dgCMatrix"
                      s0
(Intercept)  7.094187e+01
Population   5.185263e-05
Income      -2.191147e-05
Illiteracy   3.467775e-02
Murder      -3.012157e-01
HS.Grad      4.894538e-02
Frost       -5.730853e-03
Area        -7.370497e-08
```

Example: Mortality Rate

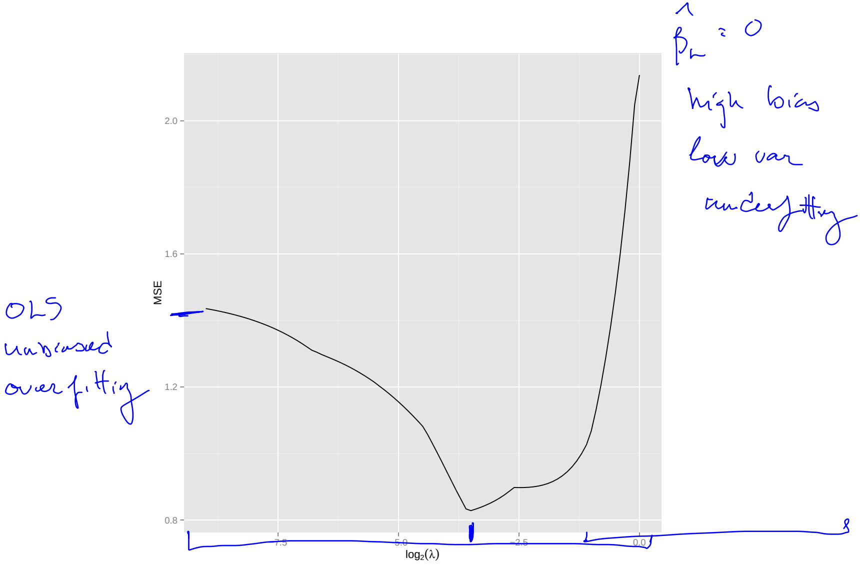
```
> model.lasso2 = glmnet(X, y, lambda = 0.01)
> coef(model.lasso2)
8 x 1 sparse Matrix of class "dgCMatrix"
                        s0
(Intercept)  7.101048e+01
Population   4.762476e-05
Income       .
Illiteracy   .
Murder      -2.944565e-01
HS.Grad      4.551701e-02
Frost       -5.542157e-03
Area         .
```

$\neq \hat{\beta}_{OLS}$ for same variables

Example: Mortality Rate

```
> model.lasso3 = glmnet(X, y, lambda = 10)
> coef(model.lasso3)
8 x 1 sparse Matrix of class "dgCMatrix"
                  s0
(Intercept) 70.8786
Population   0.0000
Income       .
Illiteracy   .
Murder       .
HS.Grad      .
Frost        .
Area         .
```

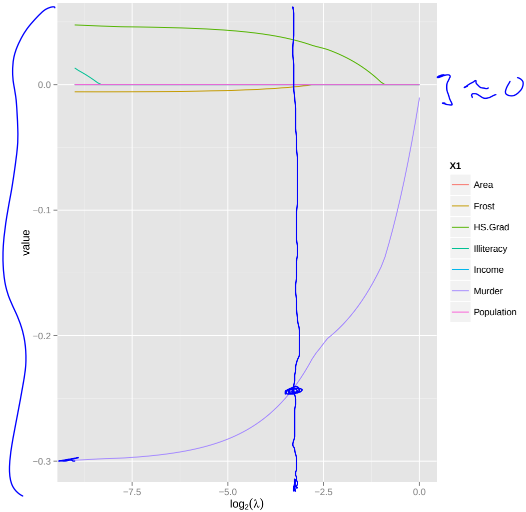
CV plot



$\hat{\beta}_\lambda = 0$
high bias
low var
underfitting
OLS
unbiased
overfitting
2.0
1.6
1.2
0.8
MSE
−7.5
−5.0
−2.5
0.0
$\log_2(\lambda)$

Coef plot

OL



$\beta \approx 0$

Example: Mortality Rate

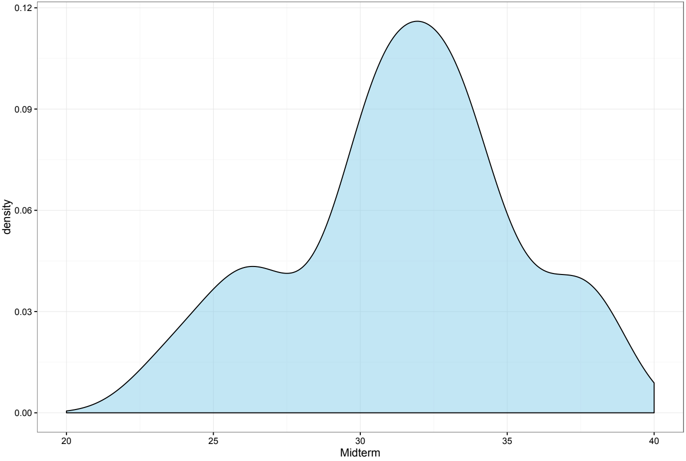
```
> Lam.Final = lam[which(apply(MSE, 2, mean) == min(apply(MSE, 2, mean)))]
> model.lasso4 = glmnet(X, y, lambda = Lam.Final)
> coef(model.lasso4)
8 x 1 sparse Matrix of class "dgCMatrix"
                        s0
(Intercept)  7.088048e+01
Population   2.786869e-05
Income       .
Illiteracy   .
Murder      -2.498481e-01
HS.Grad      3.716564e-02
Frost       -2.399294e-03
Area         .
```

Practical note

$$\frac{x_{ip} - \bar{x}_p}{sd(x_p)}$$

- In most cases, it's best to standardize predictors prior to penalizing
- Doing so ensures that the coefficients to be penalized have comparable effects on the outcome
- Not always obvious – see, e.g. categorical and binary predictors – but useful nonetheless

Midterm grades



Today's big ideas

- Ridge regression
- Lasso

- Suggested reading: Faraway Ch. 9.5, ISLR Ch 6.2