Lecture 11: Cross validation

Reading: Chapter 5

STATS 202: Data mining and analysis

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Comparing classification methods through simulation

1. Simulate data from several different known distributions with 2 predictors and a binary response variable.
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2. Compare the test error (0-1 loss) for the following methods:
   - KNN-1
   - KNN-CV (“optimal” KNN)
   - Logistic regression
   - Linear discriminant analysis (LDA)
   - Quadratic discriminant analysis (QDA)
Scenario 1

- $X_1, X_2$ standard normal.
- No correlation in either class.
Scenario 2

- $X_1, X_2$ standard normal.
- Correlation is -0.5 in both classes.
Scenario 3

- $X_1, X_2$ Student $t$ random variables.
- No correlation in either class.
Scenario 4

- $X_1, X_2$ standard normal.
- First class has correlation 0.5, second class has correlation -0.5.
Scenario 5

- $X_1, X_2$ uncorrelated, standard normal.

- Response $Y$ was sampled from:

$$P(Y = 1|X) = \frac{e^{\beta_0 + \beta_1(X_1^2) + \beta_2(X_2^2) + \beta_3(X_1X_2)}}{1 + e^{\beta_0 + \beta_1(X_1^2) + \beta_2(X_2^2) + \beta_3(X_1X_2)}}.$$
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- The true decision boundary is quadratic.
Scenario 6

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$$P(Y = 1|X) = \frac{e^{f_{\text{nonlinear}}(X_1, X_2)}}{1 + e^{f_{\text{nonlinear}}(X_1, X_2)}}.$$ 

- The true decision boundary is very rough.
Thinking about the loss function is important

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In the Kaggle competition, what is our loss function?
Validation

**Problem:** Choose a supervised method that minimizes the test error.

In addition, tune the parameters of each method:
- $k$ in $k$-nearest neighbors.
- The number of variables to include in forward or backward selection.
- The order of a polynomial in polynomial regression.

Use of a validation set is one way to approximate the test error:
- Divide the data into two parts.
- Train each model with one part.
- Compute the error on the other.
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Polynomial regression to estimate mpg from horsepower in the Auto data.
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Problem: Every split yields a different estimate of the error.
Leave one out cross-validation

- For every $i = 1, \ldots, n$:
  - train the model on every point except $i$,
  - compute the test error on the held out point.
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- For every \( i = 1, \ldots, n \):
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- Average the test errors.
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CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i^{(-i)})^2
\]

Prediction for the \( i \) sample without using the \( i \)th sample.
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\[
CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} 1(y_i \neq \hat{y}_i^{(-i)})
\]

... for a classification problem.
Computing $CV_{(n)}$ can be computationally expensive, since it involves fitting the model $n$ times.
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For linear regression, there is a shortcut:

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{y_i - \hat{y}_i}{1 - h_{ii}} \right)^2$$

where $h_{ii}$ is the leverage statistic.
\( k \)-fold cross-validation

- Split the data into \( k \) subsets or folds.
**k-fold cross-validation**

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  - train the model on every fold except the \( i \)th fold,
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\(k\)-fold cross-validation

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- Average the test errors.
LOOCV vs. \( k \)-fold cross-validation

\[ \text{Mean Squared Error} \]

- **LOOCV**
- **10-fold CV**

During \( k \)-fold CV, we train the model on less data than what is available. This introduces bias into the estimates of test error. In LOOCV, the training samples highly resemble each other, increasing the variance of the test error estimate. \( n \)-fold CV is equivalent to LOOCV.
LOOCV vs. $k$-fold cross-validation

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- $n$-fold CV is equivalent LOOCV.
Choosing an optimal model

Even if the error estimates are off, choosing the model with the minimum cross validation error often leads to a method with near minimum test error.
Choosing an optimal model

In a classification problem, things look similar.

- - - Bayes boundary

—— Logistic regression with polynomial predictors of increasing degree.
Choosing an optimal model

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The one standard error rule

Forward stepwise selection

Blue: 10-fold cross validation
Yellow: True test error
The one standard error rule

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Forward stepwise selection

- A number of models with $10 \leq p \leq 15$ have almost the same CV error.
- The vertical bars represent 1 standard error in the test error from the 10 folds.
- **Rule of thumb:** Choose the simplest model whose CV error is no more than one standard error above the model with the lowest CV error.

Blue: 10-fold cross validation
Yellow: True test error
The wrong way to do cross validation

*Reading*: Section 7.10.2 of The Elements of Statistical Learning.

We want to classify 200 individuals according to whether they have cancer or not.
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We want to classify 200 individuals according to whether they have cancer or not. We use logistic regression onto 1000 measurements of gene expression.

Proposed strategy:

- Using all the data, select the 20 most significant genes using z-tests.
- Estimate the test error of logistic regression with these 20 predictors via 10-fold cross validation.
The wrong way to do cross validation

To see how that works, let’s use the following simulated data:

- Each gene expression is standard normal and independent of all others.
- The response (cancer or not) is sampled from a coin flip — no correlation to any of the “genes”.

What should the misclassification rate be for any classification method using these predictors?

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Why is this?

- Since we only have 200 individuals in total, among 1000 variables, at least some will be correlated with the response.

- We do variable selection using *all the data*, so the variables we select have some correlation with the response in every subset or fold in the cross validation.
The **right** way to do cross validation

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- For \( i = 1, \ldots, 10 \):
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- Average the 10 test errors obtained.

In our simulation, this produces an error estimate of close to 50%. Moral of the story: Every aspect of the learning method that involves using the data — variable selection, for example — must be cross-validated.
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