Machine Learning and Data Mining
(IT4242E)

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The course's content:

- Introduction
- **Performance evaluation of the ML/DM system**
- Regression problem
- Classification problem
- Clustering problem
- Association rule mining problem

Performance evaluation (1)

- The evaluation of the performance of a ML or DM system is usually done **experimentally** rather than analytically
  - An analytical evaluation aims at proving a system is correct and complete (e.g., theorem provers in Logics)
  - *But, it is impossible to build a formal definition of a problem to be solved by a ML or DM system* (For a ML or DM problem, what are correctness and completeness?)

Performance evaluation (2)

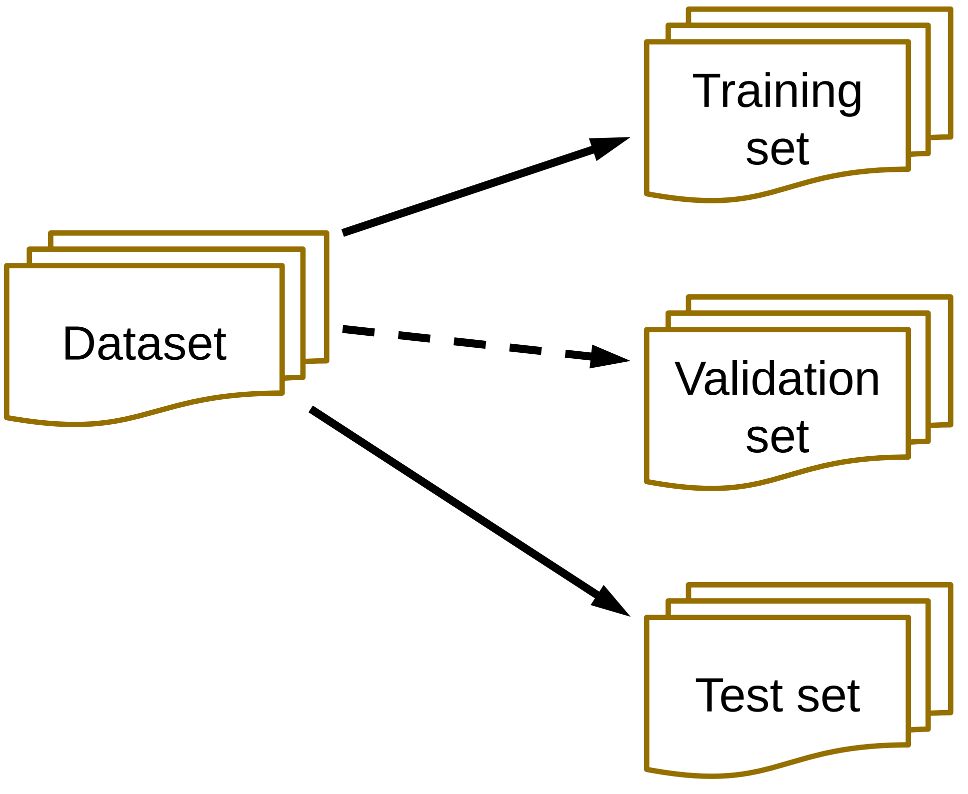
- The evaluation of the system performance should:
  - *Be done automatically by the system*, by using a set of test examples (i.e., a test set)
  - Not involve any test users
- Evaluation **methods**

  → How to have a convincing/confident evaluation of the system performance?
- Evaluation **metrics**

  → How to measure (i.e., to compute) the performance of the system?

  → Different metrics for different types of problems (e.g., classification, regression, clustering)

Evaluation methods (1)



Used to train the system

Optional, and used to optimize the values of the system's parameters

Used to evaluate the *trained* system

Evaluation methods (2)

- How to get a confident/convincing evaluation of the system performance?
  - The larger the training set is, the higher the performance of the trained system is
  - The larger the test set is, the more confident/convincing the evaluation is
  - Problem: Very difficult (i.e., rarely) to have (very) large dataset(s)
- *The system performance depends on not only ML/DM algorithms used*, but also:
  - Class distribution
  - Cost of misclassification
  - Size of the training set
  - Size of the test set

Evaluation methods (3)

- Hold-out (Splitting)
- Stratified sampling
- Repeated hold-out
- Cross-validation
  - *k*-fold
  - Leave-one-out
- Bootstrap sampling

Hold-out (Splitting)

- The whole dataset D is divided into 2 **disjoint subsets**
  - Training set D_train – To train the system
  - Test set D_test – To evaluate the performance of the trained sys.

  → $D = D\_train \cup D\_test$, and usually $|D\_train| >> |D\_test|$
- Requirements:
  - Any examples in the test set D_test must not be used in the training of the system
  - Any examples used in the training of the system (i.e., those in D_train) must not be used in the evaluation of the trained system
  - The test examples in D_test should allow an unbiased evaluation of the system performance
- Usual splitting: $|D\_train|=(2/3).|D|$, $|D\_test|=(1/3).|D|$
- **Suitable if we have a large dataset *D***

Stratified sampling

- For such datasets that is small (in size) or unbalanced, the examples in the training and test sets may not be representative
- For example: There are (very) few examples for a specific class label
- Goal: The class distribution in the training and test sets should be approximately equal to that in the original dataset (D)
- Stratified sampling
  - An approach to have a balanced (in class distribution) dataset
  - Guarantee the class distributions (i.e., the percentages of examples for class labels) in the training and tests set are approximately equal
- The stratified sampling method can not be applied to a regression problem (because for that problem the system's output is a real value, not a discrete value / class label)

Repeated hold-out

- To apply the Hold-out evaluation method for multi times (i.e., multi runs), each one uses a different training and test sets
  - For each run, a certain percentage of the dataset D ***is randomly selected*** to create the training set (possibly together with the stratified sampling method)
  - The error values (or the values of other measure metrics) *are averaged* amongst the runs to get the final (average) error value
- This evaluation method is still not perfect
  - In each run, a different test set is used
  - There are still some overlapping (i.e., repeatedly) used examples among those test sets

Cross-validation

- To avoid any overlapping amongst the used test sets (i.e., the same examples are contained in some different test sets)
- k-fold cross-validation
  - The whole dataset D is divided into k **disjoint subsets** (called "*fold*") that have approximately equal sizes
  - For each run (i.e., of the total *k* runs), a subset is circulated to use for the test set, and the remaining (k-1) subsets are used for the training set
  - The k error values (i.e., each one for each *fold*) are averaged to get the overall error value
- Usual choices of k: 10, or 5
- Often, each subset (i.e., fold) is stratified sampling (i.e., to approximate the class distribution) prior to apply the Cross-validation evaluation method
- Suitable if we have a small to medium dataset D

Leave-one-out cross-validation

- A type of the Cross-validation method
  - The number of folds is exactly the size of the original dataset (k=|D|)
  - Each fold contains just one example
- To maximally exploit the original dataset
- No random sub-sampling
- Not possible to apply the stratified sampling method

  → Because in each run (loop), the test set contains just one example
- (Very) high computational cost
- Suitable if we have a (very) small dataset D

Bootstrap sampling (1)

- The Cross-validation method applies sampling without replacement
  $\rightarrow$ For each example, *once selected (used) for the training set, then it cannot be selected (used) again (one more time)* for the training set
- The Bootstrap sampling method applies ***sampling with replacement*** to create the training set
  - Assume that the whole dataset D contains n examples
  - To sample with replacement (i.e., repeating) for n times for the dataset D to create the training set D_train that contains n examples
    - From the dataset D, randomly select an example x (but **not remove** x from the dataset D)
    - Put the example x into the training set: $D\_train = D\_train \cup x$
    - Repeat the above 2 steps for n times
  - To use the set D_train for training the system
  - To use those examples in D **but not in** D_train to create the test set: $D\_test = \{z \in D;\ z \notin D\_train\}$

Bootstrap sampling (2)

- Important notes:
  - The training set has size of n, and an example in D may **appear multi times** in `D_train`
  - The test set has size <n, and an example in D can **appear maximum to 1 time** in `D_test`
- Suitable if we have a (very) small dataset *D*

Validation set

- The examples in the test set must not be used (in any way!) in the training of the system
- In some ML/DM problems, the system's training process includes 2 tasks:
  - Task 1: To train the system (= To learn approximately the target function)
  - Task 2: To optimize the values of the system's parameters
- The test set cannot be used for the purpose of optimization of the system's parameters
- To divide the whole dataset D into 3 disjoint subsets: *training set*, *validation set*, and *test set*
- The validation set is used to optimize the values of the system's parameters and the used ML/DM algorithm's ones

  → For a parameter, **the optimal value** is the one that results in **the best performance for the validation set**

Evaluation metrics (1)

- **Accuracy**
  - →The accuracy degree of the prediction of the trained system to the test examples
- Efficiency
  - →The costs in time and memory resources needed for the training and the test of the system
- Robustness
  - →The tolerance degree of the system to noise/error/missing-value examples

Evaluation metrics(2)

- Scalability
  - →How the system's performance (e.g., training/prediction speed) varies to the size of the dataset
- Interpretability
  - →How the system's results and operation are easy to understand for users
- Complexity
  - →The complexity of the model (i.e., the target function) learned by the system

Select a trained model

- The selection of a trained model should compromise (balance) between:
  - The complexity of the trained model
  - The prediction accuracy degree of the trained model
- *Occam's razor*. A good trained model is the one that **is simple** and **achieves high accuracy (in prediction)** for the used dataset
- For example:
  - A trained classifier *`Sys1`*: (Very) simple, and rather (to a certain degree) fit to the training set
  - A trained classifier *`Sys2`*: More complex, and perfectly fit to the training set

  → *`Sys1`* is preferred to *`Sys2`*