Ch 6.2: Shrinkage - Ridge regression Lecture 17 - CMSE 381

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Dept of Computational Mathematics, Science & Engineering

Fri, Oct 11, 2024

Announcements

Last time:

Subset selection

This time:

Ridge regression

Announcements:

• HW #5 due Friday 10/18

Lec	Date			Reading	HW
#					
12	Mon	9/30	Leave one out CV	5.1.1, 5.1.2	
13	Wed	10/2	k-fold CV	5.1.3	
14	Fri	10/4	More k-fold CV,	5.1.4-5	
15	Mon	10/7	k-fold CV for classification	5.1.5	
16	Wed	10/9	Subset selection	6.1	HW #4 Due Weds 10/9
17	Fri	10/11	Shrinkage: Ridge	6.2.1	
18	Mon	10/14	Shrinkage: Lasso	6.2.2	
19	Wed	10/16	Dimension Reduction	6.3	
20	Fri	10/18	Overflow, Possibly more dimension reduction?		HW #5 Due
	Mon	10/21	No class - Fall break		Fri 10/18
	Wed	10/23	Review		
	Fri	10/25	Midterm #2		

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Section 1

Last time

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Subset selection

Algorithm 6.1 Best subset selection

- 1. Let \mathcal{M}_0 denote the *null model*, which contains no predictors. This model simply predicts the sample mean for each observation.
- 2. For $k = 1, 2, \dots p$:
 - (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors.
 - (b) Pick the best among these $\binom{p}{k}$ models, and call it \mathcal{M}_k . Here best is defined as having the smallest RSS, or equivalently largest R^2 .
- Select a single best model from among M₀,...,M_p using crossvalidated prediction error, C_p (AIC), BIC, or adjusted R².

Algorithm 6.2 Forward stepwise selection

- 1. Let \mathcal{M}_0 denote the null model, which contains no predictors.
- 2. For $k = 0, \ldots, p-1$:
 - (a) Consider all p-k models that augment the predictors in \mathcal{M}_k with one additional predictor.
 - (b) Choose the best among these p-k models, and call it \mathcal{M}_{k+1} . Here best is defined as having smallest RSS or highest R^2 .
- 3. Select a single best model from among $\mathcal{M}_0, \dots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2 .

Algorithm 6.3 Backward stepwise selection

- 1. Let \mathcal{M}_p denote the full model, which contains all p predictors.
- 2. For $k = p, p 1, \dots, 1$:
 - (a) Consider all k models that contain all but one of the predictors in M_k, for a total of k − 1 predictors.
 - (b) Choose the best among these k models, and call it \mathcal{M}_{k-1} . Here best is defined as having smallest RSS or highest \mathbb{R}^2 .
- Select a single best model from among M₀,..., M_p using crossvalidated prediction error, C_p (AIC), BIC, or adjusted R².

Section 2

Ridge Regression

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Goal

- Fit model using all p predictors
- Aim to constrain (regularize) coefficient estimates
- Shrink the coefficient estimates towards 0

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4$$

Ridge regression

Before:

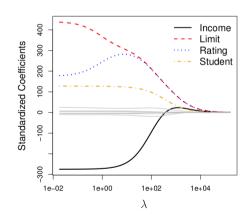
$$RSS = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j \mathsf{x}_{ij} \right)^{\frac{1}{2}}$$

After:

$$RSS = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \qquad \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$

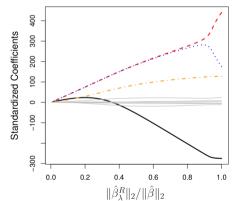
Example from the Credit data

$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$



Same Setting, Different Plot

$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2 \qquad \|\beta\|_2 = \sqrt{\sum_{j=1}^{p} \beta_j^2}$$



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Scale equivavariance (or lack thereof)

Scale equivariant: Multiplying a variable by c (cX_i) just returns a coefficient multiplied by 1/c ($1/c\beta_i$)

Solution: Standardize predictors

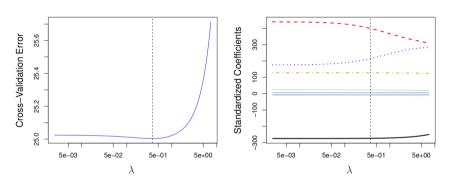
$$\widetilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \overline{x}_{j})^{2}}}$$

Using Cross-Validation to find λ

- ullet Choose a grid of λ values
- Compute the (k-fold) cross-validation error for each value of λ
- Select the tuning parameter value λ for which the CV error is smallest.
- The model is re-fit using all of the available observations and the selected value of the tuning parameter.

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LOOCV choice of λ for ridge regression and Credit data

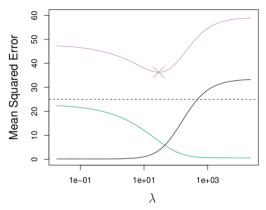


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Coding

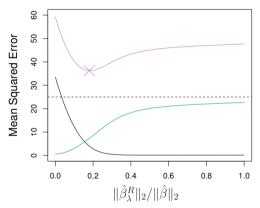
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Bias-Variance tradeoff



Squared bias (black), variance (green), and test mean squared error (purple) for simulated data.

More Bias-Variance Tradeoff



Squared bias (black), variance (green), and test mean squared error (purple) for simulated data.

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Advantages of Ridge

Ridge vs. Least Squares:

Ridge vs. Subset Selection:

Next time

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