

Testing classifier accuracy (cse352)

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Lecture Notes on Learning

Overview

- Introduction
- Basic Concept on Training and Testing
- Resubstitution (N ; N)
- Holdout ($2N/3$; $N/3$)
- x -fold cross-validation ($N-N/x$; N/x)
- Leave-one-out ($N-1$; 1)

Introduction

Predictive Accuracy Evaluation

The main methods of predictive accuracy evaluations are:

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

where N is the number of records (instances) in the dataset

Training and Testing

- REMEMBER: we must know the classification (class attribute values) of all instances (records) used in the test procedure.
- **Basic Concepts**
 - **Success:** instance (record) class is predicted correctly
 - **Error:** instance class is predicted incorrectly
 - **Error rate:** a percentage of errors made over the whole set of instances (records) used for testing
 - **Predictive Accuracy:** a percentage of well classified data in the testing data set.

Training and Testing

- **Example:**

Testing Rules (testing record #1) = record #1.class - Succ

Testing Rules (testing record #2) not= record #2.class - Error

Testing Rules (testing record #3) = record #3.class - Succ

Testing Rules (testing record #4) = instance #4.class - Succ

Testing Rules (testing record #5) not= record #5.class - Error

Error rate:

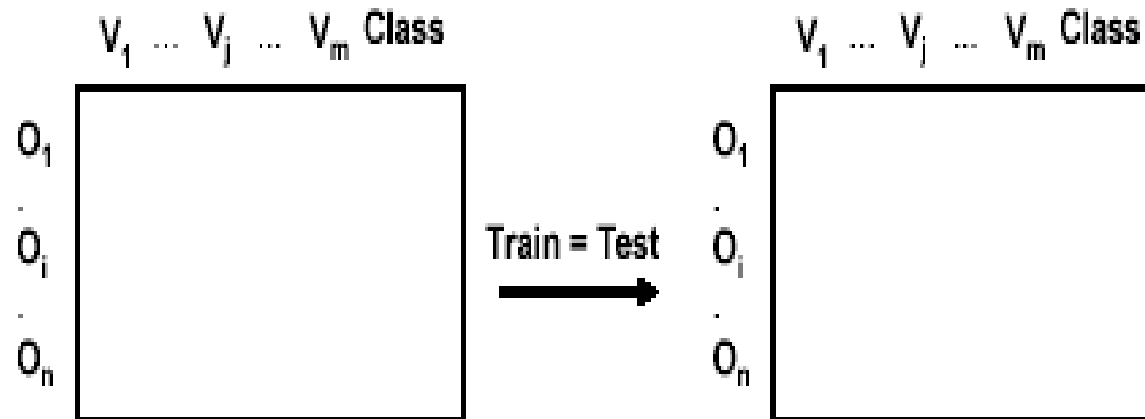
2 errors: #2 and #5

Error rate = $2/5=40\%$

Predictive Accuracy: $3/5 = 60\%$

Resubstitution (N ; N)

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



Re-substitution Error Rate

- Re-substitution error rate is obtained from training data
- **Training Data Error: uncertainty of the rules**
- The error rate is not always 0%, 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.

Re-substitution Error Rate

- Re-substitution Error Rate is usually used as the performance measure:

The training error rate reflects imprecision of the training results: **the lower, the better**

Predictive accuracy reflects how good are the training results with respect to the test data: **the higher, the better**

(N:N) re-substitution does not compute predictive accuracy

- Re-substitution error rate = training data error rate

Why not always 0%?

- The error/error rate on the training data is not always 0% because algorithms involve different (often statistical) parameters and measures that lead to uncertainties
- It is used for “**parameters tuning**”
- The error on the training data is NOT a good indicator of performance on future data since it does not measure any not yet seen data.
- Solution:
 - Split data into **training** and **test** set

Training and test set

- Training and Test data may differ in nature, but must have the same format.

Example:

Given customer data from two different towns A and B.

We train the classifier with the data from town A and we test it on data from town B, and vice-versa

Training and test set

- It is important that the test data is not used in any way to create the training rules
- In fact, learning schemes operate in three stages:
 - **Stage 1:** build the basic structure (training)
 - **Stage 2:** optimize parameter settings; can use (N:N) re-substitution (parameter tuning)
 - **Stage 3:** use test data to compute predictive accuracy/error rate

Proper procedure uses three sets: *training data, validation data and test data*

- validation data is used for parameter tuning, not test data; validation data can be the training data, or a subset of training data.

The test data cannot be used for parameter tuning!

Training and testing

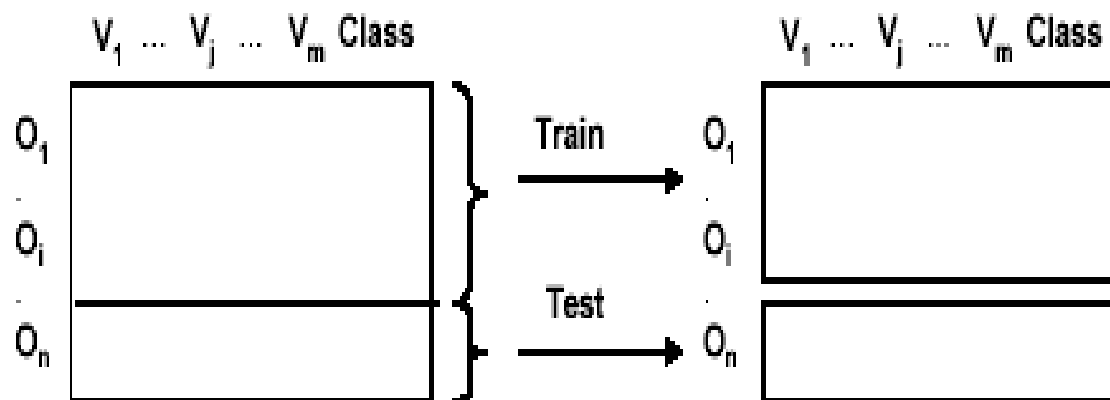
- **Generally**, the larger is the training set, the better is the classifier
- The larger the test data the more accurate the predictive accuracy, or error estimation
- Remember: the error rate of Re-substitution(N;N) can tell us ONLY whether the algorithm used in the training is good or not, or how good it is.
- **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 the data into training and test subsets (disjoint)?

Holdout

Train-and-Test (for large sample sizes) (> 1000)

dividing the given data set in

- a **training sample** for generating the classification model
- a **test sample** to test the model on independent objects with given classifications (randomly selected, 20-30% of the complete data set)



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

- The holdout method reserves a certain amount of data for testing and uses the remainder for training – so they are **disjoint!**
- Usually, one third ($N/3$) of data is used for testing, and the rest ($2N/3$) for training
- The choice of records for the train and test data is essential, so we usually perform a cycle: Train-and-test; repeat

Repeated Holdout

- Holdout can be made more reliable by repeating the process with different subsamples (subsets of data):
 1. In each iteration, a certain proportion is **randomly selected for training**, the rest of data is used for testing
 2. The error rates or predictive accuracy on the different iterations are averaged to yield an overall error rate, or predictive accuracy
- Repeated holdout still not optimum: the different test sets **overlap**

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

- The cross-validation is used to prevent the **overlap of the test sets**
- **first step:** split data into x disjoint subsets of equal size

second step: use each subset in turn for testing, the remainder for training

The error (predictive accuracy) estimates are averaged to yield an **overall error (predictive accuracy) 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; and we adopt the union of rules as the new set of rules.

A particular form of cross-validation

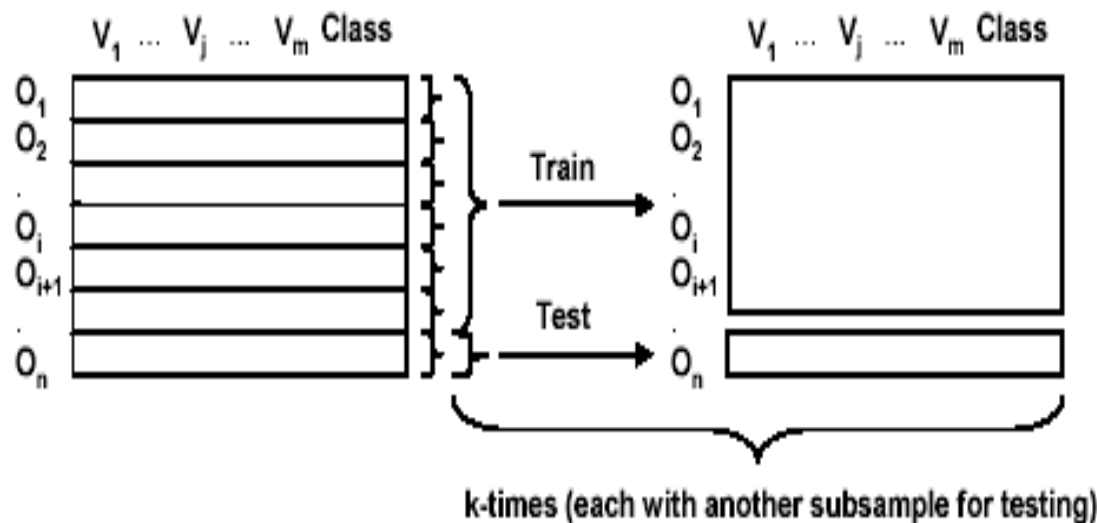
- x -fold cross-validation: $(N - N/x ; N/x)$
- If $x = N$, what happens?
- We get:
 $(N - 1 ; 1)$

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)

- Leave-one-out is a particular form of cross-validation:
 - we set number of folds to number of training instances, i.e. $x = N$.

For n instances we build classifier
(repeat the training - testing) n times

Leave-one-out Procedure

- Let $C(i)$ be the classifier (rules, patterns) built on all data except record x_i
- Evaluate $C(i)$ on x_i , and determine if it is correct or in error
- Repeat for all $i=1,2,\dots,n$.
- The total error is the proportion of all the incorrectly classified x_i
- The final set of rules (patters) is a union of all rules obtained in the process.

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

- Make best use of the data
- Involves no random sub-sampling
- Stratification is not possible
- Very computationally expensive
- MOST commonly used