Lecture 11: Cross validation

Reading: Chapter 5

STATS 202: Data mining and analysis

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Slide credits: Sergio Bacallado

Comparing classification methods through simulation

1. Simulate data from several different known distributions with 2 predictors and a binary response variable.

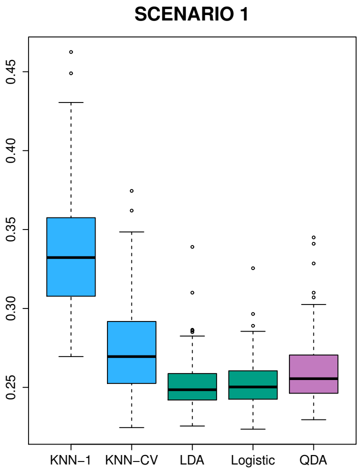
Comparing classification methods through simulation

1. Simulate data from several different known distributions with 2 predictors and a binary response variable.

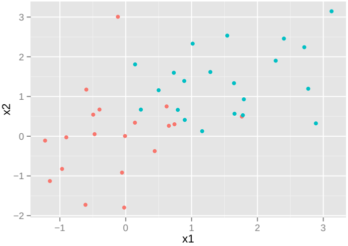
2. Compare the test error (0-1 loss) for the following methods:

   - KNN-1
   - KNN-CV ("optimal" KNN)
   - Logistic regression
   - Linear discriminant analysis (LDA)
   - Quadratic discriminant analysis (QDA)

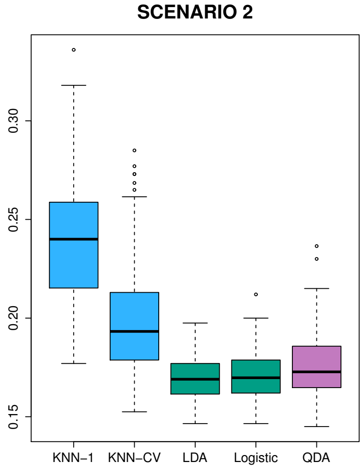
Scenario 1



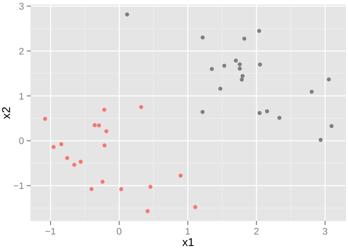
- X_1, X_2 standard normal.
- No correlation in either class.



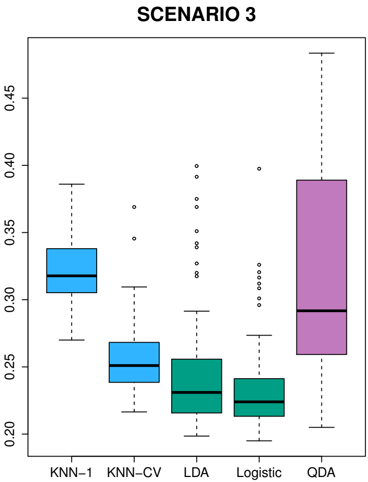
Scenario 2



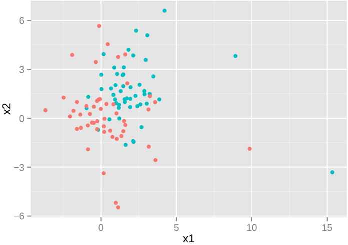
- X_1, X_2 standard normal.
- Correlation is -0.5 in both classes.



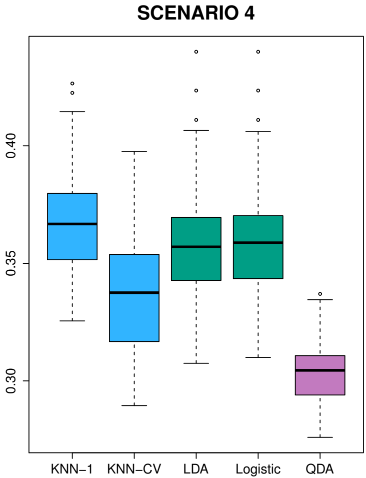
Scenario 3



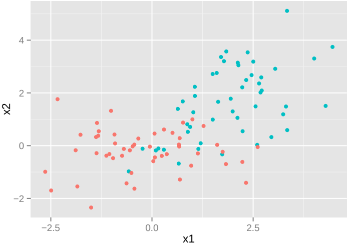
- X_1, X_2 Student t random variables.
- No correlation in either class.



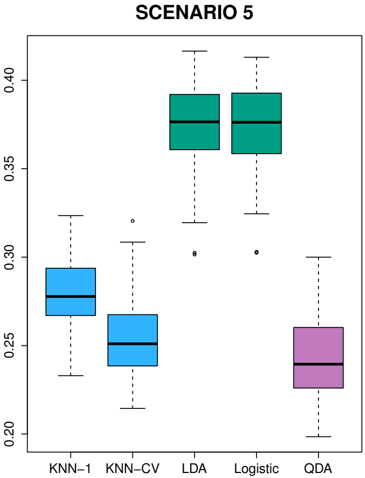
Scenario 4



- 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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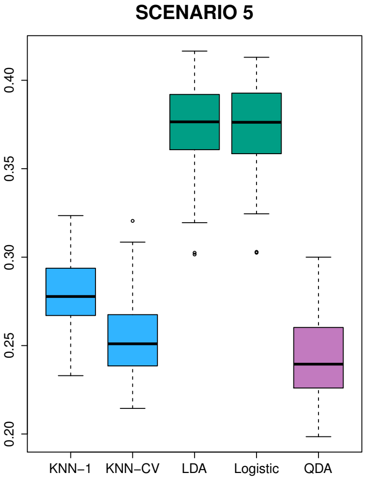

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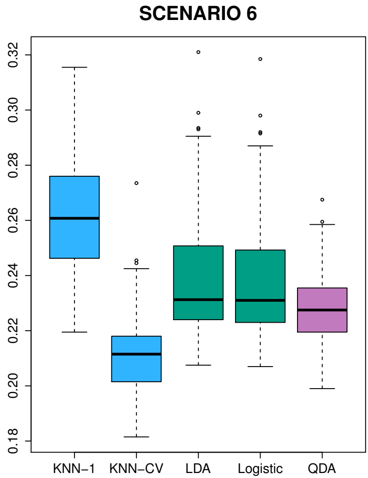
- The true decision boundary is quadratic.

Scenario 6



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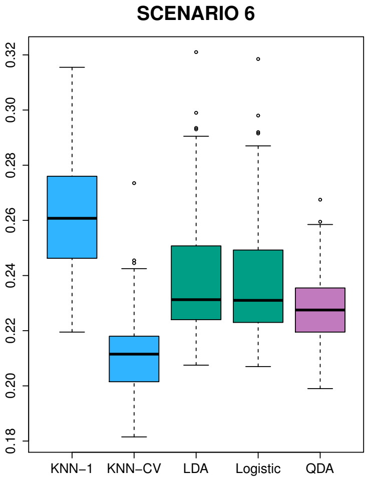

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$$P(Y = 1|X) = \frac{e^{f_{\text{nonlinear}}(X_1, X_2)}}{1 + e^{f_{\text{nonlinear}}(X_1, X_2)}}.$$

- The true decision boundary is very rough.

Thinking about the loss function is important

Most of the **regression** methods we've studied aim to minimize the RSS, while **classification** methods aim to minimize the 0-1 loss.

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In the Kaggle competition, what is our loss function?

Validation

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- k in k-nearest neighbors.
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- 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.

Validation set approach

Goal: Estimate the test error for a supervised learning method.

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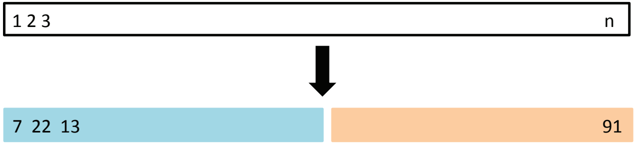

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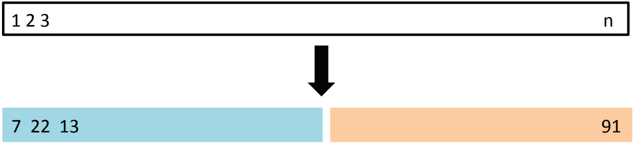

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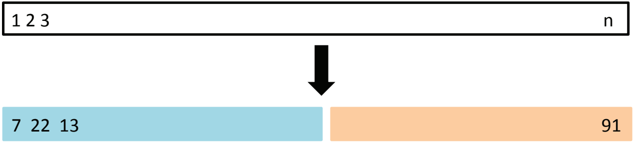
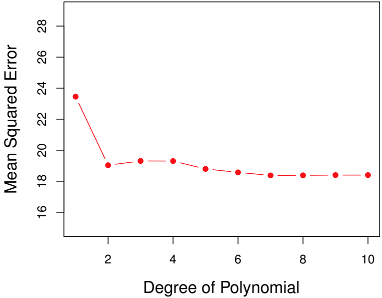
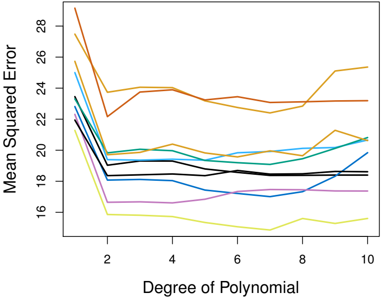


Validation set approach

Polynomial regression to estimate `mpg` from `horsepower` in the Auto data.





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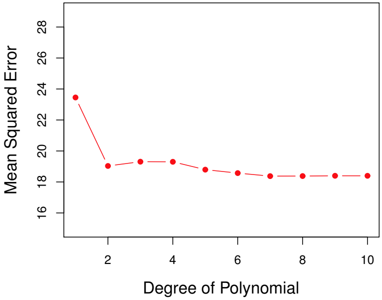
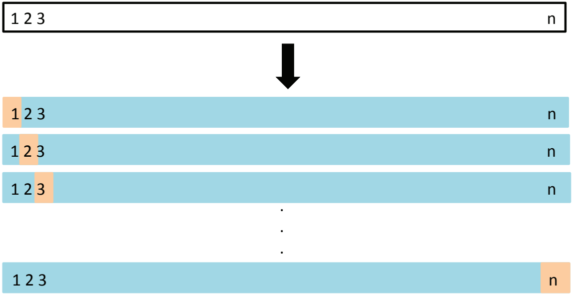


Problem: Every split yields a different estimate of the error.

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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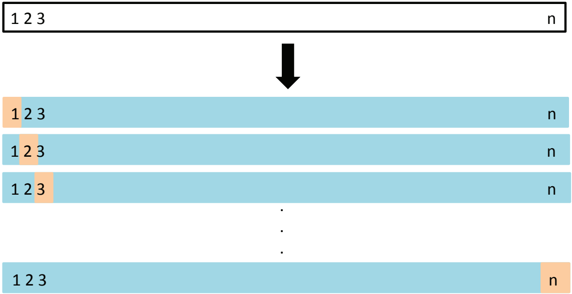

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$$\mathsf{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i^{(-i)})^2$$

Prediction for the i sample without using the ith sample.

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$$\text{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}(y_i \neq \hat{y}_i^{(-i)})$$

... for a classification problem.

Leave one out cross-validation

Computing $\mathsf{CV}_{(n)}$ can be computationally expensive, since it involves fitting the model n times.

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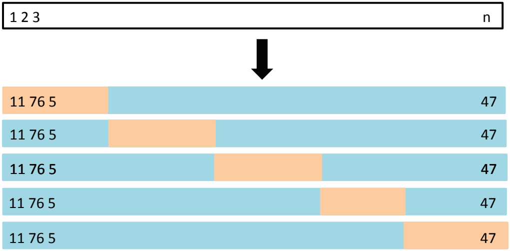
For linear regression, there is a shortcut:

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

where h_{ii} is the leverage statistic.

k-fold cross-validation

- Split the data into k subsets or *folds*.



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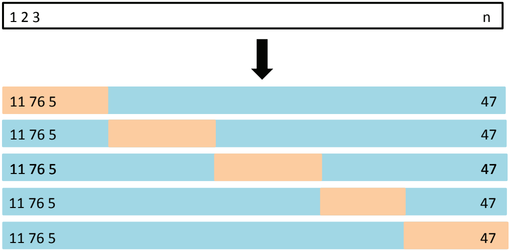

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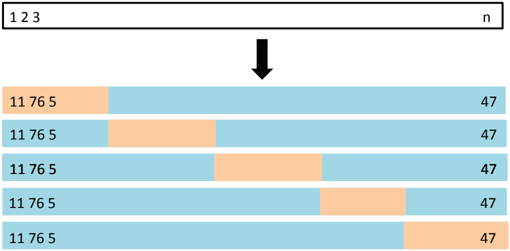
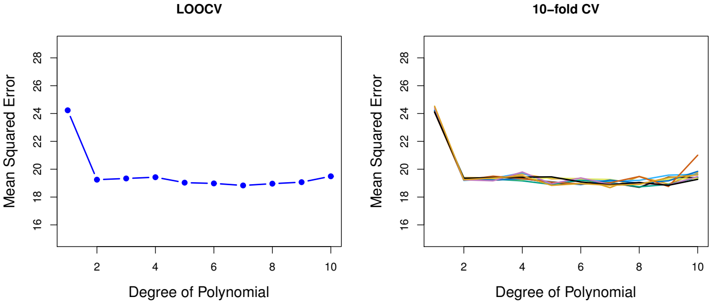
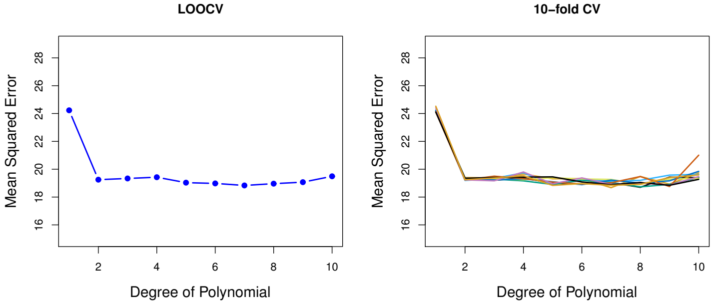


LOOCV vs. k-fold cross-validation

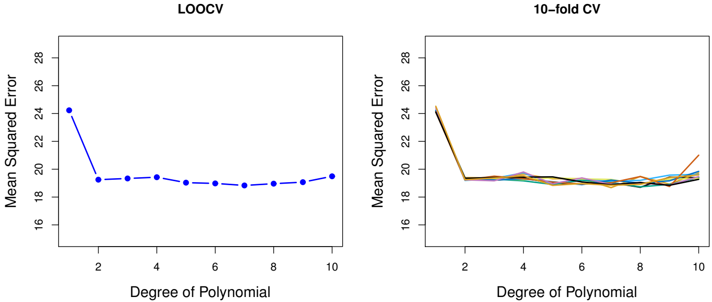


LOOCV vs. k-fold cross-validation



- k-fold CV depends on the chosen split (somewhat).

LOOCV vs. k-fold cross-validation



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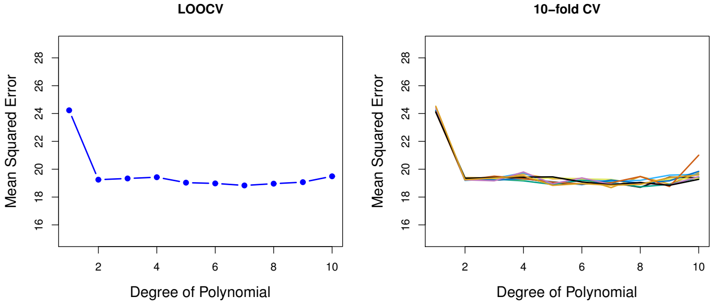

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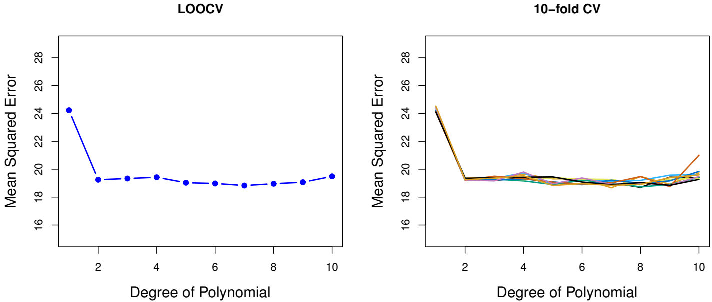
LOOCV vs. k-fold cross-validation



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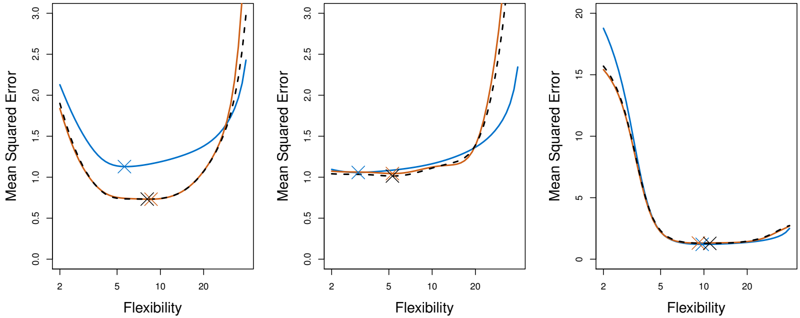
- n-fold CV is equivalent LOOCV.

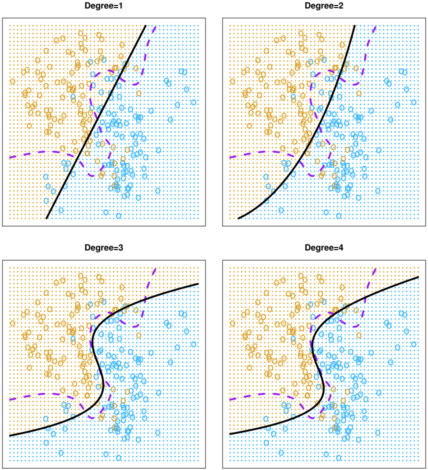
Choosing an optimal model



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.

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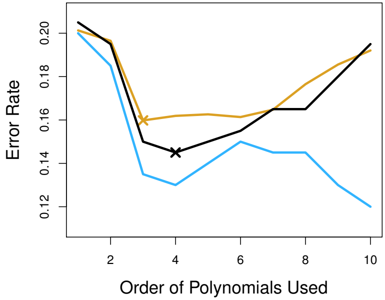
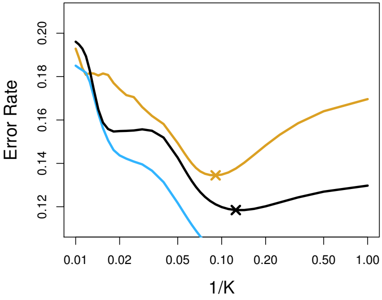
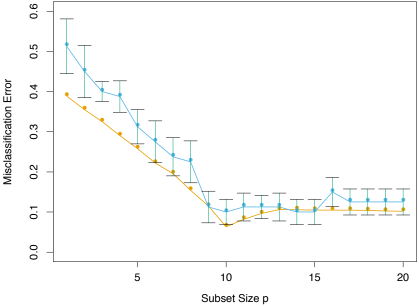




The one standard error rule

Forward stepwise selection



Blue: 10-fold cross validation
Yellow: True test error

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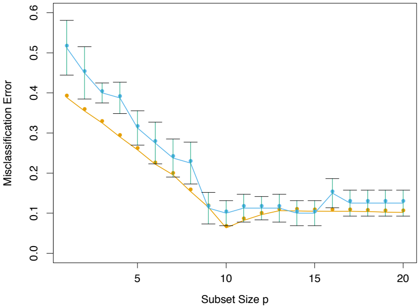

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- A number of models with $10 \leq p \leq 15$ have almost the same CV error.

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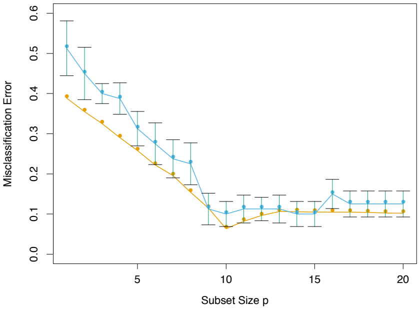

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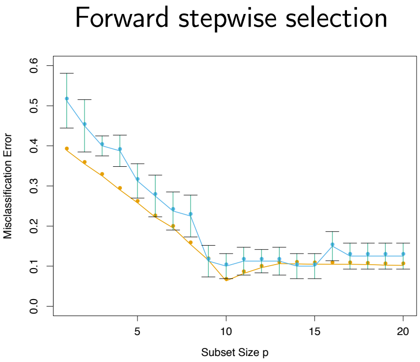

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- A number of models with $10 \leq p \leq 15$ have almost the same CV error.
- The vertical bars represent 1 standard error in the test error from the 10 folds.
- **Rule of thumb:** Choose the simplest model whose CV error is no more than one standard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

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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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.

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

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- 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?

Roughly 50%.

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We run this simulation, and obtain a CV error rate of 3%!

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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.

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- Average the 10 test errors obtained.

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In our simulation, this produces an error estimate of close to 50%.

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Moral of the story: Every aspect of the learning method that involves using the data — variable selection, for example — must be cross-validated.