

STAT 151A Lecture 30

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Remark 0.1

Method	Initial Model	Add/Drop?	Criterion
Forward	Intercept only	Add	ANY
Backward	All Variables	Drop	ANY
Stepwise	Any	Either	ANY

Reminder: You shouldn't compute p -values/CI in the same dataset you used for model selection

Interactions: Don't paly well with variable selection

Categorical Variables: Handling depends on R package (leaps, step, stepAIC)

Intuitively: as $\lambda \uparrow$ we "shrink" coefficients $\hat{\beta}_j$ in full model towards zero

Shrink approaches: Ridge vs LASSO

Remark 0.2 (How to Implement Shrinkage)

Put all variables on some scale \rightarrow standardized design matrix

\mathbf{X} drop intercept, replace each value x_{ij} by $\frac{x_{ij} - \bar{x}_j}{s_{x_j}}$

Call to new design matrix \mathbf{Z}

Also: Center $\bar{Y} \rightarrow \bar{Y} - \bar{Y}\bar{1}$

Think about OLS

$$\min_{\beta} \|\bar{y} - \mathbf{Z}\beta\|^2$$

Goal: Get good predictions while forcing β in to be a bit smaller.

Attempt:

$$\min_{\beta, S(\beta) \leq c} \|\bar{y} - \mathbf{Z}\beta\|^2$$

$$S(\beta) = \sum \beta_j^2 \text{ (Ridge)}$$

$$S(\beta) = \sum |\beta_j| \text{ (LASSO)}$$

Equivalent to the following

$$\min_{\beta} \left[\|\bar{y} - \mathbf{Z}\beta\|^2 + \lambda S(\beta) \right]$$

For any $c, \exists \lambda$ st the two problems solve the same answer

Connection to variable selection

What if we choose $S(\beta) + \sum I_{\hat{\beta}_j \neq 0}$, which gives the count of variables in the model

All subsets regression:

Problem: This is a $0-1$ penalty (L^0 norm) not smooth, makes optimization non-convex

By switching to a smoother penalty, make problems much easier computationally. Guarantees global optimum.

Remark 0.3 (Ridge Regression)

$S(\beta) = \sum \hat{\beta}_j^2$, Let us rename \mathbf{Z} as \mathbf{X}

Solve $\min \|y - \mathbf{X}\beta\|^2 + \lambda \|\beta\|^2$

$\min_{\beta} (y - \mathbf{X}\beta)^\top (y - \mathbf{X}\beta) + \lambda \beta^\top \beta$

$\min_{\beta} y^\top y - 2y^\top \mathbf{X}\beta + \beta^\top \mathbf{X}^\top \mathbf{X}\beta + \lambda \beta^\top \beta = y^\top y - 2y^\top \mathbf{X}\beta + \beta^\top [\mathbf{X}^\top \mathbf{X} + \mathbb{I}\lambda]\beta$

$\nabla_{\beta} [-2\mathbf{X}^\top y + 2(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})\beta] = 0$

$\hat{\beta}_{\lambda} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top \vec{y}$

Linear function of \vec{y}

It is not a projection

Why? Projection $\mathbb{H}\vec{y}$ satisfies $\mathbb{H}^\top = \mathbb{H}$, $\mathbb{H}\mathbb{H} = \mathbb{H}$, but regularization does not satisfy idempotency $\mathbb{H}\mathbb{H} \neq \mathbb{H}$

Remark 0.4 (Bias-Variance Tradeoff)

Assume NLM

Bias of $\hat{\beta}_{\lambda}$

$\mathbb{E} [(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top y]$

$= \mathbb{E} [(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} (\mathbf{X}^\top \mathbf{X}) (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \vec{y}] = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} (\mathbf{X}^\top \mathbf{X}) \beta = U_{\lambda} \beta$

$\text{Bias}(\hat{\beta}_{\lambda}) = \mathbb{E}(\hat{\beta}_{\lambda}) - \beta = [U_{\lambda} - \mathbb{I}]\beta$

As $\lambda \uparrow$, Bias \uparrow

Variance $\hat{\beta}^\top \hat{\beta}$ vs $\hat{\beta}_{\lambda}^\top \hat{\beta}_{\lambda}$

$\vec{y}^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top y \geq y^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top y$, strict inequality when $\lambda > 0$, $\text{Var}(\hat{\beta}) > \text{Var}(\hat{\beta}_{\lambda})$

Inference: Not allowed on same data, generally not useful since $\hat{\beta}_{\lambda,j}$ are biased