INTRODUCTION TO DATA ANALYTICS

Class # 22

Sensitivity Analysis

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TOPICS COVERED IN THIS PRESENTATION

- Introduction
- Estimation Strategies
- Accuracy Estimation
- Error Estimation
- Statistical Estimation
- Performance Estimation
- ROC Curve

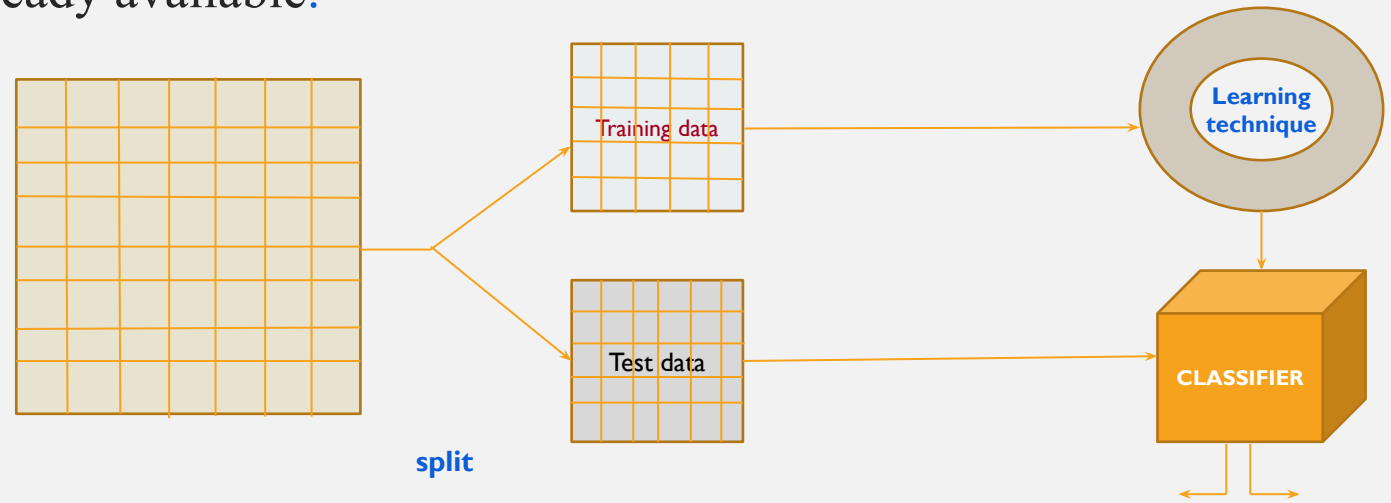
INTRODUCTION

- A classifier is used to predict an outcome of a test data
  - Such a prediction is useful in many applications
    - Business forecasting, cause-and-effect analysis, etc.
  - A number of classifiers have been evolved to support the activities.
    - Each has their own merits and demerits
- There is a need to estimate the accuracy and performance of the classifier with respect to few controlling parameters in data sensitivity
- As a task of sensitivity analysis, we have to focus on
  - Estimation strategy
  - Metrics for measuring accuracy
  - Metrics for measuring performance

Estimation Strategy

PLANNING FOR ESTIMATION

- Using some "training data", building a classifier based on certain principle is called "learning a classifier".
- After building a classifier and before using it for classification of unseen instance, we have to validate it using some "test data".
- Usually training data and test data are outsourced from a large pool of data already available.



ESTIMATION STRATEGIES

- Accuracy and performance measurement should follow a strategy. As the topic is important, many strategies have been advocated so far. Most widely used strategies are
  - Holdout method
  - Random subsampling
  - Cross-validation
  - Bootstrap approach

HOLDOUT METHOD

- This is a basic concept of estimating a prediction.
  - Given a dataset, it is partitioned into two disjoint sets called training set and testing set.
  - Classifier is learned based on the training set and get evaluated with testing set.
  - Proportion of training and testing sets is at the discretion of analyst; typically **1:1 or 2:1**, and there is a trade-off between these sizes of these two sets.
  - If the training set is too large, then model may be good enough, but estimation may be less reliable due to small testing set and vice-versa.

RANDOM SUBSAMPLING

- It is a variation of Holdout method to overcome the drawback of over-presenting a class in one set thus under-presenting it in the other set and vice-versa.
- In this method, Holdout method is repeated ***k*** times, and in each time, two **disjoint sets are chosen at random** with a predefined sizes.
- Overall estimation is taken as the average of estimations obtained from each iteration.

CROSS-VALIDATION

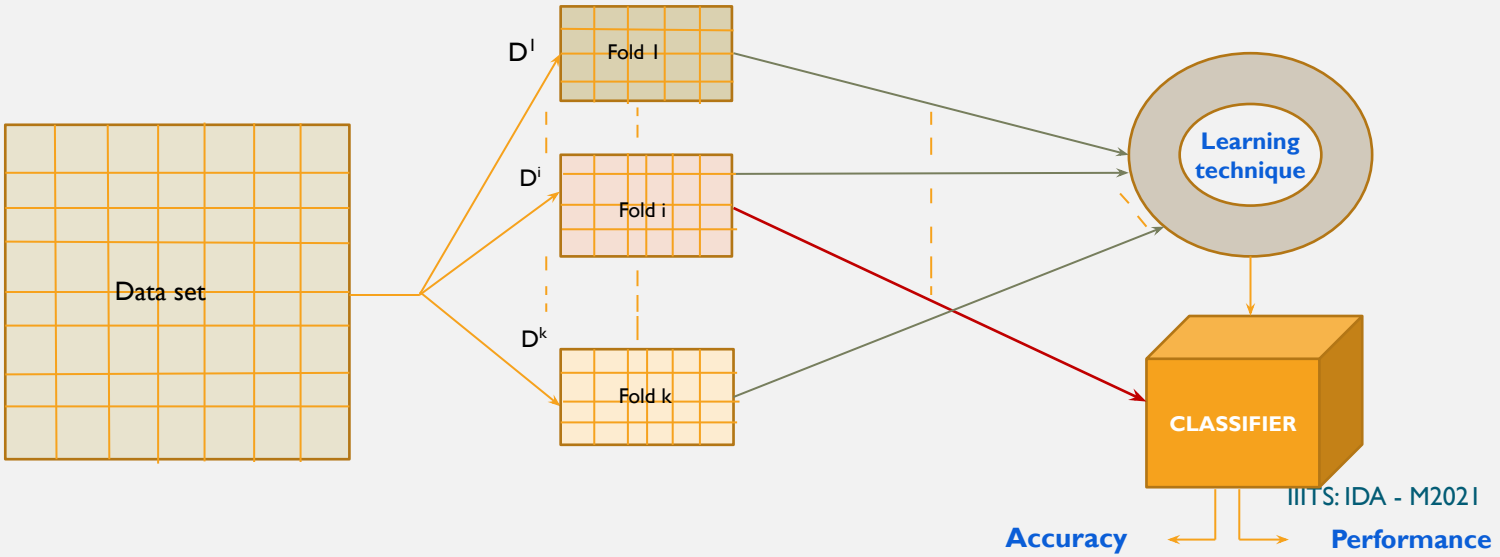
- The main drawback of Random subsampling is, it does not have control over the number of times each tuple is used for training and testing.
- Cross-validation is proposed to overcome this problem.
- There are two variations in the cross-validation method.
  - k-fold cross-validation
  - *N*-fold cross-validation

K-FOLD CROSS-VALIDATION

- Dataset consisting of N tuples is divided into k (usually, 5 or 10) equal, mutually exclusive parts or folds $(D_1, D_2, \ldots, D_k)$, and if N is not divisible by k, then the last part will have fewer tuples than other (k-1) parts.

- A series of k runs is carried out with this decomposition, and in i^{th} iteration D_i is used as test data and other folds as training data
  - Thus, each tuple is used same number of times for training and once for testing.

- Overall estimate is taken as the average of estimates obtained from each iteration.



N-FOLD CROSS-VALIDATION

- In *k*-fold cross-validation method, $\frac{k-1}{N}$ part of the given data is used in training with *k*-tests.

- *N*-fold cross-validation is an extreme case of *k*-fold cross validation, often known as "Leave-one-out" cross-validation.

- Here, dataset is divided into as many folds as there are instances; thus, all most each tuple forming a training set, building *N* classifiers.
- In this method, therefore, *N* classifiers are built from *N-1* instances, and each tuple is used to classify a single test instances.
- Test sets are mutually exclusive and effectively cover the entire set (in sequence). This is as if trained by entire data as well as tested by entire data set.
- Overall estimation is then averaged out of the results of *N* classifiers.

N-FOLD CROSS-VALIDATION : ISSUE

- So far the estimation of accuracy and performance of a classifier model is concerned, the *N*-fold cross-validation is comparable to the others we have just discussed.

- The drawback of *N*-fold cross validation strategy is that it is computationally expensive, as here we have to repeat the run *N* times; this is particularly true when data set is large.

- In practice, the method is extremely beneficial with very small data set only, where as much data as possible to need to be used to train a classifier.

BOOTSTRAP METHOD

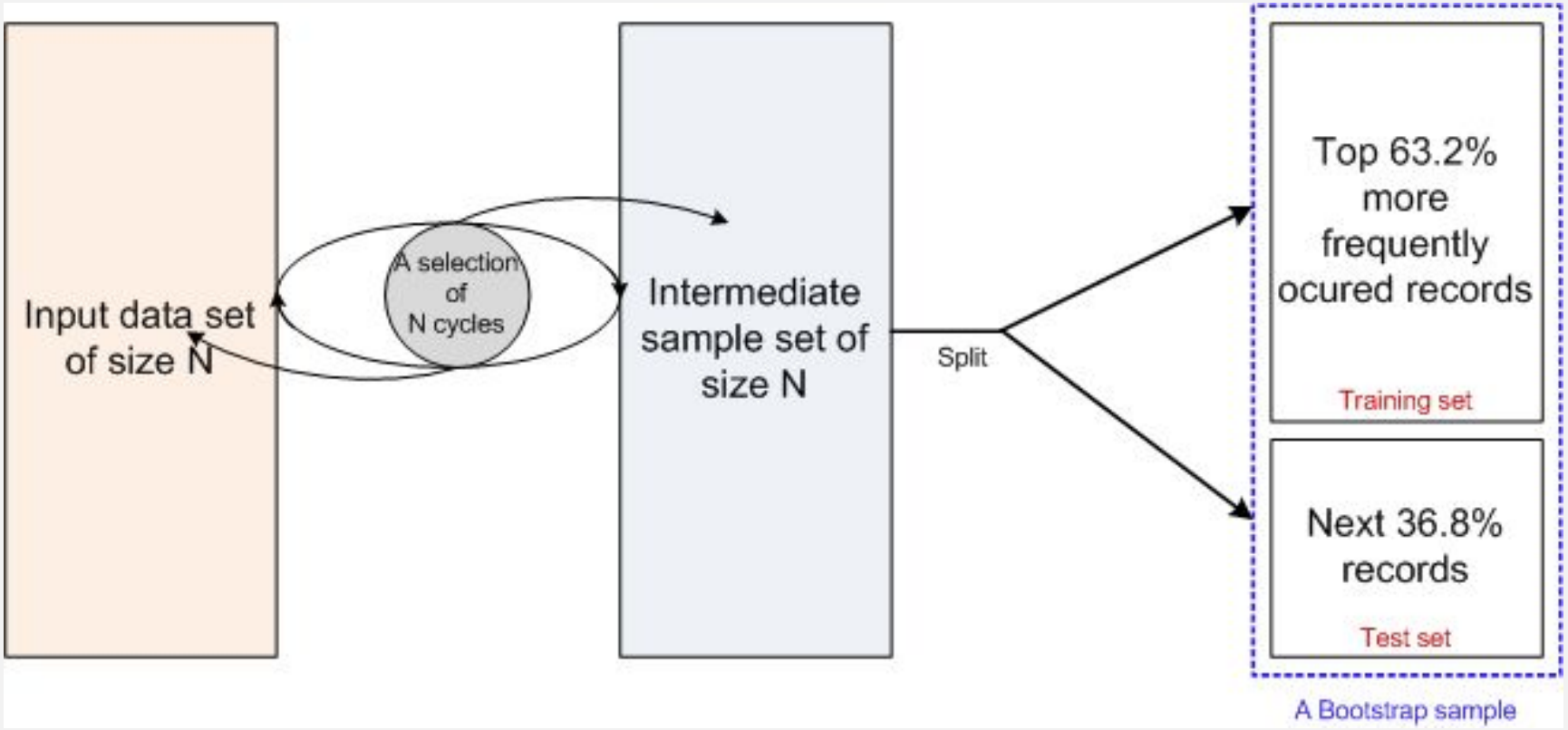
- The Bootstrap method is a variation of repeated version of Random sampling method.
- The method suggests the sampling of training records with replacement.
  - Each time a record is selected for training set, is put back into the original pool of records, so that it is equally likely to be redrawn in the next run.
  - In other words, the Bootstrap method samples the given data set uniformly with replacement.
- The rational of having this strategy is that let some records be occur more than once in the samples of both training as well as testing.
  - What is the probability that a record will be selected more than once?

BOOTSTRAP METHOD

- Suppose, we have given a data set of *N* records. The data set is sampled *N* times with replacement, resulting in a bootstrap sample (i.e., training set) of I samples.
  - Note that the entire runs are called a bootstrap sample in this method.

- There are certain chance (i.e., probability) that a particular tuple occurs one or more times in the training set
  - If they do not appear in the training set, then they will end up in the test set.
  - Each tuple has a probability of being selected $\frac{1}{N}$ (and the probability of not being selected is $\left(1-\frac{1}{N}\right)$.
  - We have to select N times, so the probability that a record will not be chosen during the whole run is $\left(1-\frac{1}{N}\right)^N$
  - Thus, the probability that a record is chosen by a bootstrap sample is $1-\left(1-\frac{1}{N}\right)^N$
  - For a large value of *N*, it can be proved that $\left(1-\frac{1}{N}\right)^N \approx e^{-1}$
  - Thus, the probability that a record chosen in a bootstrap sample is $1-e^{-1}=0.632$

BOOTSTRAP METHOD : IMPLICATION



- This is why, the Bootstrap method is also known as 0.632 bootstrap method

Accuracy Estimation

ACCURACY ESTIMATION

- We have learned how a classifier system can be tested. Next, we are to learn the metrics with which a classifier should be estimated.

- There are mainly two things to be measured for a given classifier
  - Accuracy
  - Performance

- **Accuracy estimation**
  - If N is the number of instances with which a classifier is tested and p is the number of correctly classified instances, the accuracy can be denoted as

$$\epsilon = \frac{p}{N}$$

  - Also, we can say the error rate (i.e., is misclassification rate) denoted by $\bar{\epsilon}$ is denoted by

$$\bar{\epsilon} = 1 - \epsilon$$

ACCURACY : TRUE AND PREDICTIVE

- Now, this accuracy may be true (or absolute) accuracy or predicted (or optimistic) accuracy.
- True accuracy of a classifier is the accuracy when the classifier is tested with all possible unseen instances in the given classification space.
  - However, the number of possible unseen instances is potentially very large (if it is not infinite)
  - For example, classifying a hand-written character
  - Hence, measuring the true accuracy beyond the dispute is impractical.
- Predictive accuracy of a classifier is an accuracy estimation for a given test data (which are mutually exclusive with training data).
  - If the predictive accuracy for test set is $\in$ and if we test the classifier with a different test set it is very likely that a different accuracy would be obtained.
  - The predictive accuracy when estimated with a given test set it should be acceptable without any objection

PREDICTIVE ACCURACY

Example 21.1 : Universality of predictive accuracy

- Consider a classifier model M^D developed with a training set D using an algorithm M.
- Two predictive accuracies when M^D is estimated with two different training sets T_1 and T_2 are

  $(M^D)_{T1} = 95\%$

  $(M^D)_{T2} = 70\%$

- Further, assume the size of T_1 and T_2 are

  $|T_1| = 100$ records

  $|T_2| = 5000$ records.

- Based on the above mentioned estimations, neither estimation is acceptable beyond doubt.

PREDICTIVE ACCURACY

- With the above-mentioned issue in mind, researchers have proposed two heuristic measures
  - Error estimation using **Loss Functions**
  - Statistical Estimation using **Confidence Level**
- In the next few slides, we will discus about the two estimations

Error Estimation using Loss Functions

- Let T be a matrix comprising with N test tuples

$$\begin{bmatrix} X_1 & y_1 \\ X_2 & y_2 \\ & \\ X_N & y_N \end{bmatrix}_{N\times(n+1)}$$

where X_i ($i = 1, 2, \ldots, N$) is the n-dimensional test tuples with associated outcome y_i.

- Suppose, corresponding to (X_i, y_i), classifier produces the result (X_i, y_i')
- Also, assume that $(y_i - y_i')$ denotes a difference between y_i and y_i' (following certain difference (or similarity), (e.g., $(y_i - y_i') = 0$, if there is a match else 1)

- The two loss functions measure the error between y_i (the actual value) and y_i' (the predicted value) are

Absolute error: $|y_i - y_i'|$

Squared error: $|y_i - y_i'|^2$

Error Estimation using Loss Functions

- Based on the two loss functions, the test error (rate) also called generalization error, is defined as the average loss over the test set T. The following two measures for test errors are

Mean Absolute Error (MAE): $\frac{\sum_{i=1}^{N} |y_i - y_i'|}{N}$

Mean Squared Error(MSE): $\frac{\sum_{i=1}^{N} (y_i - y_i')^2}{N}$

- Note that, MSE aggregates the presence of outlier.
- In addition to the above, a relative error measurement is also known. In this measure, the error is measured relative to the mean value $\tilde{y}$ calculated as the mean of y_i ($i = 1, 2, \ldots, N$) of the training data say D. Two measures are

Relative Absolute Error (RAE: $\frac{\sum_{i=1}^{N} |y_i - y_i'|}{\sum_{i=1}^{N} |y_i - \tilde{y}|}$

Relative Squared Error (RSE): $\frac{\sum_{i=1}^{N} (y_i - y_i')^2}{\sum_{i=1}^{N} (y_i - \tilde{y})^2}$

Statistical Estimation using Confidence Level

- In fact, if we know the value of predictive accuracy, say $\in$, then we can guess the true accuracy within a certain range given a confidence level.
- Confidence level: The concept of "confidence level " can be better understood with the following two experiments, related to tossing a coin.

- **Experiment 1:** When a coin is tossed, there is a probability that the head will occur. We have to experiment the value for this probability value. A simple experiment is that the coin is tossed many times and both numbers of heads and tails are recorded.

N=10		N=50		N=100		N=250		N=500		N=1000	
H	T	H	T	H	T	H	T	H	T	H	T
3	7	29	21	54	46	135	115	241	259	490	510
0.30	0.70	0.58	0.42	0.54	0.46	0.54	0.46	0.48	0.42	0.49	0.51

- Thus, we can say that $p \rightarrow 0.5$ after a large number of trials in each experiment.

Statistical Estimation using Confidence Level

- **Experiment 2:** A similar experiment but with different counting is conducted to learn the probability that a coin is flipped its head 20 times out of 50 trials. This experiment is popularly known as Bernoulli's trials. It can be stated as follows.

$$\mathrm{P}(X = v) = \binom{N}{v} p^v (1-p)^{N-v}$$

  - where N = Number of trials
  - v = Number of outcomes that an event occurs.
  - p = Probability that the event occur

- Thus, if $p = 0.5$, then $P(X = 20) = \binom{50}{20} 0.5^{20} \times 0.5^{30} = 0.0419$

- **Note:**
  - Also, we may note the following
    - Mean = $N \times p = 50 \times 0.5 = 25$ and Variance = $p \times (1\text{-}p) \times N = 50 \times 0.5 \times 0.5 = 12.5$

Statistical Estimation using Confidence Level

- The task of predicting the class labels of test records can also be considered as a binomial experiment, which can be understood as follows. Let us consider the following.
  - N = Number of records in the test set.
  - n = Number of records predicted correctly by the classifier.
  - $\epsilon = n/N$, the observed accuracy (it is also called the empirical accuracy).
  - $\tilde{\epsilon}$ = the true accuracy.

- Let ${\tau^L}_\alpha$ and ${\tau^U}_\alpha$ denotes the lower and upper bound of a confidence level α. Then the confidence interval for α is given by

$$P\left(\tau_\alpha^L \leq \frac{\epsilon - \tilde{\epsilon}}{\sqrt{\epsilon\,(1-\epsilon)/N}} \leq \tau_\alpha^U\right) = \alpha$$

- If τ_α is the mean of ${\tau^L}_\alpha$ and ${\tau^U}_\alpha$, then we can write

$$\tilde{\epsilon} = \epsilon \pm \tau_\alpha \times \sqrt{\epsilon\,(1-\epsilon)/N}$$

Statistical Estimation using Confidence Level

$$\tilde{\epsilon} = \epsilon \pm \tau_{\alpha} \times \sqrt{\epsilon\,(1-\epsilon)/N}$$

- A table of τ_{α} with different values of α can be obtained from any book on statistics. A small part of the same is given below.

	0.5	0.7	0.8	0.9	0.95	0.98	0.99
	0.67	1.04	1.28	1.65	1.96	2.33	2.58

- Thus, given a confidence level α, we shall be able to know the value of τ_{α} and hence the true accuracy ($\tilde{\epsilon}$), if we have the value of the observed accuracy (ϵ).

- Thus, knowing a test data set of size *N*, it is possible to estimate the true accuracy!

Statistical Estimation using Confidence Level

Example 21.2: True accuracy from observed accuracy

A classifier is tested with a test set of size 100. Classifier predicts 80 test tuples correctly. We are to calculate the following.

a) Observed accuracy

b) Mean error rate

c) Standard error

d) True accuracy with confidence level 0.95.

Solution:

a) The observed accuracy(ϵ) = 80/100 = 0.80 So error (p) = 0.2

b) Mean error rate = $p \times N = 0.2 \times N = 20$

c) Standard error rate (σ) = $\sqrt{\epsilon\,(1-\epsilon)/N} = \sqrt{\frac{0.8\times0.2}{100}} = 0.04$

d) $\tilde{\epsilon} = \epsilon \pm \tau_\alpha \times \sqrt{\epsilon\,(1-\epsilon)/N}$ = 0.8±0.04×1.96 = 0.7216 with τ_α=1.96 and α = 0.95.

Statistical Estimation using Confidence Level

Note:

- Suppose, a classifier is tested k times with k different test sets. If ϵ_i denotes the predicted accuracy when tested with test set N_i in the i-th run ($1 \leq i \leq k$), then the overall predicted accuracy is

$$\epsilon = \sum_{i=1}^{k} \frac{\epsilon_i \times N_i}{\sum N_i}$$

Thus, ϵ is the weighted average of ϵ_i values. The standard error and true accuracy at a confidence α are

$$\text{Standard error} = \sqrt{\epsilon\,(1-\epsilon)/\sum_{i=1}^{k} N_i}$$

$$\text{True accuracy} = \epsilon \pm \sqrt{\frac{\epsilon(1-\epsilon)}{\sum_{i=1}^{k} N_i}} \times \tau_\alpha$$

REFERENCE

- The detail material related to this lecture can be found in

Data Mining: Concepts and Techniques, (3rd Edn.), Jiawei Han, Micheline Kamber, Morgan Kaufmann, 2015.

Introduction to Data Mining, Pang-Ning Tan, Michael Steinbach, and Vipin Kumar, Addison-Wesley, 2014

Any question?