

Predictive Accuracy Evaluation

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Predictive Accuracy Evaluation

The main methods of predictive accuracy evaluations are:

- Resubstitution ($N ; N$);
- Holdout ($2N/3 ; N/3$)
- k -fold cross-validation ($N - N/k ; N/k$)
- Leave-one-out ($N - 1 ; 1$)

where N is the number of instances in the dataset

Predictive Accuracy Evaluation

$N = 100$

Resubstitution (100 ; 100);

Holdout (70 ; 30)

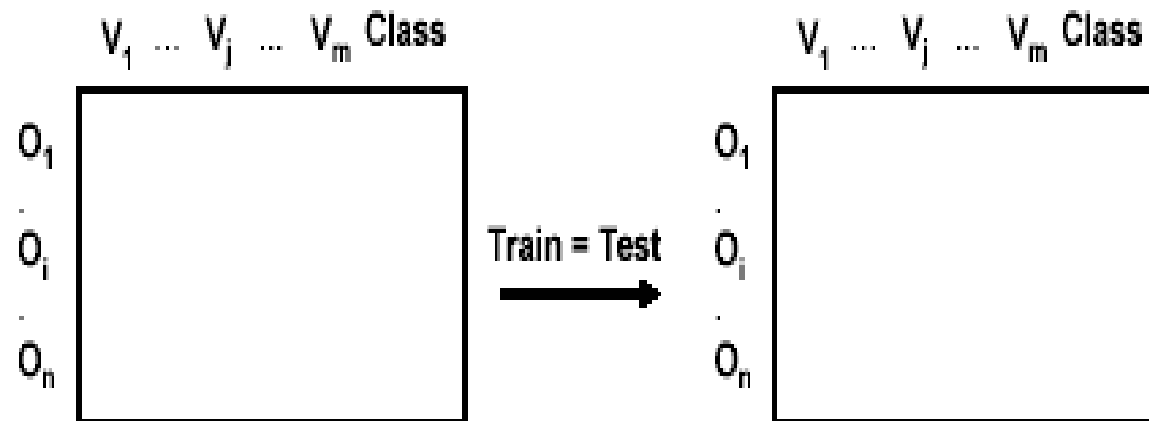
k-fold cross-validation (90 ; 10);

Leave-one-out (99 ; 1);

where N is the number of instances in the dataset

Resubstitution (N ; N)

Testing the classification model by using the given data set
(already used for „training“)



Resubstitution Error Rate

- Error rate is obtained from **training data**
- NOT always 0% error rate, but usually (and hopefully) very low!
- Resubstitution error rate indicates only how good (bad) are our results (rules, patterns, NN) on the TRAINING data; expresses some knowledge about the algorithm used

Holdout ($2N/3$; $N/3$)

- The holdout method reserves a certain amount for testing and uses the remainder for training – so they are **disjoint**!
- Usually, one third for testing, and the rest for training
- Train-and-test; repeat

Holdout ($2N/3$; $N/3$)

- **Generally**, the larger is the training the better is the classifier
- The larger the test data the more accurate the error estimate
- **Holdout procedure**: a method of splitting original data into training and test set
- **Dilemma**: ideally both training and test set should be large!
What to do if the amount of data is limited?
- How to split?

k-fold cross-validation ($N - N/k$; N/k)

- cross-validation is used to prevent the **overlap!**
- **cross-validation** avoids overlapping test sets:
 - **first step:** split data into k subsets of equal size
 - **second step:** use each subset in turn for testing, the remainder for training
 - The error estimates are averaged to yield an **overall error estimate**

Cross-validation

- Standard cross-validation: 10-fold cross-validation
- Why 10?

Extensive experiments have shown that this is the best choice to get an accurate estimate. There is also some theoretical evidence for this. *So interesting!*

Improve cross-validation

- Even better: *repeated cross-validation*

Example:

10-fold cross-validation is repeated 10 times
and results are averaged (reduce the variance)

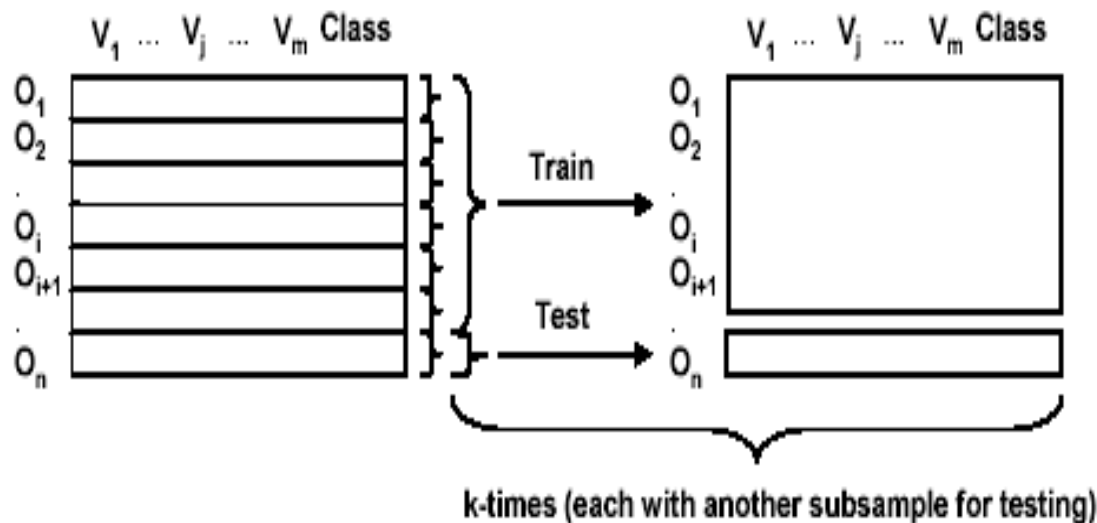
A particular form of cross-validation

- k-fold cross-validation: $(N - N/k ; N/k)$
- If $k = N$, what happens?
- We get:
- $(N - 1; 1)$
- **It is called “leave –one –out”**

Leave-one-out (N-1 ; 1)

Cross-Validation (for moderated sample sizes) → Sampling without replacement

- Dividing the given data set into **m subsamples of equal size**
 - Each subsample is tested by using a model generated from the remaining $(m-1)$ subsamples
- **Leave-One-Out**: $m = \text{Number of objects}$



Leave-one-out (N-1 ; 1)

- Make best use of the data
- Involves no random subsampling
- Stratification is not possible
- Very computationally expensive