Cross validation

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Study design

http://www2.research.att.com/~volinsky/papers/ASAStatComp.pdf
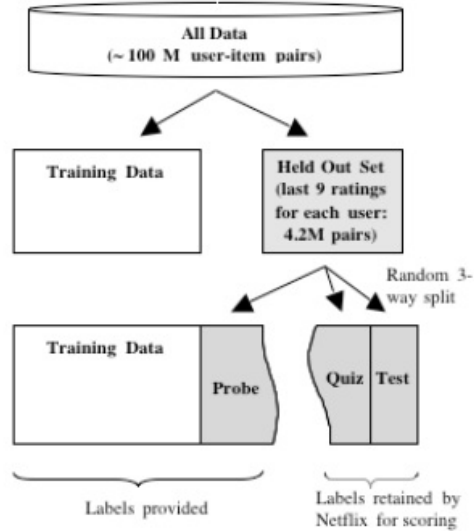
Key idea

1. Accuracy on the training set (resubstitution accuracy) is optimistic

2. A better estimate comes from an independent set (test set accuracy)

3. But we can't use the test set when building the model or it becomes part of the training set

4. So we estimate the test set accuracy with the training set.
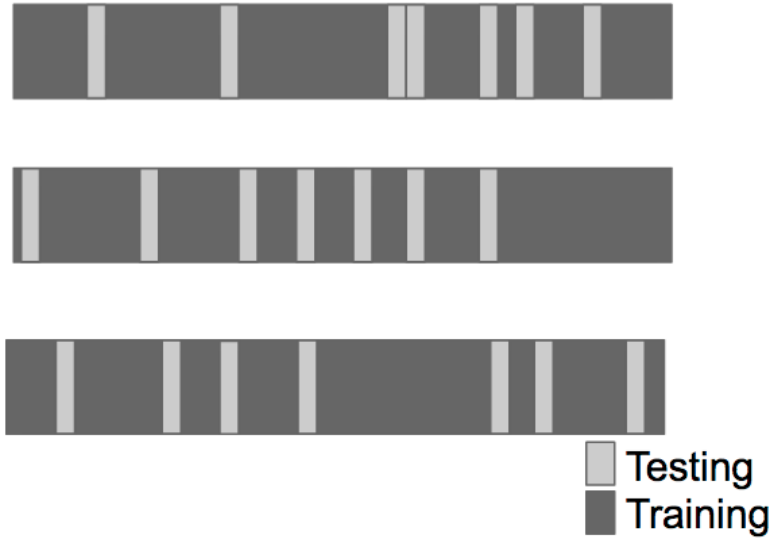
Cross-validation

Approach:

1. Use the training set

2. Split it into training/test sets

3. Build a model on the training set

4. Evaluate on the test set

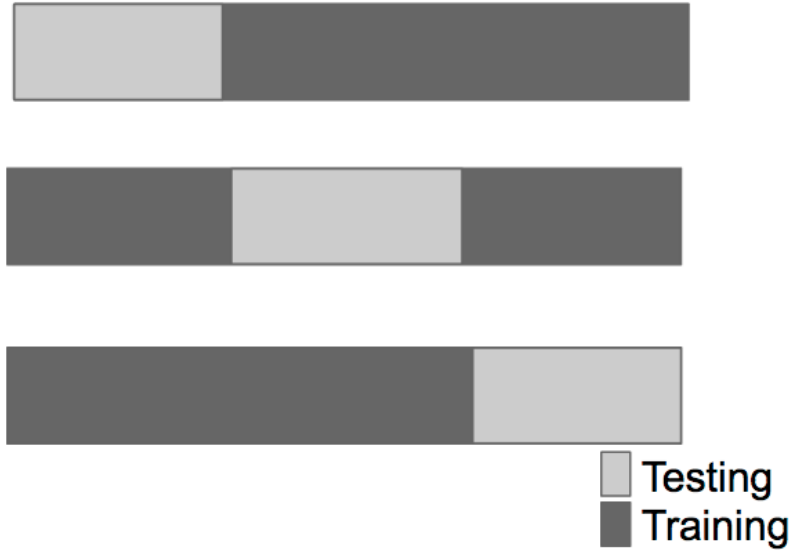5. Repeat and average the estimated errors

Used for:

1. Picking variables to include in a model

2. Picking the type of prediction function to use

3. Picking the parameters in the prediction function
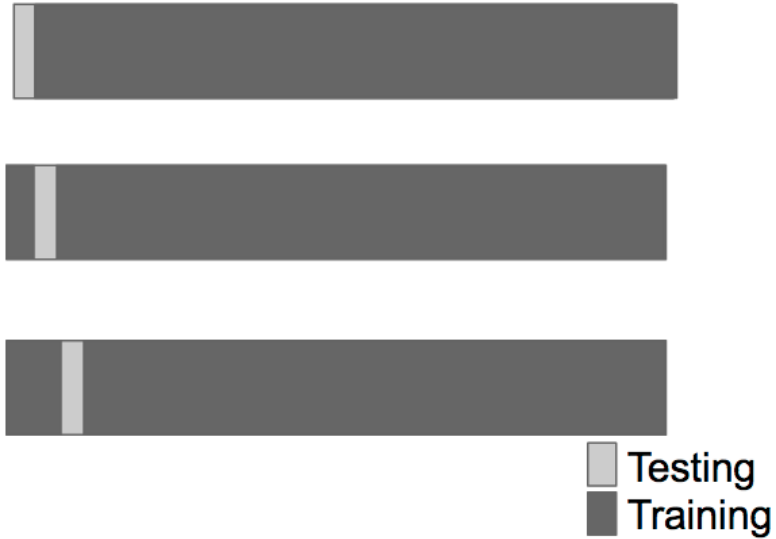
4. Comparing different predictors

Random subsampling

Testing
Training

K-fold

Testing
Training

Leave one out

Testing
Training

Considerations

- For time series data data must be used in "chunks"

- For k-fold cross validation

  - Larger k = less bias, more variance

  - Smaller k = more bias, less variance

- Random sampling must be done *without replacement*

- Random sampling with replacement is the *bootstrap*

  - Underestimates of the error

  - Can be corrected, but it is complicated (0.632 Bootstrap)

- If you cross-validate to pick predictors estimate you must estimate errors on independent data.