STAT406- Methods of Statistical Learning Lecture 6

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"Far better an approximate answer to the right question, which is often vague, than an exact answer to the wrong question, which can always be made precise."

John Tukey. The future of data analysis. Annals of Mathematical Statistics, 33(1), (1962), p. 13.

Progress report?

- Piazza - course content discussions
- Coming to “lectures” isn’t enough: read reference texts, dissect / break code on Github, discuss w/peers
- Google is not your friend

Effective degrees of freedom

- How many "effective" parameters are we using?
- In linear regression, we have p parameters
- A more general definition is as follows. For a fitting method producing $\hat{y}_1$, $\hat{y}_2$, $\ldots$, $\hat{y}_n$,

$$\text{edf} = \frac{1}{\sigma^2} \sum_{i=1}^{n} \text{cov}\left(\hat{y}_i, y_i\right)$$

Efron, B. (1986). How biased is the apparent error rate of a prediction rule? Journal of the

American Statistical Association, 81(394):461-470.

Effective degrees of freedom

- It is easy to see that for least squares predictors, we have

$$\hat{\mathbf{y}} = \mathbf{H}\,\mathbf{y}$$

with

$$\mathbf{H} = \mathbf{X}\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'$$

and

$$\text{edf} = \frac{1}{\sigma^2}\sum_{i=1}^{n} \text{cov}\left(\hat{y}_i, y_i\right) = \text{trace}\left(\mathbf{H}\right) = p$$

Effective degrees of freedom

- More in general, for any linear predictor

$$\hat{\mathbf{y}} = \mathbf{S}\,\mathbf{y}$$

  we have

$$\text{edf} = \text{trace}\,(\mathbf{S}) = \sum_{i=1}^{n} \mathbf{S}_{i,i}$$

Effective degrees of freedom

- The ridge regression fit satisfies

$$\hat{\mathbf{y}} = \mathbf{S}_\lambda \mathbf{y}$$

where

$$\mathbf{S}_\lambda = \mathbf{X} \left(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}_p \right)^{-1} \mathbf{X}'$$

$$\text{trace}\,(\mathbf{S}) = ?$$

Effective degrees of freedom

- Using the singular value decomposition (SVD) of $\mathbf{X}$

  $$\mathbf{X} = \mathbf{U} \boldsymbol{\Lambda} \mathbf{V}'$$

  where $\mathbf{U} \in \mathbb{R}^{n \times p}$, $\mathbf{V} \in \mathbb{R}^{p \times p}$ with

  $$\mathbf{U}'\mathbf{U} = \mathbf{I}_p = \mathbf{V}'\mathbf{V}$$

  and

  $$\boldsymbol{\Lambda} = \operatorname{diag}(d_1, \ldots, d_p) \, ,$$

  we have

  $$\operatorname{trace}(\mathbf{S}) = \sum_{i=1}^{p} \left(\frac{d_i^2}{d_i^2 + \lambda} \right)$$

Effective degrees of freedom

- For example, in the Air Pollution data example, if we use

$$\lambda = \exp(6)$$

we get

$$\text{edf} = 9.9$$

Model / feature selection - LASSO

- Another regularized method is given by LASSO

$$\min_{\alpha,\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \alpha - \boldsymbol{\beta}'\mathbf{x}_i\right)^2 + \lambda \sum_{j=1}^{p} \left|\beta_j\right|$$

$$\min_{\alpha,\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \alpha - \boldsymbol{\beta}'\mathbf{x}_i\right)^2 + \lambda \left\|\boldsymbol{\beta}\right\|_1$$

for some $\lambda > 0$

Model / feature selection - LASSO

- The above is equivalent to

$$\min_{\alpha,\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \alpha - \boldsymbol{\beta}' \mathbf{x}_i \right)^2$$

subject to

$$\sum_{j=1}^{p} \left| \beta_j \right| \leq K$$

for some $K > 0$

LASSO

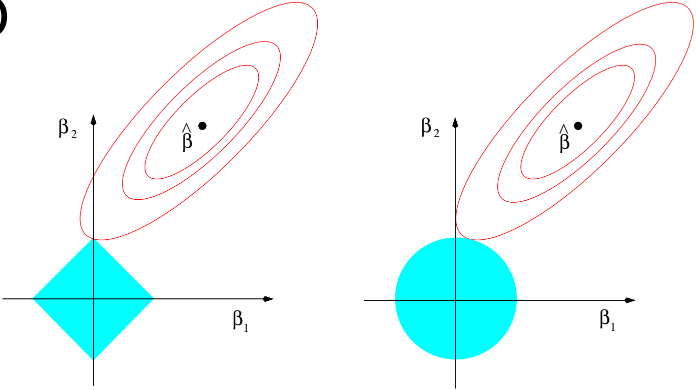
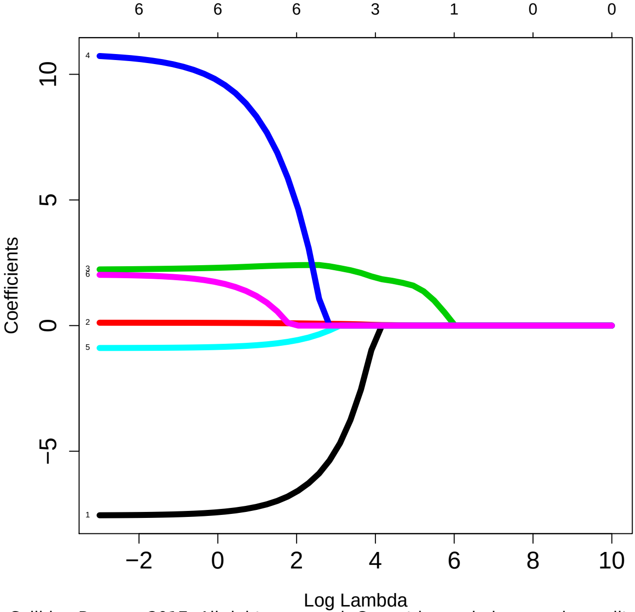


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are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

Credit data - glmnet output



Credit data - glmnet output

```
a <- glmnet(x=xm, y=yc, lambda=lambdas,
    family='gaussian', alpha=1, intercept=FALSE)

> coef(a, s=1)
7 x 1 sparse Matrix of class "dgCMatrix"
                    1
(Intercept)  .
Income      -7.4285710
Limit        0.1078894
Rating       2.3006418
Cards        9.7499618
Age         -0.8515917
Education    1.7182477
```

Credit data - glmnet output

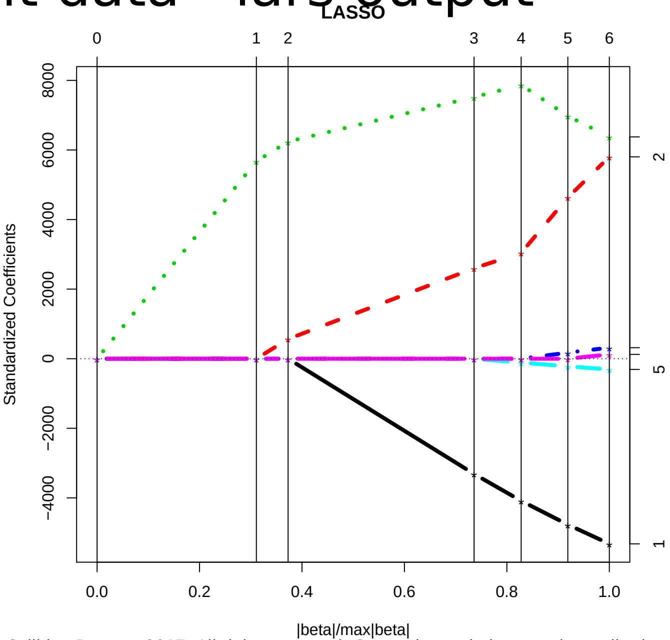
```
> coef(a, s=exp(4))
7 x 1 sparse Matrix of class "dgCMatrix"
                       1
(Intercept)  .
Income      -0.63094341
Limit        0.02749778
Rating       1.91772580
Cards        .
Age          .
Education    .
```


Credit data - another implementation

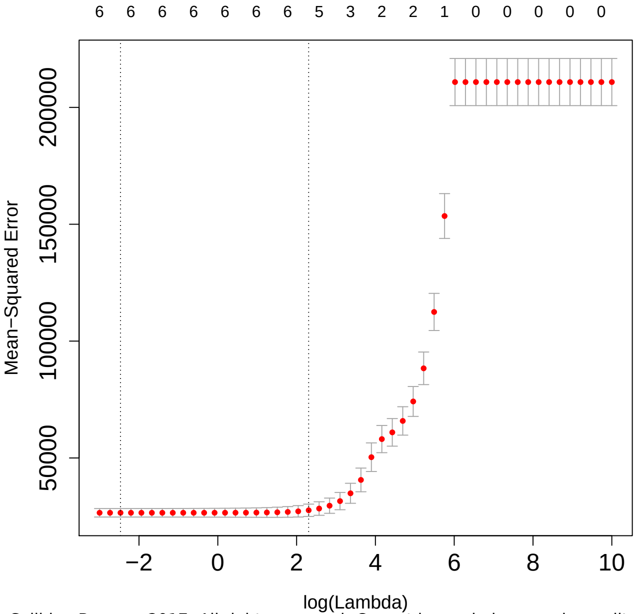
```
> library(lars)
> b <- lars(x=xm, y=yc, type='lasso', intercept=FALSE)
> coef(b)
        Income      Limit   Rating     Cards        Age Education
[1,]  0.000000 0.00000000 0.000000  0.000000  0.0000000  0.000000
[2,]  0.000000 0.00000000 1.835963  0.000000  0.0000000  0.000000
[3,]  0.000000 0.01226464 2.018929  0.000000  0.0000000  0.000000
[4,] -4.703898 0.05638653 2.433088  0.000000  0.0000000  0.000000
[5,] -5.802948 0.06600083 2.545810  0.000000 -0.3234748  0.000000
[6,] -6.772905 0.10049065 2.257218  6.369873 -0.6349138  0.000000
[7,] -7.558037 0.12585115 2.063101 11.591558 -0.8923978  1.998283
> b

Call:
lars(x = xm, y = yc, type = "lasso", intercept = FALSE)
R-squared: 0.878
Sequence of LASSO moves:
     Rating Limit Income Age Cards Education
Var       3     2      1   5     4         6
Step      1     2      3   4     5         6
```

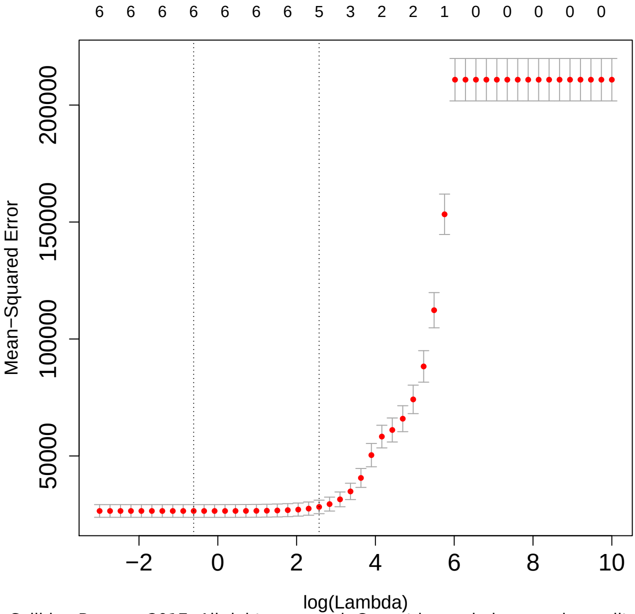
Credit data - lars output



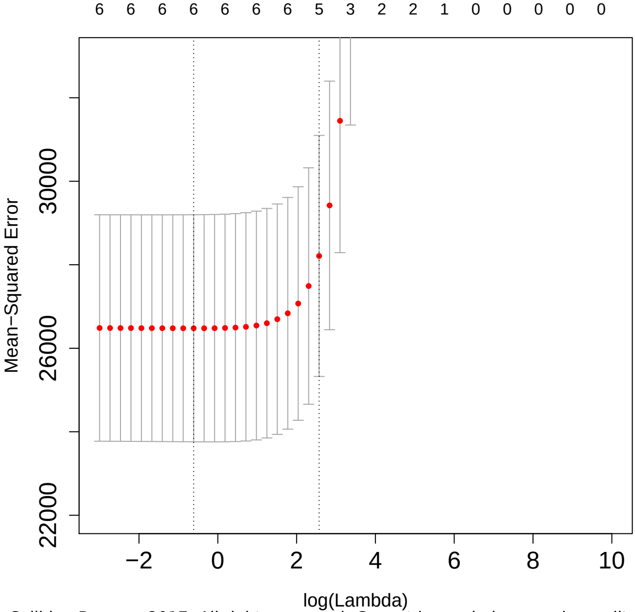
Credit data - CV - glmnet



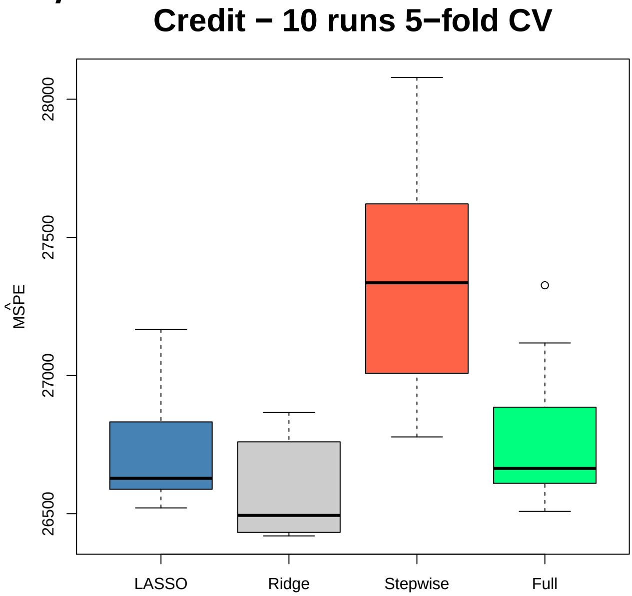
Credit data - CV - another run



Credit data - CV - zoom



Model / feature selection - LASSO



Model / feature selection - LASSO

- Worse estimated MSPE than Ridge Regression in this case
- It provides a sequence of explanatory variables, an ordered set of models
- Much like stepwise, but with better MSPE in this case

Model / feature selection - LASSO

- Why does it work? It is the convex proxy for the “nuclear norm”
- Also generates infinitely many estimates, but there’s a clever algorithm
- Inference?

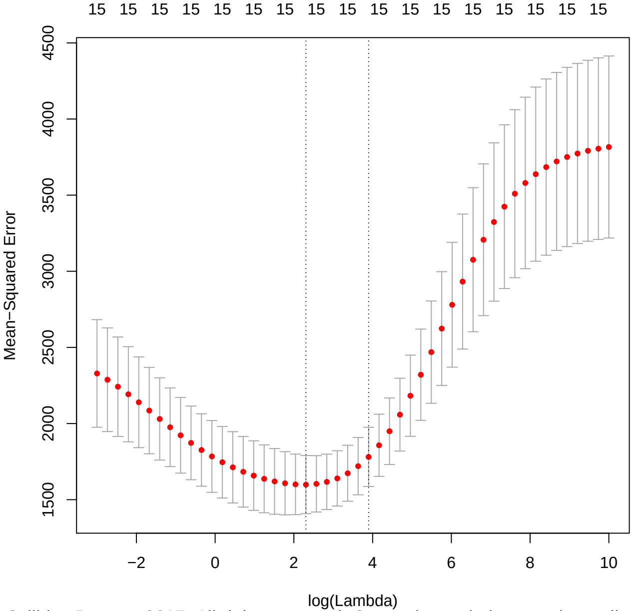
Air pollution example

- There are correlated covariates
- LASSO solution picks one of each group early on and relegates the rest to the end of the sequence
- Ridge Regression includes all variables always

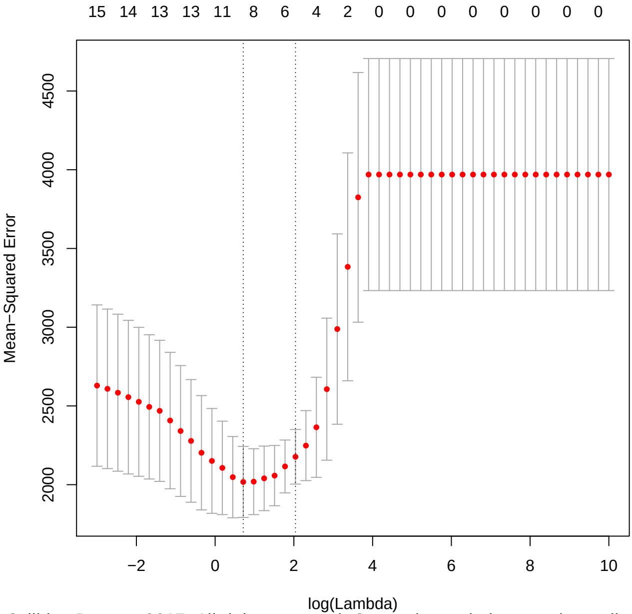
Air pollution example

```
airp <- read.table('..-30861_CSV-1.csv',
    header=TRUE, sep=',')
y <- as.vector(airp$MORT)
xm <- as.matrix(airp[, names(airp) != 'MORT'])
# Ridge
set.seed(123)
air.l2 <- cv.glmnet(x=xm, y=y, lambda=lambdas,
    nfolds=5, alpha=0, family='gaussian',
    intercept=TRUE)
# LASSO
set.seed(23)
air.l1 <- cv.glmnet(x=xm, y=y, lambda=lambdas,
    nfolds=5, alpha=1, family='gaussian',
    intercept=TRUE)
```


Air pollution - Ridge



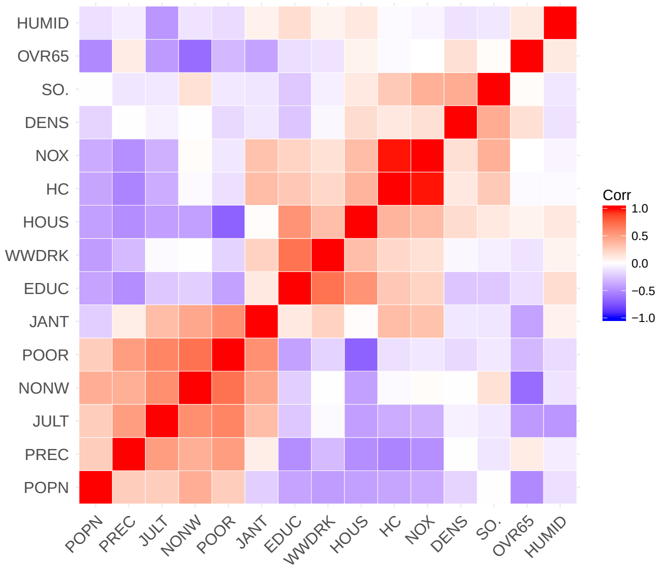
Air pollution - LASSO



Air pollution example

	Ridge	LASSO
(Intercept)	1179.335	1100.355
PREC	1.570	1.503
JANT	−1.109	−1.189
JULT	−1.276	−1.247
OVR65	−2.571	.
POPN	−10.135	.
EDUC	−8.479	−10.510
HOUS	−1.164	−0.503
DENS	0.005	0.004
NONW	3.126	3.979
WWDRK	−0.476	−0.002
POOR	0.576	.
HC	−0.035	.
NOX	0.064	.
SO.	0.240	0.228
HUMID	0.372	.

Air pollution - Correlations



Model / feature selection - LASSO

- Oracle - consistency
- Problem: when $n < p$, LASSO will only choose up to n variables
- When covariates are correlated, LASSO will typically pick any one of them, and ignore the rest
- Ridge Regression, on the other hand, combines the coefficients of correlated covariates, but doesn't provide sparse models

Elastic Net

- Elastic Net is a compromise between the two:

$$\min_{\beta_0, \boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \boldsymbol{\beta}' \mathbf{x}_i \right)^2 + \lambda \left[\alpha \|\boldsymbol{\beta}\|_1 + \frac{(1-\alpha)}{2} \|\boldsymbol{\beta}\|_2^2 \right]$$

for some $\lambda > 0$ and $0 \leq \alpha \leq 1$.

Elastic Net

- $\alpha = 0 \quad \longrightarrow \quad$ Ridge Regression
- $\alpha = 1 \quad \longrightarrow \quad$ LASSO

- α also needs to be chosen...
- How would you find a good choice for α?

Air pollution example

- There are correlated covariates
- LASSO solution picks one of each group early on and relegates the rest to the end of the sequence
- Ridge Regression includes all variables always
- EN with $\alpha = 0.10$ gives a nice path of solutions...
- CV? bivariate search, unless α can be chosen beforehand