Ch 6.1: Subset Selection

Lecture 11 - CMSE 381

Michigan State University
::
Dept of Computational Mathematics, Science & Engineering

Feb 21, 2024

Announcements

Last time

- Boostrapping

Covered in this lecture

- Subset selection
- Forward and Backward Selection
- Ridge regression

Announcements:

- HW #6 posted and due next Wednesday
- Spring break next week

Section 1

Last time

Goals of fitting a given model

Up to now, we've focused on standard linear model: $Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$ and done least squares estimation. *Translation: Minimize RSS* $= \sum_i (y_i - \hat{y}_i)^2$

Prediction accuracy

- If the true relationship is approximately linear, least squares estimates have low bias
- If $n \gg p$, then least squares also has low variance
- If n not much larger than p, then high variability, overfitting, poor predictions
- If $n < p$ then no unique solution so can't use at all
- Goal on next slide: shrink/constrain number of variables to improve accuracy

Goals of fitting a given model

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Model Interpretability

- Often, many variables included aren't associated with response
- Including them leads to unnecessary complexity in the model
- Idea: Set these coefficients to 0 (or close to zero)
- Goal on next slide: Do some automatic feature selection / variable selection to get rid of unnecessary variables

Goal of next chapter

Classes of methods

- Subset selection: identify subset of predictors, fit model using least squares on smaller set of variables
- Shrinkage:
  - Estimated coeff are shrunken towards zero relative to the least squares estimate
- Dimension reduction: Project the p-dimensional data into M-dimensional subspace, $M < p$.

Section 2

Best Subset Selection

Brute-force, but too slow...

All subsets of 4 variables ($2^4 = 16$)

- $\emptyset$

- X_1
- X_2
- X_3
- X_4

- X_1 X_2
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- X_1 X_2 X_3 X_4

The game: fit the model 2^n times, score each, pick one with best score

One way of breaking this up

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 $k = 1, 2, \ldots p$:

   (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.

3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

- Part 2b goes for lowest training score, Part 3 then goes for lowest testing score.
- Step 2 is computational infeasable for large p

Group work: calculate by hand

We train a model using four variables, X_1, X_2, X_3, X_4. We're interested in getting a subset of the variables to use. The following table shows the mean squared error and the R^2 value computed for the model learned using each possible subset of variables.

	Training MSE (x10^7)	k-fold CV Testing Error
Null model	8.76	10.08
X1	8.63	9.98
X2	7.42	8.01
X3	8.16	8.3
X4	8.33	9.06
X1,X2	4.33	7.47
X1,X3	5.82	5.22
X1,X4	3.17	4.23
X2,X3	4.07	3.78
X2,X4	3.31	4.01
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X1,X3,X4	2.97	4.23
X2,X3,X4	2.98	3.17
X1,X2,X3,X4	2.16	4.39

1. What subset of variables is found for each of the sets $\mathcal{M}_0, \mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3, \mathcal{M}_4$ when using best subset selection?
2. What subset of variables is returned using best subset selection?

Extra work space

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Section 3

Forward Selection

What's the problem?

- Checking 2^p models is not reasonable for large p, $p > 40$
- The next bits are finding alternatives to Step 2

Forward Stepwise Selection

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 $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

An example for Forward Stepwise Selection

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Group work: by hand same example with forward example

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1. What subset of variables is found for each of the sets $\mathcal{M}_0, \mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3, \mathcal{M}_4$ when using forward selection?
2. What subset of variables is returned using forward subset selection?

Extra work space if it helps

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Pros and Cons of Forward Stepwise

Pros:

- Computationally cheaper
- Number of models fit is

$$1 + \sum_{k=0}^{p-1}(p-k) = 1 + \frac{p(p+1)}{2}$$

which is way better than 2^p

Cons:

- Not guaranteed to find the best model
- As example: if best 1-variable model is X_1, but best 2-variable model is $X_2 X_3$, then forward selection won't find it.
- Is this a con? Maybe just a limitation If $n < p$, then can only construct models $\mathcal{M}_0 \cdots \mathcal{M}_{n-1}$

Section 4

Backward Selection

Backward stepwise selection

Algorithm 6.3 *Backward stepwise selection*

1. Let $\mathcal{M}_p$ denote the *full* model, which contains all p predictors.
2. For $k = p, p-1, \ldots, 1$:
   (a) Consider all k models that contain all but one of the predictors in $\mathcal{M}_k$, for a total of $k-1$ predictors.
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Group work: by hand same example with backward

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Pros:

- Computationally cheaper
- Number of models fit is still

$$1 + \sum_{k=1}^{p} k = 1 + \frac{p(p+1)}{2}$$

which is way better than 2^p

Cons:

- Not guaranteed to find the best model
- Unlike forward selection, this can't be used at all if $n < p$

Section 5

Alternatives for Approximating Test Error

Remembering what we're doing

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 $k = 1, 2, \dots p$:
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Now we're focusing on step 3

Algorithm 6.2 *Forward stepwise selection*

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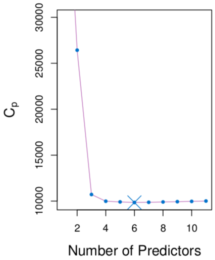
3. Select a single best model from among $\mathcal{M}_0, \dots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

The goal is to come up with ways to adjust the training scores to get something that better approximates testing scores

The C_p estimate

$$C_p = \frac{1}{n}(\mathrm{RSS} + 2d\hat{\sigma}^2)$$



Example using `Credit`

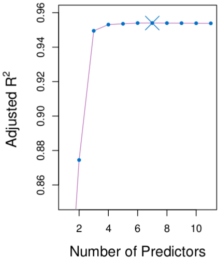
- The p does nothing. It's not our usual p. WTF
- d is the number of predictors you're using to fit
- $\hat{\sigma}^2$ is an estimate of $\mathrm{Var}(\varepsilon)$

- Penalty increases with more d, so aims for fewer predictors
- This acts to adjust for the overfitting decrease in RSS from higher d
- One can show that if $\hat{\sigma}^2$ is an unbiased estimate of σ^2, then C_p is an unbiased estimate of test MSE.
- So.... aim for model with lowest C_p
- This example takes a 6 variable model

Adjusted R^2

$$R^2 = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}}$$

$$\text{adjusted } R^2 = 1 - \frac{\mathrm{RSS}/(n-d-1)}{\mathrm{TSS}/(n-1)}$$



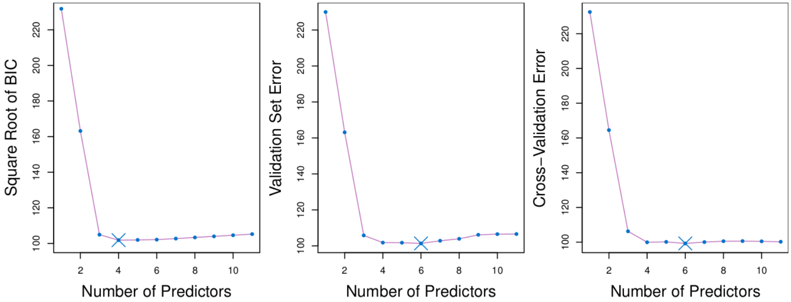
- $TSS = \sum (y_i - \bar{y})^2$ total sum of squares
- A large value means small test error, so we want the R^2 to go up
- RSS always decreases as number of variables increases, but $RSS/(n-d-1)$ could go up or down.

- Idea is that including additional variables to the model that are noise leads to small decrease in RSS.
- In that case, d always up by 1, so $\frac{RSS}{n-d-1}$ will increase, causing R^2 to decrease
- View this as penalizing adding unnecessary variables

Comparisons

- C_p has rigorous justifications that we're gonna skip
- R^2 is intuitive, but doesn't really come with theoretical justification
- These equations presented are in the case of least squares fit.

All this vs. Validation and Cross Validation



- The goal was to approximate test error, so why not do validation or CV instead?
- Historically, CV was computationally prohibitive. These tools were an alternative to deal with the same question but with much cheaper computation

Section 6

Ridge Regression

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
- Lasso

Ridge regression

Before:

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

- $\lambda \geq 0$ is a tuning paramter to figure out separately.
- Second term is called “shrinkage penalty”
- $\lambda = 0$ means least squares estimate

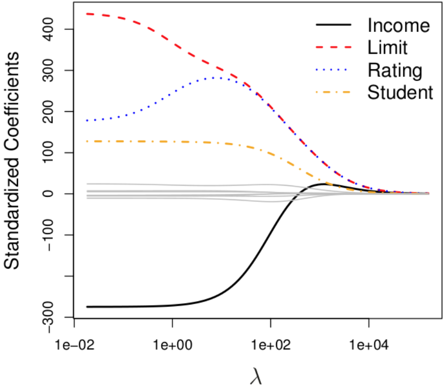
After:

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

- As $\lambda \to \infty$ impact of shrinkage penalty grows, ridge regression coeff will go towards 0
- Not applied to the intercept
- call coefficients found by ridge regression $\hat{\beta}_\lambda^R = (\beta_{1,\lambda}^R, \cdots, \beta_{p,\lambda}^R \cdots)$

Example from the Credit data

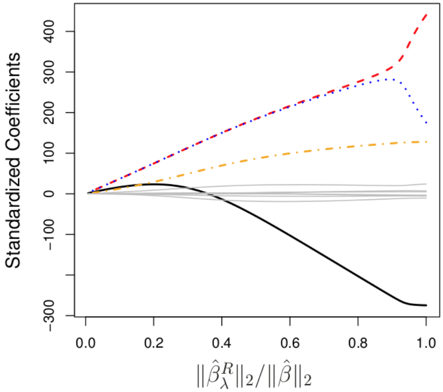
$$RSS + \lambda \sum_{j=1}^{p} \beta_j^2$$



- Left x-axis, $\lambda \approx 0$
- Each line is the predicted coefficient value for a single variable
- as λ increases everything goes to 0, basically giving the null model at the right end

Same Setting, Different Plot

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



- $\hat{\beta}$ is the vector of least squares coeff estimates
- $\|\cdot\|$ measures distance from 0
- $\|\hat{\beta}_\lambda^R\|/\|\hat{\beta}\|$ ranges from 1 (when $\lambda = 0$) down to 0
- Amount the coefficient estimates have been shrunk

Scale equivavariance (or lack thereof)

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

- Ex: `income variable`.
- Least squares is scale equivariant
- Ridge regression very much is not
- $X_j\hat{\beta}^R_{j,\lambda}$ depends not only on λ but also on values of other predictors

Solution: Standardize predictors

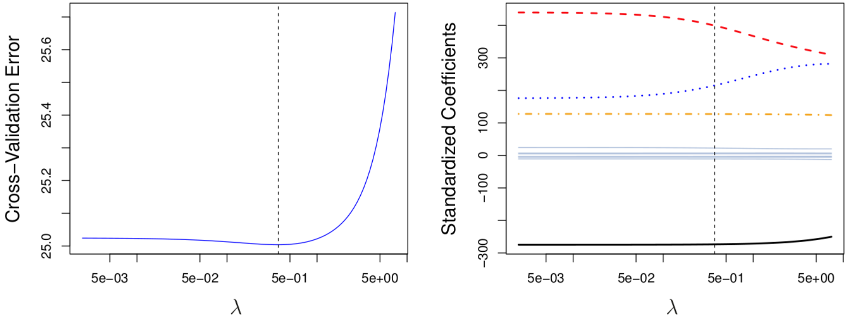
$$\widetilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \overline{x}_j)^2}}$$

- Denominator is estimated standard deviation of the jth predictor
- Standardized predictors will all have a standard deviation of one
- Previous figures showe standardized ridge regression coeffs on the y-axis

Using Cross-Validation to find λ

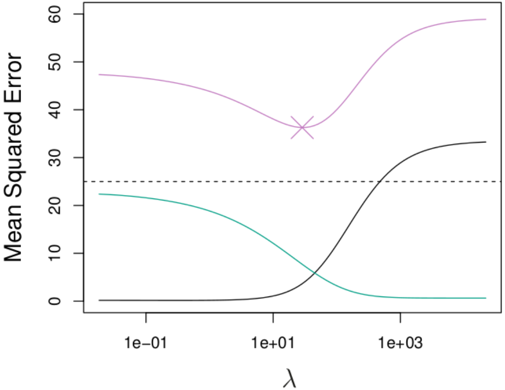
- Choose a grid of λ values
- Compute the (k-fold) cross-validation error for each value of λ
- Select the tuning parameter value λ for which the CV error is smallest.
- The model is re-fit using all of the available observations and the selected value of the tuning parameter.

LOOCV choice of λ for ridge regression and Credit data



- Dashed vertical lines indicate the selected value of λ.
- In this case, small λ so optimal fit involves small amount of shrinkage relative to least squares
- The dip is not very pronounced, so there is rather a wide range of values that would give a very similar error.
- In a case like this we might simply use the least squares solution.

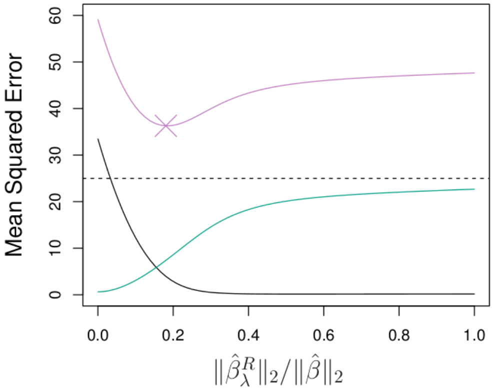
Bias-Variance tradeoff



Squared bias (black), variance (green), and test mean squared error (purple) for simulated data. *Horizontal dashed line is minimum possible test MSE*

- Bias-variance tradeoff
- Minimum MSE achieved around $\lambda = 30$
- High variance means MSE for $\lambda = 0$ (least squares) and $\lambda = \infty$ (null model) are basically the same

More Bias-Variance Tradeoff



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

Advantages of Ridge

Ridge vs. Least Squares:

- Previous slide and ability to lower variance
- Ridge regression works best in situations where the least squares estimates have high variance
- Can trade off small increase in bias for a large decrease in variance

Ridge vs. Subset Selection:

- So much better computationally!
- Only fits a single model rather than 2^p
- Tricks available to find the optimal λ without CV