STAT406- Methods of Statistical Learning Lecture 5

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Comparing models

- For Gaussian errors we have

$$\text{AIC} \; = \; n \, \log \left(\frac{\text{RSS}}{n} \right) \; + \; 2\,p + \text{constant}$$

where

$$\text{RSS} \; = \sum_{i=1}^{n} r_i^2 \,,$$

the **constant** depends on n, not on p

Comparing models

- However, many times we find

$$\text{AIC} = \frac{1}{n}\,\frac{1}{\hat{\sigma}^2}\left(\text{RSS} + 2\,p\,\hat{\sigma}^2\right) + \text{constant}$$

(e.g. [JWHT13])

Where does this expression come from?

Comparing models

- Regularity assumptions are needed
  - This is an asymptotic approximation, n should be large
  - One of the models should include truth
  - $\theta_1 \neq \theta_2 \ \Rightarrow f(y, \theta_1) \neq f(y, \theta_2)$
  - Standard large-sample MLE assumptions to obtain asymptotic normality

Comparing models

- AIC suggests a submodel
- Prediction-wise the full model is better
- AIC can be highly variable

“Smoother” model selection

- Ridge regression
- Can be thought as a type of “prediction taming”
- It is a member of a larger class called “shrinkage methods”
- However, its origins are rather different

Without loss of generality...

- If covariates are centered, $\sum_{i=1}^n \mathbf{x}_i = \mathbf{0}$

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

satisfies

$$\hat{\alpha}_n = \frac{1}{n} \sum_{i=1}^n y_i = \bar{y}_n \, ,$$

and

$$\hat{\boldsymbol{\beta}}_{LS} = \left(\mathbf{X}' \mathbf{X} \right)^{-1} \mathbf{X}' \mathbf{Y} \, ,$$

Without loss of generality...

- We can always assume that

$$\sum_{i=1}^{n} \mathbf{x}_i = \mathbf{0}$$

and hence

$$\hat{\alpha}_n = \frac{1}{n} \sum_{i=1}^{n} y_i = \bar{y}_n \, ,$$

- In what follows, there is no intercept

Shrinkage methods

- When covariates are correlated, LS estimators can be highly variable

$$\hat{\beta}_{LS} = \left(\mathbf{X}'\mathbf{X}\right)^{-1} \mathbf{X}' \mathbf{Y}$$

$$\mathrm{var}\left(\hat{\beta}_n\right) = \sigma^2 \left(\mathbf{X}'\mathbf{X}\right)^{-1}$$

- When $\mathbf{X}'\mathbf{X}$ is close to singular...

Ridge Regression

- One way to "avoid" this problem is to add a "ridge" to $\mathbf{X}'\mathbf{X}$...

$$\hat{\beta}_{RR} = \left(\mathbf{X}'\mathbf{X} + \lambda\,\mathbf{I}_p\right)^{-1}\mathbf{X}'\mathbf{Y}$$

where $\lambda > 0$ and

$$\mathbf{I}_p = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ 0 & \cdots & \ddots & 0 \\ 0 & \cdots & \cdots & 1 \end{pmatrix}$$

Ridge Regression

- This is equivalent to solving

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

Ridge Regression

- And also equivalent to solving

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

subject to

$$\sum_{j=1}^{p} \beta_j^2 \ \leq \ C$$

for some $C > 0$

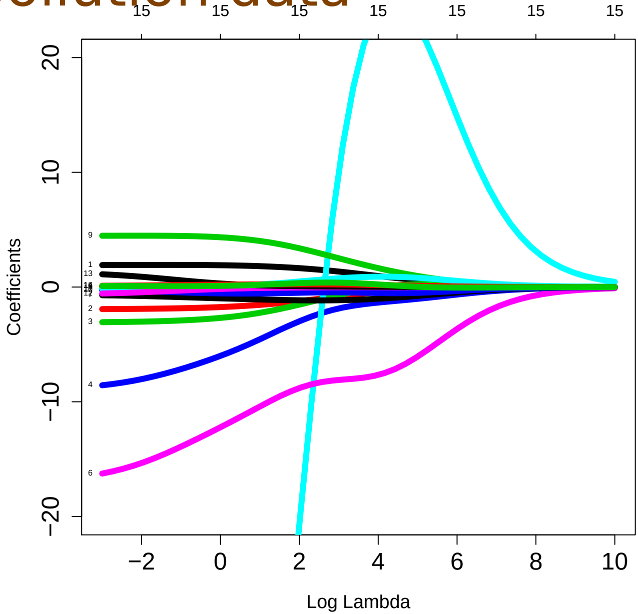
Bias / variance trade-off

- Ridge regression was originally proposed as a “hack” to “push” $\mathbf{X}'\mathbf{X}$ away from singularity
- It can also be thought as a way of reducing the variance of $\hat{\beta}_n$
- This may increase the bias of the estimator, but if the variance is reduced even more, we might gain overall in expected squared error performance...

Ridge regression

- We now have a sequence ("path") of estimators (one for each $\lambda > 0$)
- $\mathbf{X}'\mathbf{X} + \lambda\,\mathbf{I}_p$ is always non-singular for $\lambda > 0$ (why?)
- Why are they called "shrinkage methods"?

Air pollution data



Questions

- What does λ measure?
- How do I choose one among these infinitely many “solutions”?

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

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