Model Selection

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How do we measure our models' ability to predict unseen data, when we only have access to training data?

Cross-validation

The most common method to evaluate model **generalization** performance is cross-validation.

It is used in two essential data analysis phases: Model Selection and Model Assessment.

Cross-validation

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Model Selection

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Consider an SVM example: what predictors should be included?, interactions?, data transformations? Use a kernel? Which kernel?

Another example is the value of hyper-parameters to use when training.

Which kind of algorithm to use, linear regression vs. K-nearest neighbors vs. SVM

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The same question can be asked of a kernel parameter in an SVM.

Cross-validation

Cross-validation is a resampling method to obtain estimates of **expected prediction error rate** (or any other performance measure on unseen data).

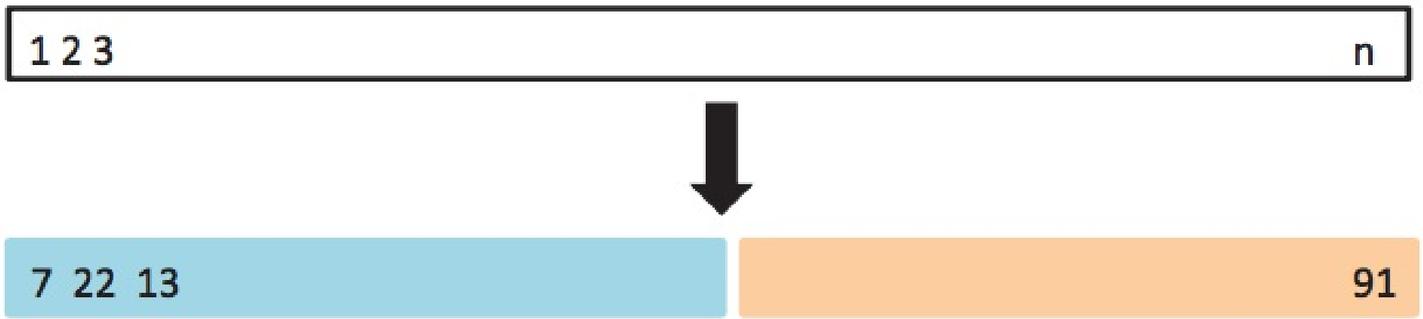
In some instances, you will have a large predefined test dataset **that you should never use when training**.

In the absence of access to this kind of dataset, cross validation can be used.

Validation Set

The simplest option to use cross-validation is to create a validation set, where our dataset is **randomly** divided into training and validation sets.

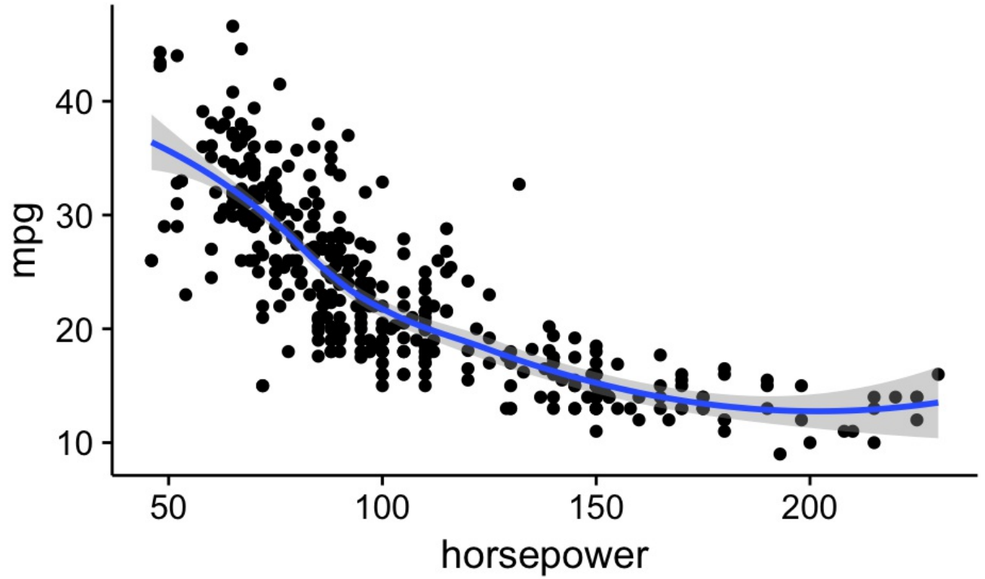
Then the validation is set aside, and not used at until until we are ready to compute **test error rate** (once, don't go back and check if you can improve it).



Validation Set

Let's look at an example using automobile data, where we want to build a regression model to predict miles per gallon given other auto attributes.

A linear regression model is not appropriate for this dataset. Use polynomial regression as an illustrative example.



Validation Set

For polynomial regression, our regression model (for a single predictor X) is given as a d degree polynomial.

$$Y = b + w_1 x + w_2 x^2 + \cdots + w_d x^d$$

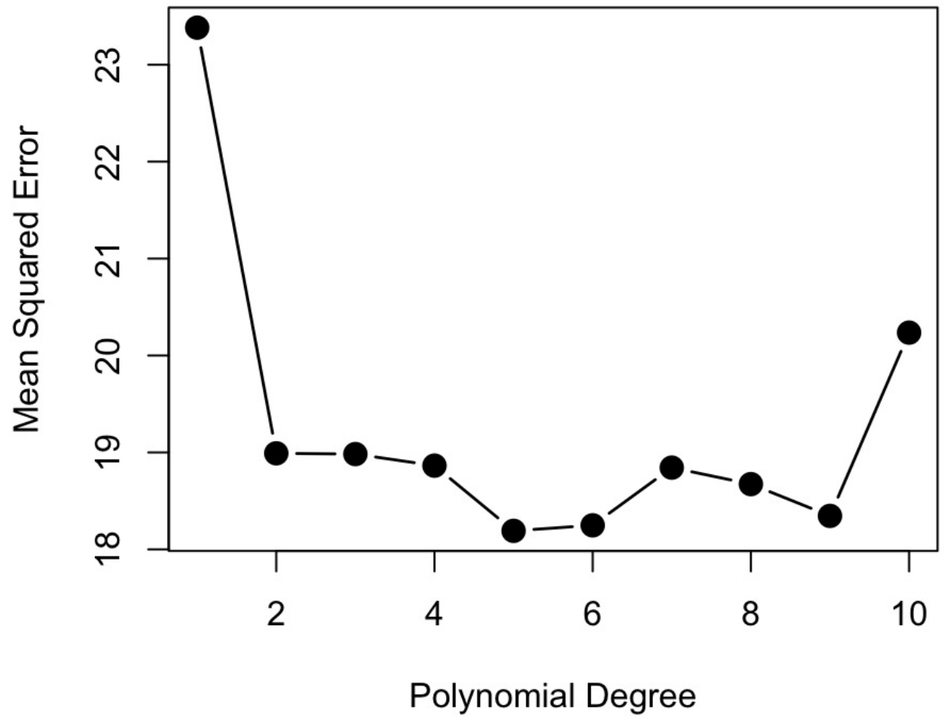
For model selection, we want to decide what degree d we should use to model this data.

Validation Set

Using the validation set method, split our data into a training set,

fit the regression model with different polynomial degrees d on the training set,

measure test error on the validation set.



Resampled validation set

The validation set approach can be prone to sampling issues.

It can be highly variable as error rate is a random quantity and depends on observations in training and validation sets.

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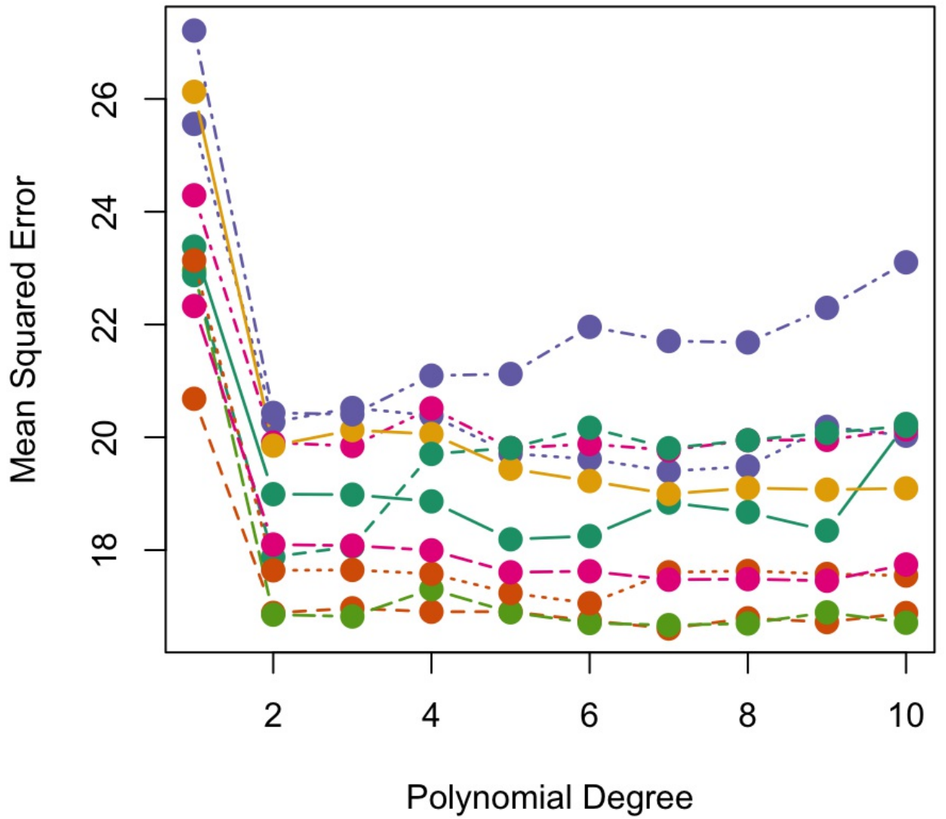
We can improve our estimate of test error by averaging multiple measurements of it (remember the law of large numbers).

Resampled validation set

Resample validation set 10 times (yielding different validation and training sets) and averaging the resulting test errors.



Leave-one-out Cross-Validation

This approach still has some issues.

Each of the training sets in our validation approach only uses 50% of data to train, which leads to models that may not perform as well as models trained with the full dataset and thus we can overestimate error.

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To alleviate this situation, we can extend our approach to the extreme: Make each single training point it's own validation set.

Leave-one-out Cross-Validation

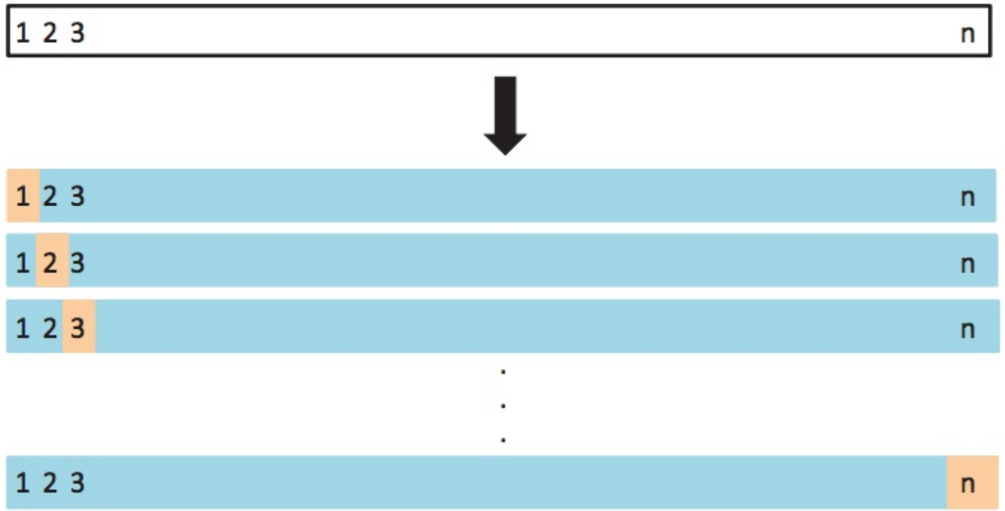
Procedure:

For each observation i in data set:

a. Train model on all but i-th observation

b. Predict response for i-th observation

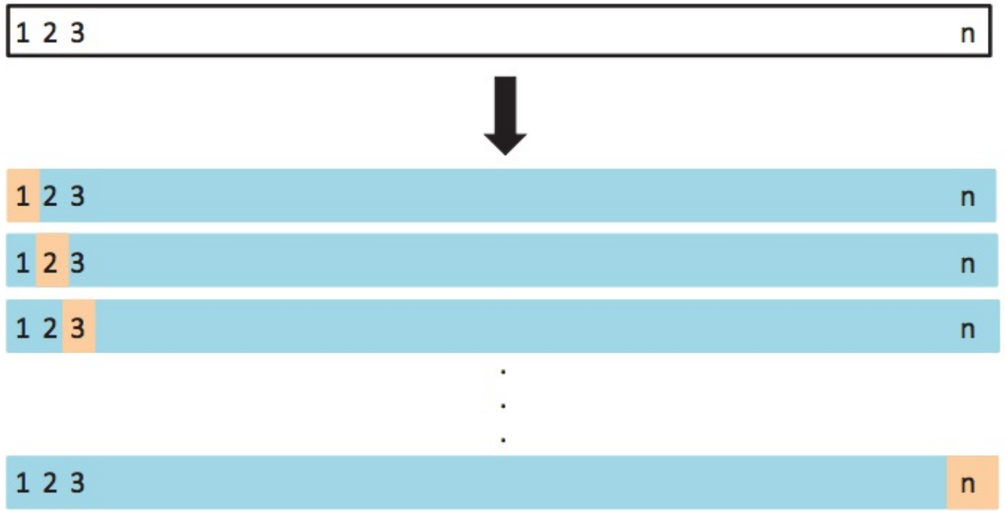
c. Calculate prediction error



Leave-one-out Cross-Validation

This gives us the following cross-validation estimate of error.

$$CV_{(n)} = \frac{1}{n}\sum_i (y_i - \hat{y}_i)^2$$



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Advantages:

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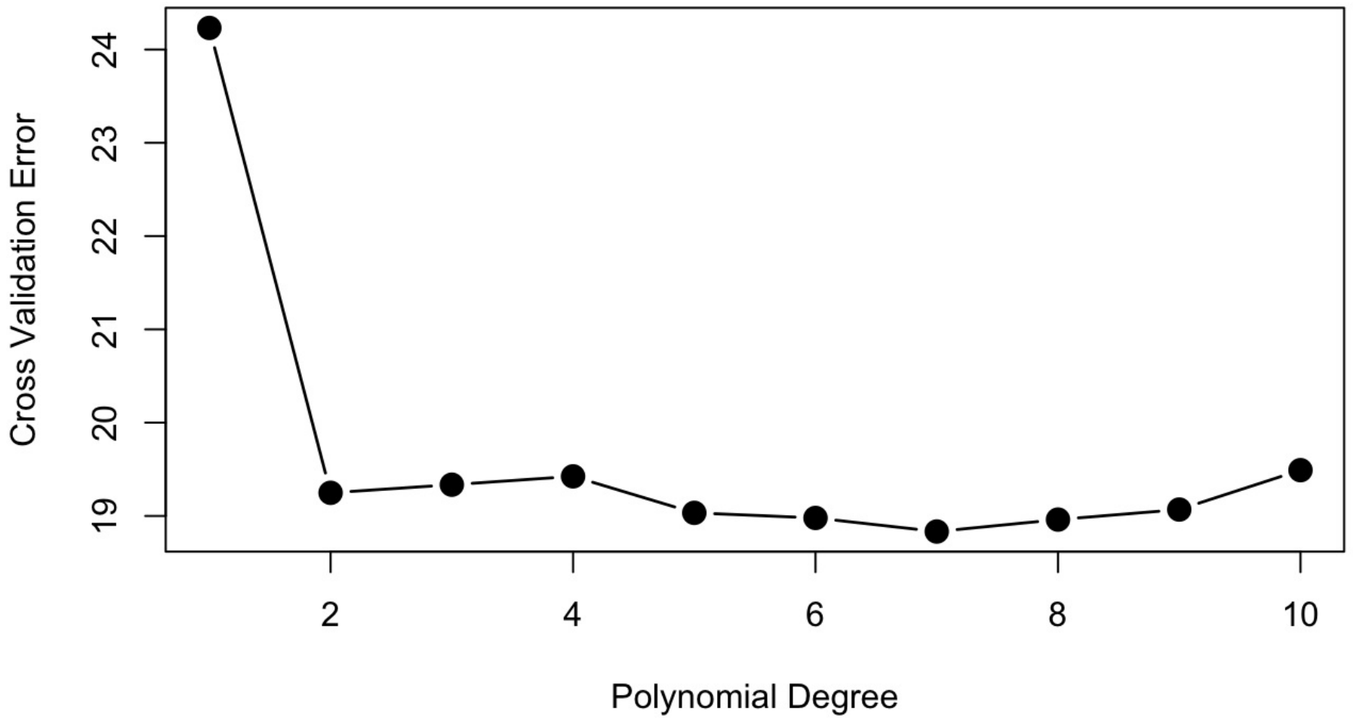
Disadvantages:

- Depending on the models we are trying to fit, it can be very costly to train $n-1$ models.
- Error estimate for each model is highly variable (since it comes from a single datapoint).

Leave-one-out Cross-Validation

On our running example



k-fold Cross-Validation

This discussion leads us to the most commonly used cross-validation approach k-fold Cross-Validation.

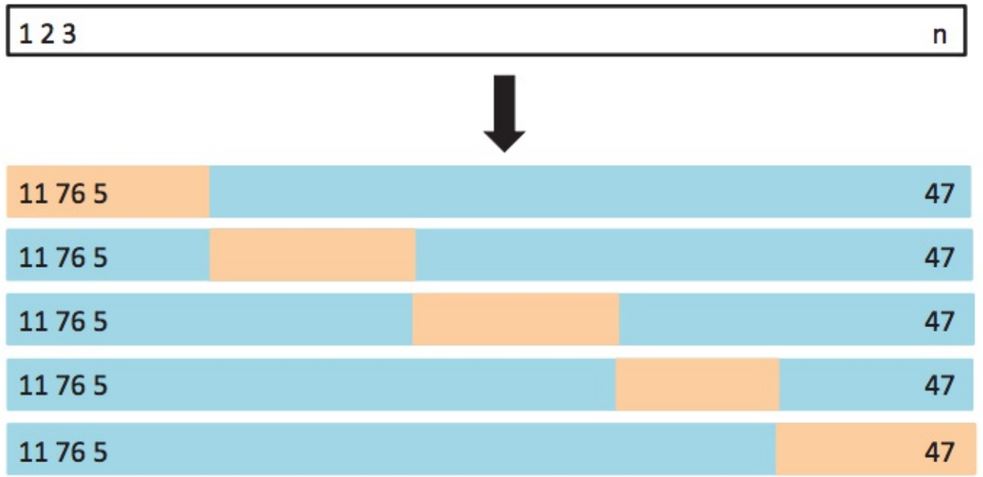
k-fold Cross-Validation

Procedure:

Partition observations randomly into k groups (folds).

For each of the k groups of observations:

- Train model on observations in the other $k-1$ folds
- Estimate test-set error (e.g., Mean Squared Error) on this fold



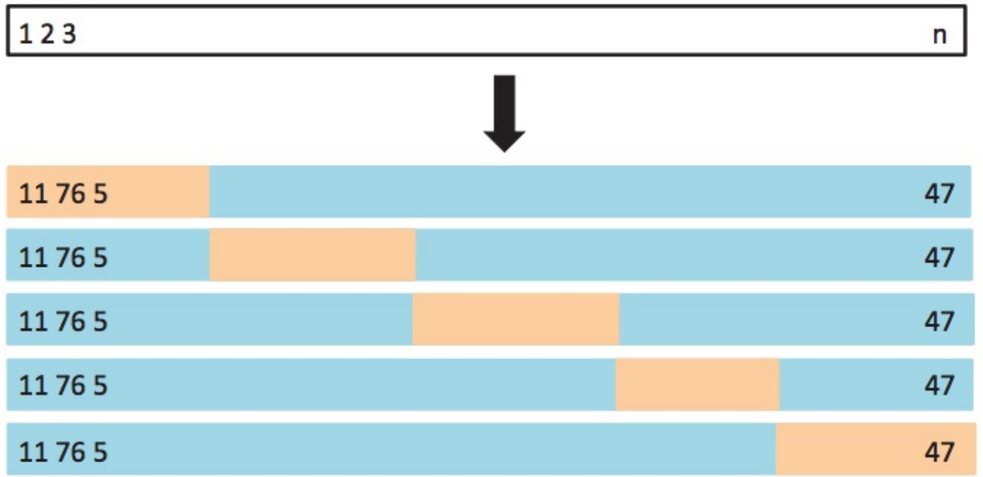
k-fold Cross-Validation

Procedure:

Compute average error across k folds

$$CV_{(k)} = \frac{1}{k} \sum_{i} MSE_i$$

where MSE_i is mean squared error estimated on the i-th fold



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- Fewer models to fit (only k of them)
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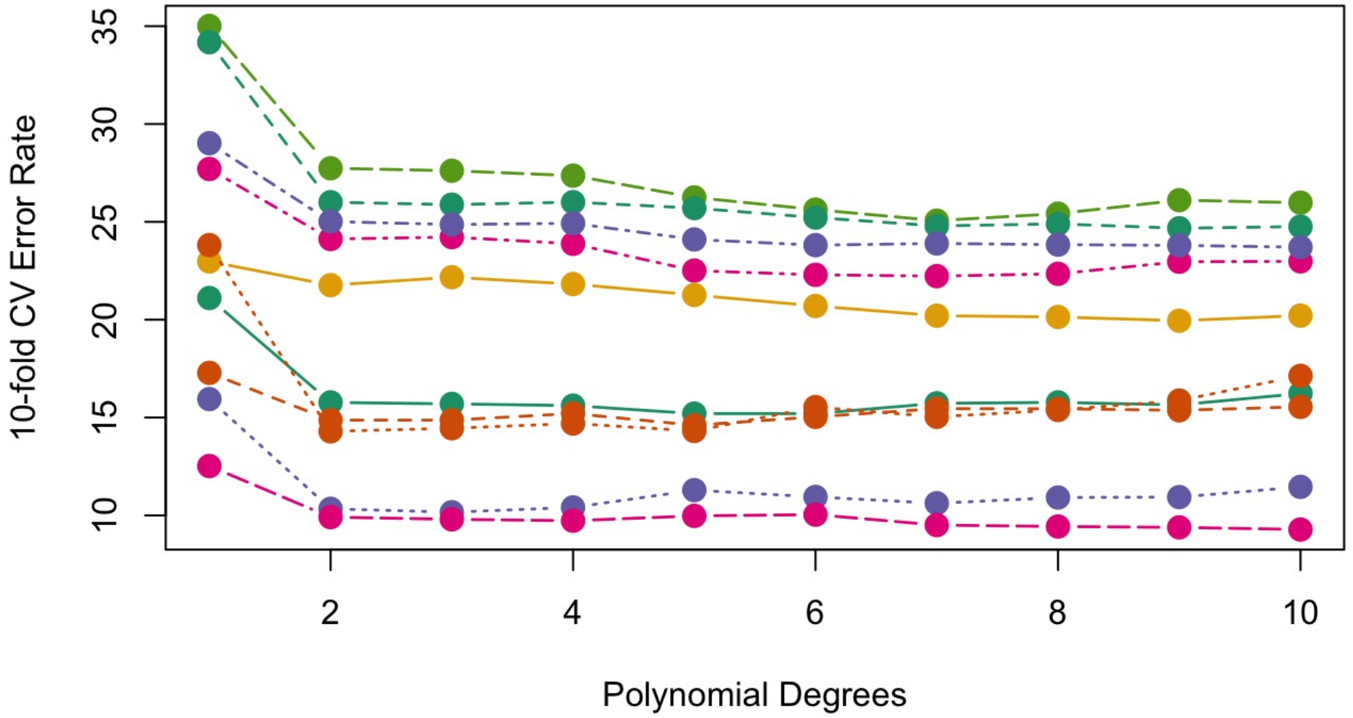
It can be shown that there is a slight bias (over estimating usually) in error estimate obtained from this procedure.

k-fold Cross-Validation

Running Example



Cross-Validation in Classification

Each of these procedures can be used for classification as well.

In this case we would substitute MSE with performance metric of choice.
E.g., error rate, accuracy, TPR, FPR, AUROC.

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In this case we would substitute MSE with performance metric of choice. E.g., error rate, accuracy, TPR, FPR, AUROC.

Note however that not all of these work with LOOCV (e.g. AUROC since it can't be defined over single data points).

Evaluating Classification

The AUROC statistic

The AUROC statistic is related to the Mann-Whitney non-parametric statistical test for distributional differences.

Null hypothesis: for randomly drawn pair of samples from two populations, it is equally likely that sample from first population is greater than sample from second population.

Evaluating Classification

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The AUROC statistic is related to the Mann-Whitney non-parametric statistical test for distributional differences.

Null hypothesis: for randomly drawn pair of samples from two populations, it is equally likely that sample from first population is greater than sample from second population.

Specifically, if x_A and x_B are drawn randomly from populations A and B respectively, $P(x_A < x_B) = P(x_A > x_B)$.

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Consider a classifier C trained to distinguish between two classes, using a training set containing n_A and n_B instances for each of the two classes respectively.

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Denote as C_i the score given by classifier i with higher C_i indicating predictions for class A.

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Use the Mann-Whitney test to verify that scores for class A are greater than scores for class B

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Use the Mann-Whitney test to verify that scores for class A are greater than scores for class B

Null hypothesis: $P(C_i < C_j) = P(C_j < C_i)$ for randomly drawn pairs C_i from class A and C_j from class B.

Evaluating Classification

The AUROC statistic

The Mann-Whitney test uses the U statistic to perform this test:

$$U = \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} \frac{I\{C_i > C_j\}}{n_A n_B}$$

This is an empirical estimate of $P(C_i > C_j)$, which under the null hypothesis of the Mann-Whitney test is 0.5.

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It can be shown that U is exactly the AUCROC.

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Note that the U statistic, and thus AUROC, is only dependent on the rank of scores c_i not on their magnitude.

This implies that we can compare AUCROC for classifiers that produce scores in different scales, e.g., probabilities or not.

Evaluating Classification

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The relationship to the Mann-Whitney test also permits to use its inferential tools on AUCROC statistics.

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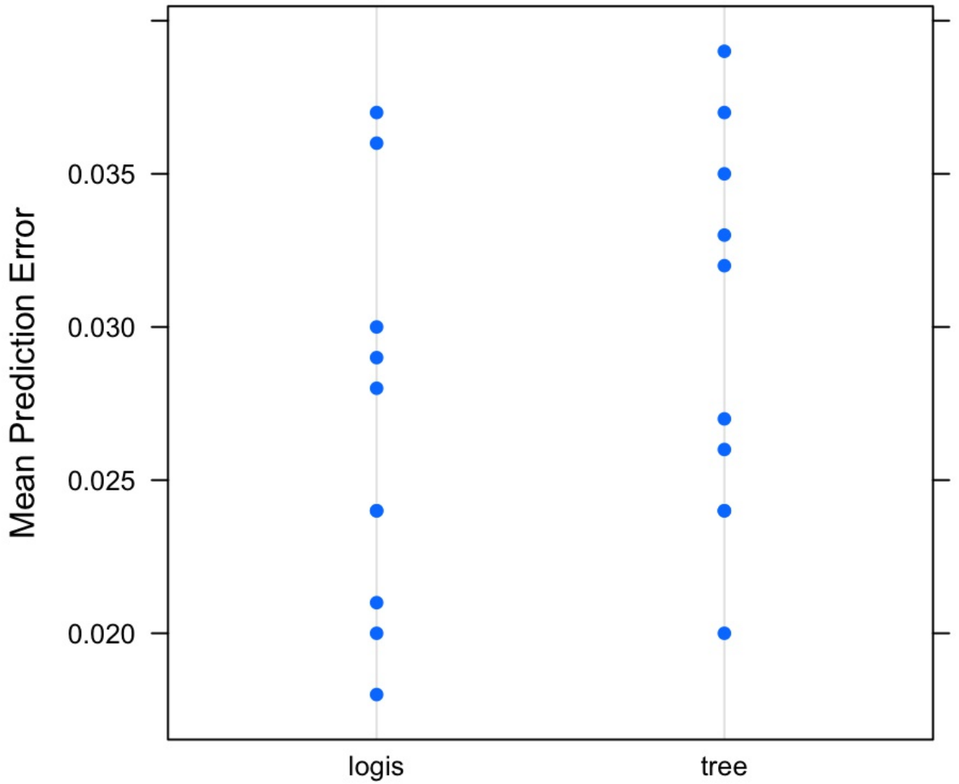
There are methods to compare AUCROC statistics from multiple classifiers. See http://ieeexplore.ieee.org/document/6851192/ for the most practical.

Comparing models using cross-validation

Suppose you want to compare two classification models (logistic regression vs. a decision tree) on the `Default` dataset. We can use Cross-Validation to determine if one model is better than the other, using a t-test for example.



Comparing models using cross-validation

Using hypothesis testing:

term	estimate	std.error	statistic	p.value
(Intercept)	0.0267	0.0020306	13.148828	0.0000000
methodtree	0.0030	0.0028717	1.044677	0.3099998

In this case, we do not observe any significant difference between these two classification methods.

Summary

Model selection and assessment are critical steps of data analysis.

Resampling methods are general tools used for this purpose.

k-fold cross-validation can be used to provide larger training sets to algorithms while stabilizing empirical estimates of expected prediction error