Lecture 13: Model selection and regularization

Reading: Sections 6.1-6.2.1

STATS 202: Data mining and analysis

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- However, adding predictors does not necessarily improve the test error.
- Selecting significant predictors is hard when n is not much larger than p.
- When $n < p$, there is no least squares solution:

$$\hat{\beta} = \underbrace{(\mathbf{X}^T\mathbf{X})}_{\text{Singular}}{}^{-1}\mathbf{X}^T y.$$

So, we must find a way to select fewer predictors.

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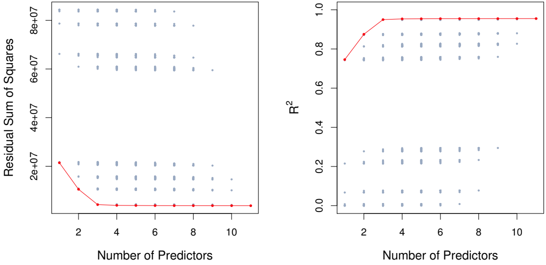

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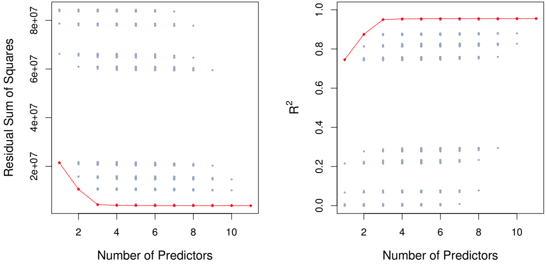

- Naturally, the RSS and R^2 improve as we increase k.

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$$\frac{1}{n\hat{\sigma}^2}(\mathsf{RSS} + 2k\hat{\sigma}^2)$$

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3. **Adjusted R^2:**

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

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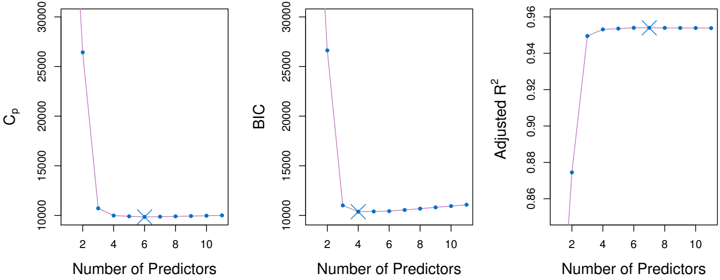
How do they compare to cross validation:

- They are much less expensive to compute.
- They are motivated by asymptotic arguments and rely on model assumptions (eg. normality of the errors).
- Equivalent concepts for other models (e.g. logistic regression).

Example

Best subset selection for the Credit dataset.



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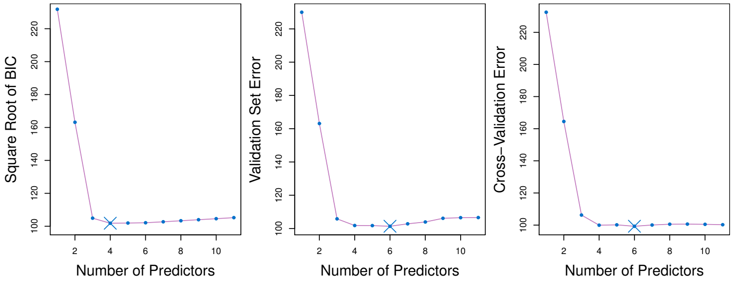
Cross-validation vs. the BIC.



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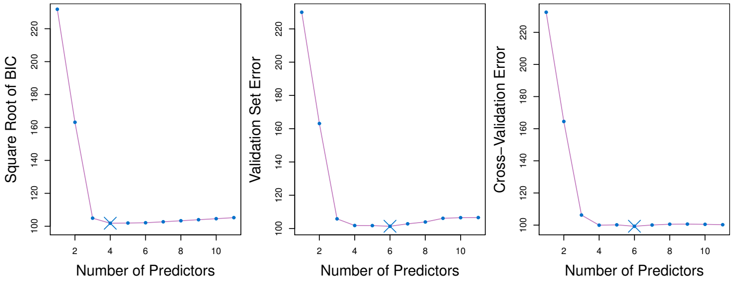

Recall: In k-fold cross validation, we can estimate a standard error or accuracy for our test error estimate. Then, we apply the **one standard-error rule**.

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2. If for a fixed k, there are too many possibilities, we increase our chances of overfitting. The model selected has *high variance*.

In order to mitigate these problems, we can restrict our search space for the best model.

This reduces the variance of the selected model at the expense of an increase in bias.

Forward 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.

Forward selection vs. best subset

# Variables	Best subset	Forward stepwise
One	rating	rating
Two	rating, income	rating, income
Three	rating, income, student	rating, income, student
Four	cards, income	rating, income,
	student, limit	student, limit

TABLE 6.1. *The first four selected models for best subset selection and forward stepwise selection on the* Credit *data set. The first three models are identical but the fourth models differ.*

Backward 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.
   (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 R^2.
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  - Backward: $\{X_1, X_2, X_3\} \to \{X_1, X_2\} \to \{X_2\}$

Other stepwise selection strategies

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The idea is to perform a linear regression, while *regularizing* or *shrinking* the coefficients $\hat{\beta}$ toward 0.

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- Extreme example: set $\hat{\beta}$ to 0 – variance is 0!
- There are Bayesian motivations to do this: the prior tends to shrink the parameters.

Ridge regression

Ridge regression solves the following optimization:

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

In blue, we have the RSS of the model.

In red, we have the squared ℓ_2 norm of β, or $\|\beta\|_2^2$.

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The parameter λ is a tuning parameter. It modulates the importance of fit vs. shrinkage.

We find an estimate $\hat{\beta}^R_\lambda$ for many values of λ and then choose it by cross-validation. Fortunately, this is no more expensive than running a least-squares regression.

Ridge regression

In least-squares linear regression, scaling the variables has no effect on the fit of the model:

$$Y = X_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p.$$

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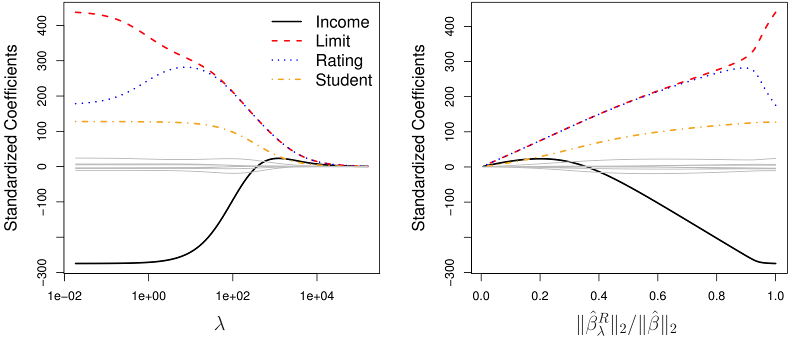
In practice, what do we do?

- Scale each variable such that it has sample variance 1 before running the regression.
- This prevents penalizing some coefficients more than others.

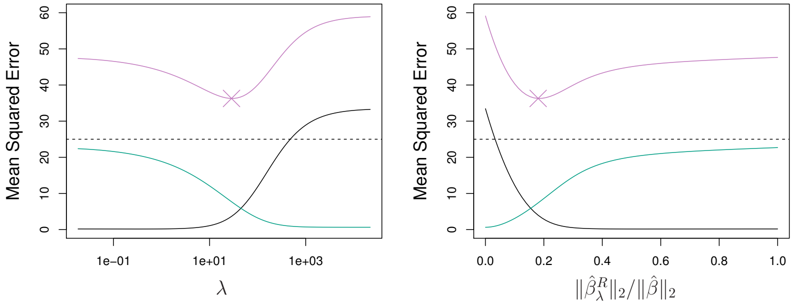
Example. Ridge regression

Ridge regression of `default` in the Credit dataset.



Bias-variance tradeoff

In a simulation study, we compute bias, variance, and test error as a function of λ.



Cross validation would yield an estimate of the test error.

Selecting λ by cross-validation