Classification

3.1 Introduction

Classification is the process where a model or classifier is constructed to predict *categorical labels* of unknown data. Classification problems aim to identify the characteristics that indicate the group to which each case belongs. This pattern can be used both to understand the existing data and to predict how new instances will behave.

Definition: Classification is the task of learning a target function *f* that maps each attribute set *X* to one of the predefined class label *Y*.

For example, classification of loan applicants as "safe" or "risky" for the bank, whether a customer with a given profile will buy a new computer or not, whether a patient is a good candidate for a surgical procedure or not etc.

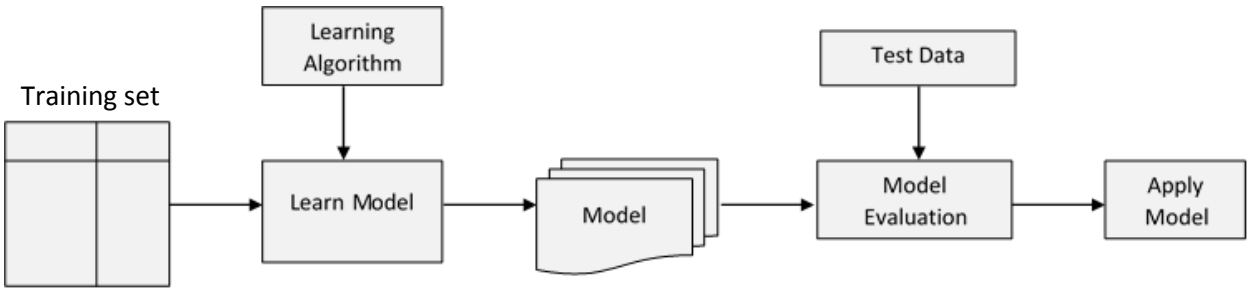
Data classification is a two-step process:

I. Model construction

In the first step, a classifier is built describing a predetermined set of data classes or concepts. This is the learning step (or training phase), where a classification algorithm builds the classifier by analyzing or "learning from" a training set made up of database tuples and their associated class labels.

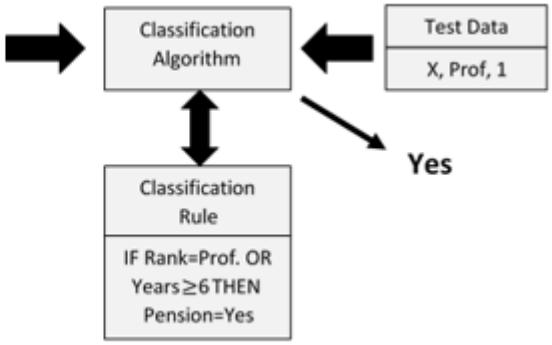
II. Model usage

In the second step, the model is used for classification. Test data are used to estimate the accuracy of the classification rules. If the accuracy is considered acceptable, the rules can be applied to the classification of new data tuples.



Example:

Name	Rank	Years	Pension
A	Prof.	2	Yes
B	Asst. Prof.	2	No
C	Asst. Prof.	6	Yes
D	Asst. Prof.	7	Yes
E	Prof.	5	Yes



Issues Regarding Classification

i. Preparing the Data for Classification

Data cleaning: This refers to the preprocessing of data in order to remove or reduce *noise* (by applying smoothing techniques, for example) and the treatment of *missing values* (e.g., by replacing a missing value with the most commonly occurring value for that attribute, or with the most probable value based on statistics).

Relevance analysis: Many of the attributes in the data may be redundant. Correlation analysis can be used to identify whether any two given attributes are statistically related. For example, a strong correlation between attributes A_1 and A_2 would suggest that one of the two could be removed from further analysis.

Data transformation and reduction: The data may be transformed by normalization, particularly when neural networks or methods involving distance measurements are used in the learning step. Normalization involves scaling all values for a given attribute so that they fall within a small specified range, such as -1.0 to 1.0, or 0.0 to 1.0. Data can also be reduced by applying methods such as binning, histogram analysis, and clustering.

ii. Evaluating Classification Methods

Classification methods can be compared and evaluated according to the following criteria:

Accuracy: The accuracy of a classifier refers to the ability of a given classifier to correctly predict the class label of new or previously unseen data (i.e., tuples without class label information).

Speed: This refers to the computational costs involved in generating and using the given classifier or predictor.

Robustness: This is the ability of the classifier or predictor to make correct predictions given noisy data or data with missing values.

Scalability: This refers to the ability to construct the classifier or predictor efficiently given large amounts of data.

Types of Classifiers:

- Decision Tree classifier
- Rule Based Classifier
- Nearest Neighbor Classifier
- Bayesian Classifier
- Artificial Neural Network (ANN) Classifier

3.2 Decision Tree Classifier

Decision tree is a collection of *decision nodes*, connected by *branches*, extending downward from the *root node* until terminating in *leaf nodes*. Beginning at the root node, which by convention is placed at the top of the decision tree diagram, attributes are tested at the decision nodes, with each possible outcome resulting in a branch. Each branch then leads either to another decision node or to a terminating leaf node.

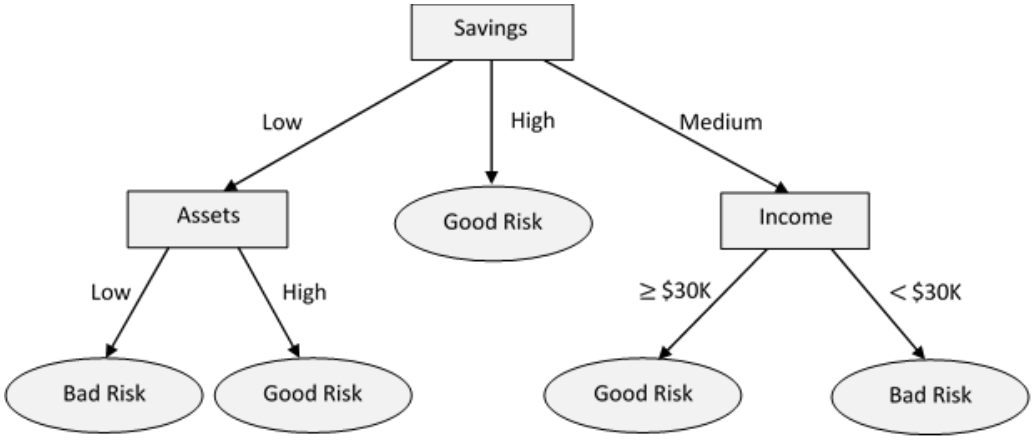


Figure 1. Decision tree for the credit risk data.

The problem of constructing a decision tree can be expressed recursively. First, select an attribute to place at the root node and make one branch for each possible value. This splits up the example set into subsets, one for every value of the attribute. Now the process can be repeated recursively for each branch, using only those instances that actually reach the branch. If at any time all instances at a node have the same classification, stop developing that part of the tree.

"How are decision trees used for classification?" Given a tuple, ***X***, for which the associated class label is unknown, the attribute values of the tuple are tested against the decision tree. A path is traced from the root to a leaf node, which holds the class prediction for that tuple (***X***). Decision trees can easily be converted to classification rules as well.

The only (and the most important) thing left to decide is how to determine which attribute to split on, given a set of examples with different classes. Consider the weather data in the *table 1*. There are four possibilities for root node (*Outlook, Temperature, Humidity* and *Wind*). Which is the best choice? The number of *yes* and *no* classes are shown at the leaves. Any leaf with only one class—*yes* or *no*—will not have to be split further, and the recursive process down that branch will terminate. Because we seek small trees, we would like this to happen as soon as possible. If we had a measure of the purity of each node, we could choose the attribute that produces the purest child nodes.

Attribute Selection Measures

An attribute selection measure is an approach for selecting the splitting criterion that "best" separates a given data partition, *D*, of class-labeled training tuples into individual classes. If we were to split *D* into smaller partitions according to the outcomes of the splitting criterion, ideally each partition would be pure (i.e. all of the tuples that fall into a given partition would belong to the same class). Conceptually, the "best" splitting criterion is the one that most closely results in such a scenario. Attribute selection measure is also known as splitting rules because they determine how the tuples at a given nodes are to be split.

There are three popular attribute selection measures—information gain, gain ratio, and gini index.

a. Information Gain

Information gain is used by ID3 algorithm. The attribute with the highest information gain is chosen as the splitting attribute for node N. This attribute minimizes the information needed to

classify the tuples in the resulting partitions and reflects the least randomness or "impurity" in these partitions.

The expected information needed to classify a tuple in *D* is given by

$$Info(D) = -\sum_{i=1}^{m} P_i \, log_2(P_i)$$

Where P_i= probability that an arbitrary tuple D belongs to class C_i

At this point, the information we have is based solely on the proportions of tuples of each class. *Info(D)* is also known as the entropy of *D*.

Now, suppose we were to partition the tuples in D on some attribute A having v distinct values, $\{a_1, a_2, \ldots, a_V\}$ as observed from the training data. Attribute A can be used to split D into v partitions or subsets, $\{D_1, D_2, \ldots, D_v\}$, where D_j contains those tuples in D that have outcome a_j of A. How much more information would we still need (after the partitioning) in order to arrive at an exact classification? This amount is measured by

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{D} \times Info(D_j)$$

$|D_j|/D$ acts as the weight of the j^{th} partition. $Info_A(D)$ is the expected information required to classify a tuple from *D* based on the partitioning by *A*.

Finally the information gain of any attribute A can be calculated as:

$$Gain(A) = Info(D) - Info_A(D)$$

In other words, *Gain(A)* tells us how much would be gained by branching on *A*. The attribute *A* with the highest information gain, (*Gain*(*A*)), is chosen as the splitting attribute at node *N*. This is equivalent to saying that we want to partition on the attribute *A* that would do the "best classification," so that the amount of information still required to finish classifying the tuples is minimal (i.e., minimum $Info_A(D)$).

Example 1: Decision tree using information gain.

Table below presents a training set, D, of class-labeled tuples randomly selected from the weather dataset consisting of weather information of last 14 days and whether a match was played on that day or not. Now using the decision tree we need to predict whether the game will happen or not in the day with testing attributes.

Day	Outlook	Temperature	Humidity	Wind	Play_Tennis?
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Table 1. Weather data

In this example, the class label attribute, play_tennis, has two distinct values (*yes, no*); therefore, there are two distinct classes (i.e., $m = 2$). Let class C_1 correspond to *yes* and class C_2 correspond to *no*. There are nine tuples of class *yes* and five tuples of class *no*. A (root) node *N* is created for the tuples in *D*. To find the splitting criterion for these tuples, we must compute the information gain of each attribute.

We first compute the expected information needed to classify a tuple in *D* as,

$$Info(D) = -\left[\frac{9}{14} log_2\left(\frac{9}{14}\right) + \frac{5}{14} log_2\left(\frac{5}{14}\right)\right] = 0.940\ bits$$

Next, we need to compute the expected information requirement for each attribute. Let's start with the attribute *Outlook*. We need to look at the distribution of *yes* and *no* tuples for each category of *age*. For the *Outlook* category *sunny*, there are two *yes* tuples and three *no* tuples *(total five)*. For the category *Overcast*, there are four *yes* tuples and zero *no* tuples *(total four)*. For the category *Rain*, there are three *yes* tuples and two *no* tuples *(total five)*.

So, the expected information needed to classify a tuple in *D* if the tuples are partitioned according to *Outlook* is

$$Info_{Outlook}(D) = \frac{5}{14} \times \left[-\frac{2}{5} log_2\left(\frac{2}{5}\right) - \frac{3}{5} log_2\left(\frac{3}{5}\right)\right] + \frac{4}{14} \times \left[-\frac{4}{4} log_2\left(\frac{4}{4}\right) - \frac{0}{4} log_2\left(\frac{0}{4}\right)\right]$$
$$+ \frac{5}{14} \times \left[-\frac{3}{5} log_2\left(\frac{3}{5}\right) - \frac{2}{5} log_2\left(\frac{2}{5}\right)\right] = 0.694\ bits$$

Hence, the gain in information from such a partitioning would be

$$Gain(Outlook) = Info(D) - Info_{Outlook}(D) = 0.940 - 0.694 = 0.246\ bits$$

Similarly,

$$Info_{Humidity}(D) = \frac{7}{14} \times \left[-\frac{3}{7} log_2\left(\frac{3}{7}\right) - \frac{4}{7} log_2\left(\frac{4}{7}\right)\right] + \frac{7}{14} \times \left[-\frac{6}{7} log_2\left(\frac{6}{7}\right) - \frac{1}{7} log_2\left(\frac{1}{7}\right)\right]$$
$$= 0.787\ bits$$

Hence, the gain in information from such a partitioning would be

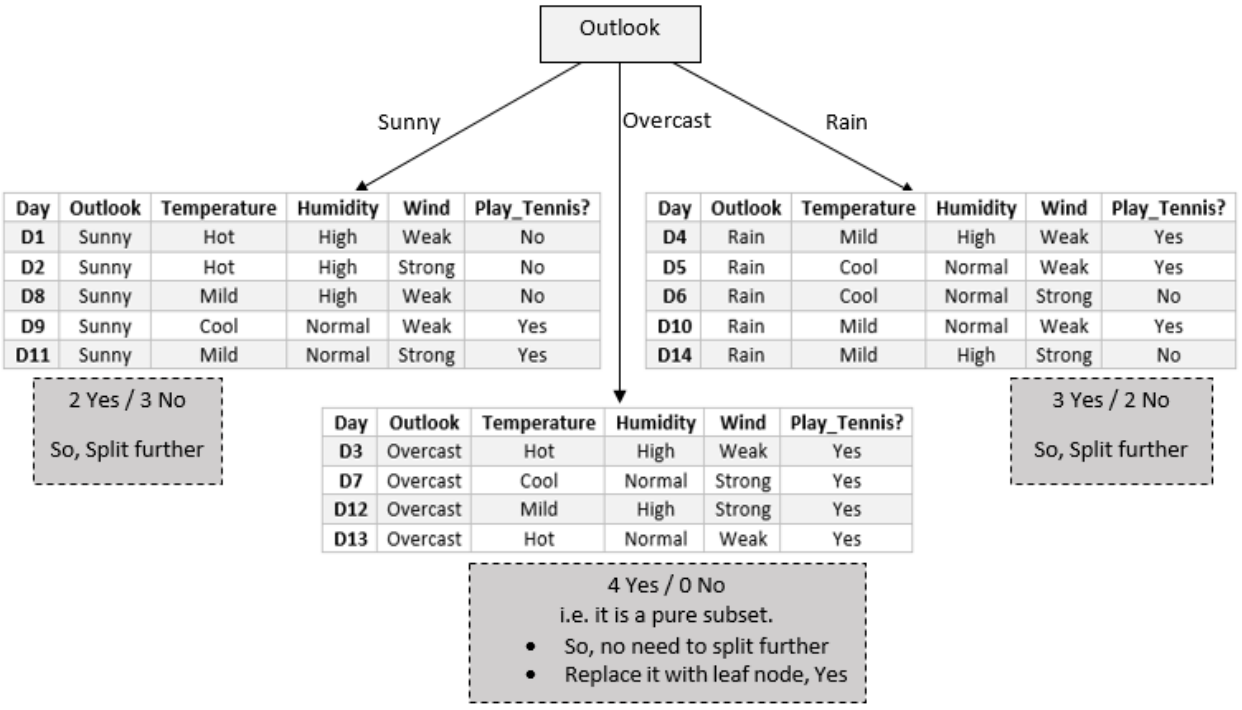
$$Gain(Humidity) = Info(D) - Info_{Humidity}(D) = 0.940 - 0.787 = 0.153\ bits$$

In similar way we can compute,

Gain(Temperature)= 0.031 bits

Gain(Wind)=0.048 bits

Because *Outlook* has the highest information gain *(0.246)* among the attributes, it is selected as the splitting attribute. Node *N* is labeled with *Outlook*, and branches are grown for each of the attribute's values. The tuples are then partitioned accordingly. *So, initially our decision tree will look like:*



Day	Outlook	Temperature	Humidity	Wind	Play_Tennis?
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes

2 Yes / 3 No

So, Split further

Day	Outlook	Temperature	Humidity	Wind	Play_Tennis?
D3	Overcast	Hot	High	Weak	Yes
D7	Overcast	Cool	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes

4 Yes / 0 No

i.e. it is a pure subset.

- So, no need to split further
- Replace it with leaf node, Yes

Day	Outlook	Temperature	Humidity	Wind	Play_Tennis?
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D10	Rain	Mild	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

3 Yes / 2 No

So, Split further

Notice that the tuples falling into the partition for *Outlook = overcast* all belong to the same class. Because they all belong to class *"yes,"* a leaf should therefore be created at the end of this branch and labeled with *"yes"*.

As we can see, for Outlook being sunny, there are 2 yes and 3 no. So we have to further split the decision tree. To do so, we need to compute information gain of attributes for the sub table on the left using same methods as above.

So, $$Info(D) = -\left[\frac{2}{5}log_2\left(\frac{2}{5}\right) + \frac{3}{5}log_2\left(\frac{3}{5}\right)\right] = 0.970\ bits$$

So, the expected information needed to classify a tuple in *D* if the tuples are partitioned according to *Outlook* is

$$Info_{Temperature}(D) = \frac{2}{5} \times \left[-\frac{0}{2}log_2\left(\frac{0}{2}\right) - \frac{2}{2}log_2\left(\frac{2}{2}\right)\right] + \frac{2}{5} \times \left[-\frac{1}{2}log_2\left(\frac{1}{2}\right) - \frac{1}{2}log_2\left(\frac{1}{2}\right)\right]$$

$$+\frac{1}{5} \times \left[-\frac{1}{1}log_2\left(\frac{1}{1}\right) - \frac{0}{1}log_2\left(\frac{0}{1}\right)\right] = 0.400\ bits$$

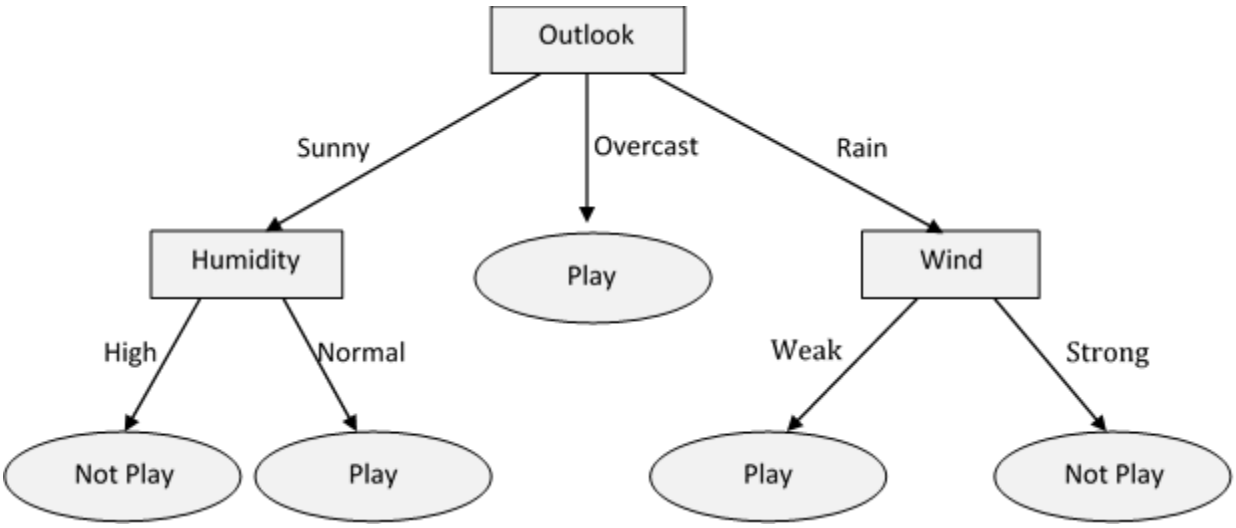
$$Gain(Temperature) = Info(D) - Info_{Temperature}(D) = 0.970 - 0.400 = 0.570\ bits$$

In similar way we can compute,

Gain(Humidity)=0.970 bits

Gain(Wind)=0.020 bits

So, we select Humidity as splitting criteria. In similar way, we can compute information gain for all attributes in right sub table. In the right sub table, Wind will be our splitting criteria. So our final decision tree will be as follows:



b. Gain Ratio

The information gain measure is biased toward tests with many outcomes. That is, it prefers to select attributes having a large number of values. C4.5, a successor of ID3, uses an extension to information gain known as *gain ratio*, which attempts to overcome this bias. It applies a kind of normalization to information gain using a "split information" value defined analogously with *Info*(*D*) as

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times log_2\left(\frac{|D_j|}{|D|}\right)$$

This value represents the potential information generated by splitting the training data set, *D*, into *v* partitions, corresponding to the *v* outcomes of a test on attribute *A*. Note that, for each outcome, it considers the number of tuples having that outcome with respect to the total number of tuples in *D*. It differs from information gain, which measures the information with respect to classification that is acquired based on the same partitioning. The gain ratio is defined as

$$GainRatio(A) = \frac{Gain(A)}{SplitInfo_A(D)}$$

The attribute with the maximum gain ratio is selected as the splitting attribute.

For example

A test on *Temperature* splits the data of Table 1 into three partitions, namely *cool*, *mild*, and *hot*, containing four, six, and four tuples, respectively. To compute the gain ratio of *Temperature*, we first compute

$$SplitInfo_A(D) = -\left[\frac{4}{14}log_2\left(\frac{4}{14}\right) + \frac{6}{14}log_2\left(\frac{6}{14}\right) + \frac{4}{14}log_2\left(\frac{4}{14}\right)\right] = 0.926\ bits$$

From above example, we have Gain(Temperature)=0.031 bits

Therefore, GainRatio(Temperature)=0.031/0.926=0.033 bits.

c. Gini Index

The Gini index is used in CART. Using the notation described above, the Gini index measures the impurity of D, a data partition or set of training tuples, as

$$Gini(D) = 1 - \sum_{i=1}^{m} P_i^2$$

Where, p_i is the probability that a tuple in D belongs to class C_i and is estimated by $|C_{i,D}|/|D|$. The sum is computed over m classes.

The Gini index considers a binary split for each attribute. Let's first consider the case where A is a discrete-valued attribute having v distinct values, $\{a_1, a_2, \ldots, a_v\}$, occurring in D. To determine the best binary split on A, we examine all of the possible subsets that can be formed using known values of A.

When considering a binary split, we compute a weighted sum of the impurity of each resulting partition. For example, if a binary split on A partitions D into D_1 and D_2, the gini index of D given that partitioning is

$$Gini_A(D) = \frac{|D_1|}{|D|}Gini(D_1) + \frac{|D_2|}{|D|}Gini(D_2)$$

For each attribute, each of the possible binary splits is considered. The reduction in impurity that would be incurred by a binary split on a discrete- or continuous-valued attribute A is

$Gini(A) = Gini(D) - Gini_A(D)$.

----------*Refer Text Book*----------

Tree Pruning

When a decision tree is built, many of the branches will reflect anomalies in the training data due to noise or outliers. Tree pruning methods address this problem of *overfitting* the data. Such

methods typically use statistical measures to remove the least reliable branches. The pruned trees are smaller and less complex. The dual goal of pruning is reduced complexity of the final classifier as well as better predictive accuracy by the reduction of overfitting and removal of sections of a classifier that may be based on noisy data. A tree that is too large risks overfitting the training data and poorly generalizing to new samples.

A small tree might not capture important structural information about the sample space. But it is hard to tell when a tree algorithm should stop because it is impossible to tell if the addition of a single extra node will dramatically decrease error. A common strategy is to grow the tree until each node contains a small number of instances then use pruning to remove nodes that do not provide additional information.

Pruning should reduce the size of a learning tree without reducing predictive accuracy as measured by a test set or using cross-validation.

Approaches:

i Pre pruning

In the pre pruning approach, a tree is "pruned" by halting its construction early (e.g. by deciding not to further split or partition the subset of training tuples at a given node). Upon halting, the node becomes a leaf. The leaf may hold the most frequent class among the subset tuples or the probability distribution of those tuples. When constructing a tree, measures such as statistical significance, information gain, Gini index, and so on can be used to assess the goodness of a split. If partitioning the tuples at a node would result in a split that falls below a pre specified threshold, then further partitioning of the given subset is halted. There are difficulties, however, in choosing an appropriate threshold. High thresholds could result in oversimplified trees, whereas low thresholds could result in very little simplification.

ii Post pruning

Post pruning removes subtrees from a "fully grown" tree. A subtree at a given node is pruned by removing its branches and replacing it with a leaf. The leaf is labeled with the most frequent class among the subtree being replaced. Post pruning is done by computing the cost complexity. The cost complexity for each internal node N and the complexity if it were to be replaced by a leaf node is computed. If pruning would result in lower cost complexity, it would be pruned.

3.3 Rule Based Classifier

Large decision trees are difficult to understand because each node has a specific context established by the outcomes of tests at antecedent nodes. To make a decision tree model more readable, a path to each leaf can be transformed into an IF - THEN production rule. The IF part consists of all tests on a path, and the THEN part is a final classification. Rules in this form are called *decision rules.* Rules are a good way of representing information or bits of knowledge. An IF-THEN rule is an expression of the form

IF *condition* THEN *conclusion*.

An example is rule *R*1,

R1: IF *age = youth* AND *student = yes* THEN *buys computer = yes*.

The "IF"-part (or left-hand side) of a rule is known as the rule antecedent or precondition. The "THEN"-part (or right-hand side) is the rule consequent. In the rule antecedent, the condition consists of one or more *attribute tests* (such as *age = youth*, and *student = yes*) that are logically ANDed. The rule's consequent contains a class prediction (in this case, we are predicting whether a customer will buy a computer). *R*1 can also be written as

R1: (*age = youth*) ∧ (*student = yes*)) ⇒ (*buys computer = yes*).

If the condition (that is, all of the attribute tests) in a rule antecedent holds true for a given tuple, we say that the rule antecedent is satisfied (or simply, that the rule is satisfied) and that the rule covers the tuple.

A rule R can be assessed by its coverage and accuracy

- Given a tuple X from a data D
- n_{covers}: Number of tuples covered by R
- $n_{correct}$: Number of tuples correctly classify by R
- |D|: Number of tuples in D

We can define the coverage and accuracy of *R* as

$$Coverage\ (R) = \frac{n_{covers}}{|D|}$$

$$accuracy\ (R) = \frac{n_{correct}}{n_{covers}}$$

For example,

In the training set for buys_computer in table 2, for the rule R1 above,

$n_{covers} = 2$ [*antecedent part is true for 2 tuples. i.e two tuples have age=youth as well as student = yes*]

$n_{correct} = 2$ [*both antecedent part and consequent parts are true for 2 tuples*]

So,

$$Coverage\ (R) = \frac{2}{14} = 14.28\%$$

And,

$$accuracy\ (R) = \frac{2}{2} = 100\%$$

How does a rule based classifier work?

If a rule is satisfied by a testing tuple X, a rule is said to be triggered. But triggering may not necessarily lead the rule to be fired. If more than one rule is triggered, we have a potential problem. What if they each specify a different class? Or what if no rule is satisfied by ***X***? In such situation, three cases may arise:

Case I

If only rule is satisfied, then the rule fires by returning the class prediction for ***X***.

Case II

If more than one rule is triggered, we need a conflict resolution strategy to figure out which rule gets to fire and assign its class prediction to ***X***. There are many possible strategies. Rule ordering or rule ranking or rule priority can be set in case of rules conflict. A rule ordering may be class-based or rule-based.

- *Rule-based ordering*: Individual rules are ranked based on their quality i.e. according to accuracy, coverage etc.
- *Class-based ordering*: Rules that belong to the same class appear together. The class are sorted in decreasing order of importance.

When rule-based ordering is used, the rule set is known as a decision list.

Case III

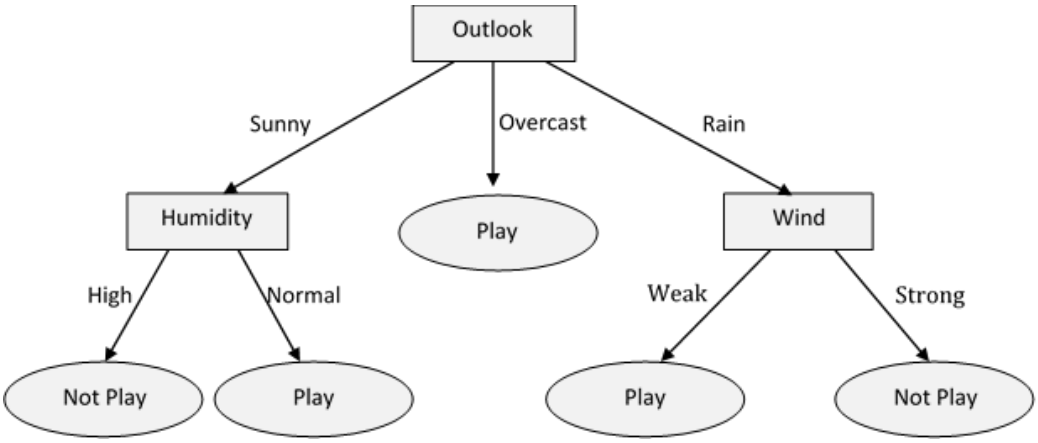
If any instance not triggered by any rule, use default class for classification. Mostly most frequent class is assigned as default class which is usually the most frequent class.

Rule extraction from decision tree

Decision tree classifiers are a popular method of classification. It is easy to understand how decision trees work and they are known for their accuracy. But decision trees can become large and difficult to interpret.

To extract rules from a decision tree, one rule is created for each path from the root to a leaf node. Each splitting criterion is logically ANDed to form the rule antecedent (IF part). Leaf node holds the class prediction for rule consequent (THEN part).

For example,



For the decision tree above, there are five possible rules which can be extracted (because there are five leaf nodes). They are as follows:

*R*1: IF *Outlook = sunny* AND *Humidity = High* THEN *Play_Tennis = no*

*R*2: IF *Outlook = sunny* AND *Humidity = Normal* THEN *Play_Tennis = yes*

*R*3: IF *Outlook = Overcast* THEN *Play_Tennis = yes*

*R*4: IF *Outlook = Rain* AND *Wind = Weak* THEN *Play_Tennis = yes*

*R*5: IF *Outlook = Rain* AND *Wind = Strong* THEN *Play_Tennis = no*

3.4 Nearest Neighbor Classifier

The nearest neighbor classifier uses the training tuples are stored in an *n*-dimensional pattern space to classify the testing tuple. A ***k***-nearest-neighbor classifier searches the pattern space for the *k* training tuples that are closest to the unknown tuple. These *k* training tuples are the *k* "nearest neighbors" of the unknown tuple. For *k*-nearest-neighbor classification, the unknown tuple is assigned the most common class among its *k* nearest neighbors. When *k* = 1, the unknown tuple is assigned the class of the training tuple that is closest to it in pattern space. k-nearest neighbor is an

example of *instance-based learning*, in which the training data set is stored, so that a classification for a new unclassified record may be found simply by comparing it to the most similar records in the training set.

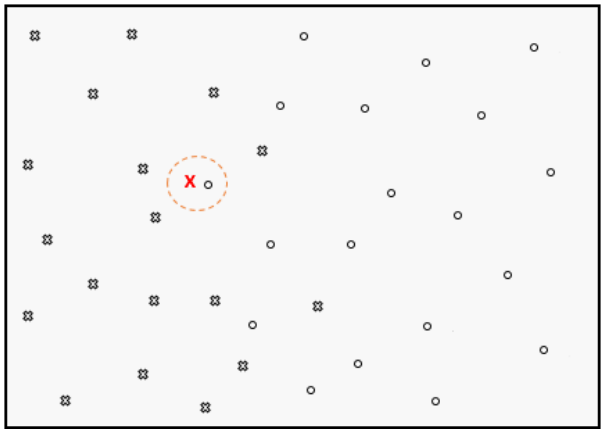
Nearest neighbor classifier requires:

- Set of stored records
- Distance matric to compute distance between records. For distance calculation any standard approach can be used such as Euclidean distance.
- The value of 'K', the number of nearest neighbor to retrieve.

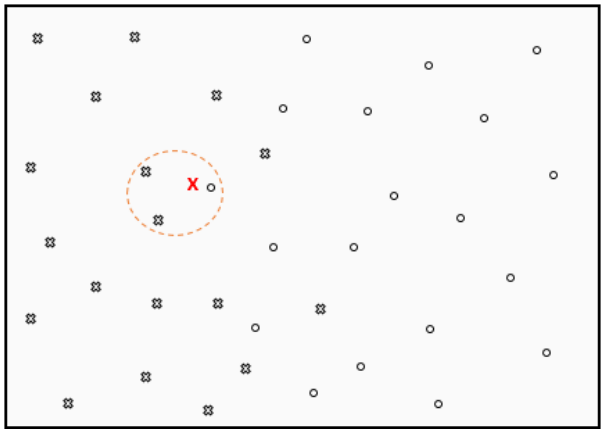
To classify the unknown records:

- Compute distance to other training records.
- Identify the k-nearest neighbor.
- Use class label nearest neighbors to determine the class label of unknown record. In case of conflict, use the majority vote for classification.

For Example,



1-NN classifies X as ○



3-NN classifies X as ⊠

Issues with kNN classifier

i. Choosing the value of K

- One of challenge in classification is to choose the appropriate value of K. If K is too small, it is sensitive to noise points. If K is too large, neighbor may include points from other classes.
- With the change of value of K, the classification result may vary as in example above.

ii. Scaling Issue

- Attribute may have to be scaled to prevent distance measure from being dominated by one of attributes. E.g. Height, Temperature etc.

iii. Distance computing for non-numeric data.

iv. Missing values

Disadvantages

i. Poor accuracy when data have noise and irrelevant attributes

ii. Computationally expensive

3.5 Bayesian Classifier

Bayesian classifiers are statistical classifiers. They can predict class membership probabilities, such as the probability that a given tuple belongs to a particular class. Bayesian classification is based on Bayes' theorem, named after Thomas Bayes (1702-1761). Naïve Bayesian classifiers assume that the effect of an attribute value on a given class is independent of the values of the other attributes. *Bayesian classifier have minimum error rate compared to all other classifiers. It also has high accuracy and speed for large database.*

Bayes Theorem

Let X be a data sample whose class label is unknown. Let H be some hypothesis: such that the data sample X belongs to a specific class C. We want to determine the probability that the hypothesis H holds given the observed data sample X (i.e. P(H|X)). P(H|X) is the *posterior probability* representing our confidence in the hypothesis after X is given. In contrast, P(H) is the *prior probability* of H for any sample, regardless of how the data in the sample look. The posterior probability P(H|X) is based on more information than the prior probability P(H). The Bayesian theorem provides a way of calculating the posterior probability P(H|X) using probabilities P(H), P(X), and P(X|H). The basic relation is:

$$P(H|X) = \frac{P(X|H) \times P(H)}{P(X)}$$

Or, the probability that an event H occurs given that another event X has already occurred is equal to the probability that the event X occurs given H has already occurred multiplied by probability that event H occurs divided by probability of occurrence of X.

For example, suppose our world of data tuples is confined to customers described by the attributes *age* and *income*, and that ***X*** is a 35-year-old customer with an income of $40,000. Suppose that *H* is the hypothesis that our customer will buy a computer. Then,

$P(H|\boldsymbol{X})$ → the probability that customer ***X*** will buy a computer given that we know the customer's age and income. It is the posterior probability, or *a posteriori probability*, of *H* conditioned on ***X***

$P(\boldsymbol{X}|H)$ → the probability that a customer, ***X***, is 35 years old and earns $40,000, given that we know the customer will buy a computer. It is the posterior probability of ***X*** conditioned on *H*.

$P(H)$ → the probability that any given customer will buy a computer, regardless of age, income, or any other information. It is the prior probability, or *a priori probability*, of *H*.

$P(\boldsymbol{X})$ → the probability that a person from our set of customers is 35 years old and earns $40,000. It is the prior probability of ***X***.

Naïve Bayesian Classification

Let *D* be a training set of tuples and their associated class labels.

Given a tuple, ***X***, the classifier will predict that ***X*** belongs to the class having the highest posterior probability, conditioned on ***X***. That is, the naïve Bayesian classifier predicts that tuple ***X*** belongs to the class C_i if and only if

$P(C_i|\boldsymbol{X}) > P(C_j|\boldsymbol{X})$ for $1 \leq j \leq m,\ j \neq i$

Where,

$$P(C_i|X) = \frac{P(X|C_i) \times P(C_i)}{P(X)}$$

Here, P(X) is constant for all classes. So, only $P(X|C_i) \times P(C_i)$ needs to be maximized.

It would be extremely computationally expensive to compute $P(\boldsymbol{X}|Ci)$. In order to reduce computation in evaluating $P(\boldsymbol{X}|Ci)$, the naïve assumption of class conditional independence is made. This presumes that the values of the attributes are conditionally independent of one another, given the class label of the tuple (i.e., that there are no dependence relationships among the attributes). Thus,

$$P(X|C_i) = \prod_{k=1}^{n} P(X_k|C_i)$$
$$= P(X_1|C_i) \times P(X_2|C_i) \times P(X_3|C_i) \times \cdots P(X_n|C_i)$$

For example,

ID	Age	Income	Student	Credit_Rating	Buy_Computer?
1	Youth	High	No	Fair	No
2	Youth	High	No	Excellent	No
3	Middle_aged	High	No	Fair	Yes
4	Senior	Medium	No	Fair	Yes
5	Senior	Low	Yes	Fair	Yes
6	Senior	Low	Yes	Excellent	No
7	Middle_aged	Low	Yes	Excellent	Yes
8	Youth	Medium	No	Fair	No
9	Youth	Low	Yes	Fair	Yes
10	Senior	Medium	Yes	Fair	Yes
11	Youth	Medium	Yes	Excellent	Yes
12	Middle_aged	Medium	No	Excellent	Yes
13	Middle_aged	High	Yes	Fair	Yes
14	Senior	Medium	No	Excellent	No

Table 2: Buys_Computer data

Test data: X:(Age=Youth, Income=Medium, Student=Yes, Credit_Rating=Fair)

Let C_1: Buys_Computer=Yes

C_2: Buys_Computer=No

So,

$P(C_1)$=P(Buys_Computer=Yes) $= 9/14 = 0.643$

$P(C_2)$=P(Buys_Computer=No) $= 5/14 = 0.357$

To compute, $P(X|C_i)$ for i=1,2 we first compute following conditional probabilities:

$P(\text{Age} = \text{Youth} \mid \text{Buys\_Computer} = \text{Yes}) = 2/9 = 0.222$

$P(\text{Age} = \text{Youth} \mid \text{Buys\_Computer} = \text{No}) = 3/5 = 0.600$

$P(\text{Income} = \text{Medium} \mid \text{Buys\_Computer} = \text{Yes}) = 4/9 = 0.444$

$P(\text{Income} = \text{Medium} \mid \text{Buys\_Computer} = \text{No}) = 2/5 = 0.400$

$P(\text{Student} = \text{Yes} \mid \text{Buys\_Computer} = \text{Yes}) = 6/9 = 0.667$

$P(\text{Student} = \text{Yes} \mid \text{Buys\_Computer} = \text{No}) = 1/5 = 0.200$

$P(\text{Credit\_Rating} = \text{Fair} \mid \text{Buys\_Computer} = \text{Yes}) = 6/9 = 0.667$

$$P(\text{Credit\_Rating} = \text{Fair} \mid \text{Buys\_Computer} = \text{No}) = 2/5 = 0.400$$

Hence,

$$P(X|C_1)=P(X|\ \text{Buys\_Computer}=\text{Yes})= P(\text{Age} = \text{Youth} \mid \text{Buys\_Computer} = \text{Yes}) \times P(\text{Income} = \text{Medium} \mid \text{Buys\_Computer} = \text{Yes}) \times P(\text{Student} = \text{Yes} \mid \text{Buys\_Computer} = \text{Yes}) \times P(\text{Credit\_Rating} = \text{Fair} \mid \text{Buys\_Computer} = \text{Yes})$$

$$= 0.222 \times 0.444 \times 0.667 \times 0.667$$

$$= 0.044$$

$$P(X|C_2)=P(X|\ \text{Buys\_Computer}=\text{No}) = P(\text{Age} = \text{Youth} \mid \text{Buys\_Computer} = \text{No}) \times P(\text{Income} = \text{Medium} \mid \text{Buys\_Computer} = \text{No}) \times P(\text{Student} = \text{Yes} \mid \text{Buys\_Computer} = \text{No}) \times P(\text{Credit\_Rating} = \text{Fair} \mid \text{Buys\_Computer} = \text{No})$$

$$= 0.600 \times 0.400 \times 0.200 \times 0.400$$

$$= 0.019$$

To find class C_i that maximizes $P(X|C_i)P(C_i)$, we compute,

$$P(X|\ \text{Buys\_Computer}=\text{Yes}) \times P(\text{Buys\_Computer}=\text{Yes})=0.444\times0.643=0.028$$

$$P(X|\ \text{Buys\_Computer}=\text{No}) \times P(\text{Buys\_Computer}=\text{No})=0.019\times0.357=0.007$$

Therefore Naïve Bayesian Classifier classifies

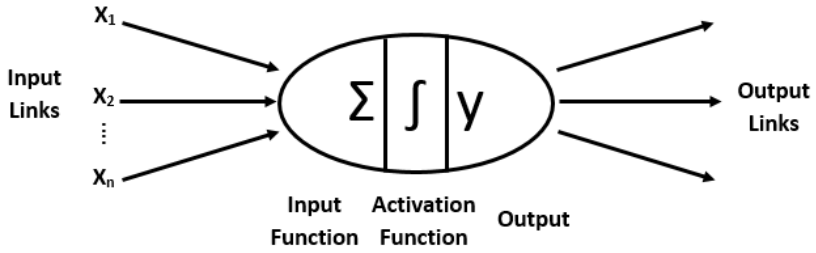
X:(Age=Youth, Income=Medium, Student=Yes, Credit_Rating=Fair)

as class Buys_Computer=**Yes**

3.6 Artificial Neural Network Classifier

An Artificial Neural Network is an abstract computational model of the human brain. The human brain has an estimated 10^{11} tiny units called neurons. These neurons are interconnected with an estimated 10^{15} links. Similar to the brain, an ANN is composed of artificial neurons (or processing units) and interconnections. When we view such a network as a graph, neurons can be represented as nodes (or vertices) and interconnections as edges. Although the term ANN is most commonly used, other names include "neural network", parallel distributed processing (PDP) system, connectionist model, and distributed adaptive system. ANNs are also referred to in the literature as neurocomputers.

An Artificial Neural Network (ANN) is a massive parallel distributed processor made up of simple processing units. It has the ability to learn experiential knowledge expressed through interunit connection strengths, and can make such knowledge available for use.

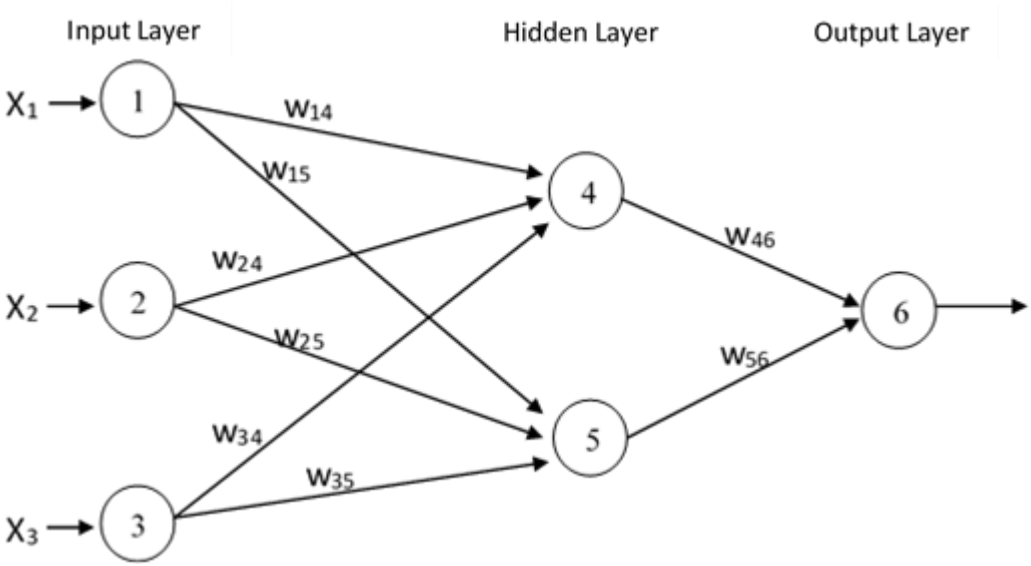


ANN represents a very basic level to imitate the type of nonlinear learning that occurs in the nature. The inputs (x) are collected from upstream neurons (or the data set) and combined through a combination function such as summation (Σ), which is then input into a (usually nonlinear) activation function to produce an output response (y), which is then channeled downstream to other neurons.

Backpropagation learns by iteratively processing a data set of training tuples, comparing the network's prediction for each tuple with the actual known *target* value. For each training tuple, the weights are modified so as to minimize the mean squared error between the network's prediction and the actual target value. These modifications are made in the "backwards" direction, that is, from the output layer, through each hidden layer down to the first hidden layer (hence the name *backpropagation*). Although it is not guaranteed, in general the weights will eventually converge, and the learning process stops.

Before training the network topology must be designed by:

i. *Specifying number of input nodes/units:* Depends upon number of independent variable in data set.
ii. *Specifying Number of hidden layers:* Generally only one layer is considered in most of the problem. Two layers can be designed for complex problem. Number of nodes in the hidden layer can be adjusted iteratively.
iii. *Number of output nodes/units:* Depends upon number of class labels of the data set.
iv. *Learning rate:* Can be adjusted iteratively.
v. *Learning algorithm:* Any appropriate learning algorithm can be selected during training phase.
vi. *Bias value:* Can be adjusted iteratively.



Algorithm

1. Initialize the weight and inputs
2. Calculate the outputs as

   For input layer j, $O_j = I_j$

   For output and hidden layer,

$$I_j = \sum W_{ij} O_i$$

$$O_j = \frac{1}{1 + e^{-I_j}}$$

3. Calculate the error as

   For output layer

$$Err_j = O_j(1 - O_j)(T - O_j)$$

   For hidden layer

$$Err_j = O_j(1 - O_j) \sum_k Err_k \, W_{jk}$$

4. Update the weights

$$W_{ij}(new) = W_{ij}(Old) + \Delta W_{ij}$$

   Where,

$$\Delta W_{ij} = (l) Err_j O_i$$

   Where, l is the learning rate.

Advantages

i. High tolerance of noisy data
ii. Classify patterns on which they have not been trained
iii. Can be used in various applications such as handwriting recognition, image classification, text narration etc.
iv. Parallelization can be implemented

Disadvantages

i. Require long training time
ii. Requires number of parameters whose best value is unknown
iii. Difficulty to interpret the meaning of weights and hidden network

3.7 Issues: Overfitting, Validation and Model Comparison

Overfitting

Overfitting refers to a model that models the training data too well. Overfitting occurs when a statistical model describes random error or noise instead of the underlying relationship. This means that the noise or random fluctuations in the training data is picked up and learned as concepts by the model. The problem is that these concepts do not apply to new data and negatively impact the models ability to generalize.

Overfitting generally occurs when a model is excessively complex, such as having too many parameters relative to the number of observations. A model which has been overfit will generally have poor predictive performance. In order to avoid Overfitting, it is necessary to use additional techniques (e.g. cross validation, pruning (Pre or Post), model comparison etc.

Reason

- Noise in training data.
- Incomplete training data.
- Flaw in assumed theory

Underfitting:

It refers to a model that can neither model the training data nor generalize to new data. An underfit machine learning model is not a suitable model and will be obvious as it will have poor performance on the training data. Underfitting is often not discussed as it is easy to detect given a good performance metric. The remedy is to move on and try alternate machine learning algorithms.

How to Limit Overfitting

Both Overfitting and underfitting can lead to poor model performance. But by far the most common problem in applied machine learning is overfitting.

Overfitting is such a problem because the evaluation of machine learning algorithms on training data is different from the evaluation we actually care the most about, namely how well the algorithm performs on unseen data.

There are two important techniques that you can use when evaluating machine learning algorithms to limit overfitting:

- Use a resampling technique to estimate model accuracy.
- Hold back a validation dataset.

Validation

Validation is the process of evaluating the model using the **training dataset.** It is done by a resampling techinique called cross validation

Cross validation (The holdout method)

Datasets can be categorized into three types: the *training* data, the *validation* data, and the *test* data. The training data is used by one or more learning methods to come up with classifiers. The validation data is used to optimize parameters of those classifiers, or to select a particular one. Then the test data is used to calculate the error rate of the final, optimized, method.

The real problem occurs when there is not a vast supply of data available. In many situations the training data must be classified manually—and so must the test data, of course, to obtain error estimates. This limits the amount of data that can be used for training, validation, and testing, and the problem becomes how to make the most of a limited dataset. From this dataset, a certain amount is held over for testing—this is called the *holdout* procedure—and the remainder is used for training (and, if necessary, part of that is set aside for validation).

***k*-fold cross-validation**

In ***k***-fold cross-validation, the initial data are randomly partitioned into k mutually exclusive subsets or "folds," $D_1, D_2 \ldots, D_k$, each of approximately equal size. Training and testing is performed k times. In iteration i, partition Di is reserved as the test set, and the remaining partitions are collectively used to train the model. That is, in the first iteration, subsets $D_2, \ldots, D_k$ collectively serve as the training set in order to obtain a first model, which is tested on D_1; the second iteration

is trained on subsets D_1, D_3, . . . , D_k and tested on D_2; and so on. Unlike the holdout and random subsampling methods above, here, each sample is used the same number of times for training and once for testing. For classification, the accuracy estimate is the overall number of correct classifications from the *k* iterations, divided by the total number of tuples in the initial data.

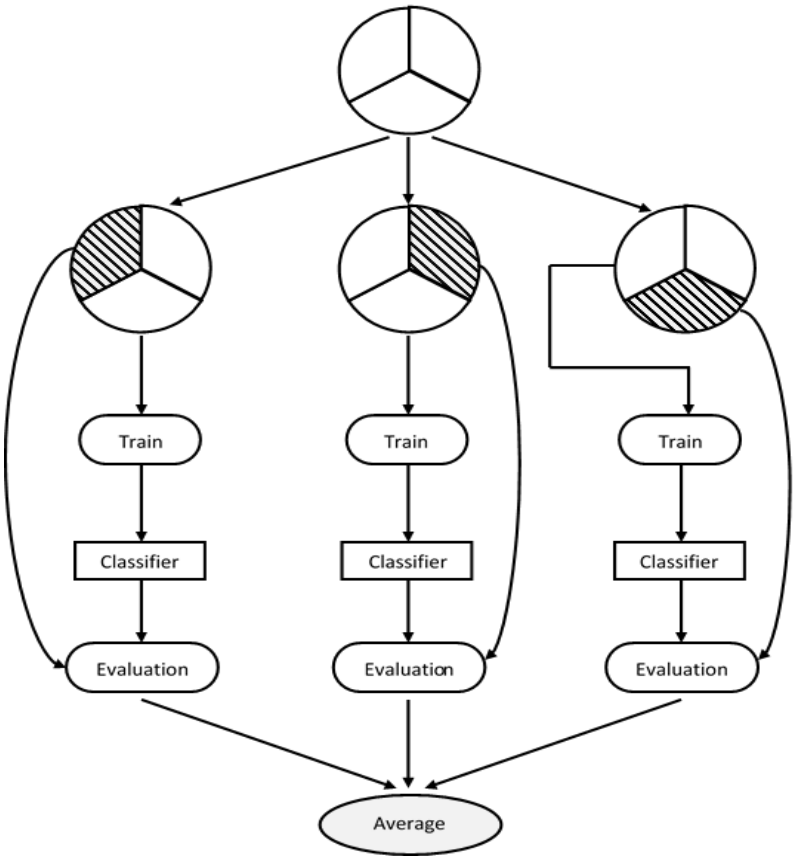


Figure 2. k-fold Cross Validation

Model Comparison

Models can be evaluated based on the output using different method:

i. Confusion Matrix
ii. ROC Analysis

Confusion Matrix

A confusion matrix, sometimes called a classification matrix, is used to assess the prediction accuracy of a model. It measures whether a model is confused or not, that is, whether the model is making mistakes in its predictions or not.

In the two-class case with classes *yes* and *no*, buys computer or not, plays golf or not and so on, a single prediction has the four different possible outcomes shown in Table 3. Given *m* classes, a confusion matrix is a table of at least size *m* by *m*. An entry, $CM_{i,j}$ in the first *m* rows and *m* columns indicates the number of tuples of class *i* that were labeled by the classifier as class *j*.

	Predicted Class			
Actual Class		***Yes***	***No***	***Total***
	Yes	True Positive	True Negative	P
	No	False Positive	False Negative	N
	Total	P'	N'	*P+N*

Table 3: Confusion Matrix

***True positive* (TP)** refer to the positive tuples that were correctly labeled by the classifier.

***True Negative* (TN)** are the negative tuples that were correctly labeled by the classifier.

A ***false positive* (FP)** occurs when the outcome is incorrectly predicted as *yes* (or positive) when it is actually *no* (negative). e.g., tuples of class *buys_computer = no* for which the classifier predicted *buys_computer = yes*

A ***false negative* (FN)** occurs when the outcome is incorrectly predicted as negative when it is actually positive. e.g., tuples of class *buys_computer = yes* for which the classifier predicted *buys_computer = no*

Accuracy is not always the best measure of the quality of the classification model. It is especially true for the real - world problems where the distribution of classes is unbalanced. For example, if the problem is classification of healthy persons from those with the disease. In many cases the medical database for training and testing will contain mostly healthy persons (99%), and only small percentage of people with disease (about 1%). In that case, no matter how good the accuracy of a model is estimated to be, there is no guarantee that it reflects the real world. Therefore, we need other measures for model quality. In practice, several measures are developed, and some of the best known are as follows:

$$Accuracy = \frac{TP+TN}{P+N}$$

$$Error\ Rate = \frac{FP+FN}{P+N}$$

$$Precision = \frac{TP}{TP+FP}$$

$$Recall = \frac{TP}{TP+FN}$$

$$Specificity = \frac{TN}{FP+TN}$$

---Refer notes for example---

ROC Analysis

ROC curves are a useful visual tool for comparing two classification models. The name ROC stands for *Receiver Operating Characteristic*. A ROC curve shows the trade-off between the true positive rate or sensitivity (proportion of positive tuples that are correctly identified) and the false-positive rate (proportion of negative tuples that are incorrectly identified as positive) for a given model. That is, given a two-class problem, it allows us to visualize the trade-off between the rate at which the model can accurately recognize 'yes' cases versus the rate at which it mistakenly identifies 'no' cases as 'yes' for different "portions" of the test set. Any increase in the true positive rate occurs at the cost of an increase in the false-positive rate. The area under the ROC curve is a measure of the accuracy of the model. A typical example is a diagnostic process in medicine, where it is necessary to classify the patient as being with or without disease. For these types of problems, two different yet related error rates are of interest. The False Acceptance Rate (FAR) is the ratio of the number of test cases that are incorrectly "accepted" by a given model to the total number of cases. For example, in medical diagnostics, these are the cases in which the patient is wrongly predicted as having a disease. On the other hand, the False Reject Rate (FRR) is the ratio of the number of test cases that are incorrectly "rejected" by a given model to the total number of cases. In order to plot an ROC curve for a given classification model, *M*, the model must be able to return a probability or ranking for the predicted class of each test tuple. That is, we need to rank the test tuples in decreasing order, where the one the classifier thinks is most likely to belong to the positive or 'yes' class appears at the top of the list. The vertical axis of an ROC curve represents the true positive rate. The horizontal axis represents the false-positive rate. An ROC curve for *M* is plotted as follows. Starting at the bottom left-hand corner (where the true positive rate and false-positive rate are both 0), we check the actual class label of the tuple at the top of the list. If we have a true positive (that is, a positive tuple that was correctly classified), then on the ROC curve, we move up and plot a point. If, instead, the tuple really belongs to the 'no' class, we have a false positive.

On the ROC curve, we move right and plot a point. This process is repeated for each of the test tuples, each time moving up on the curve for a true positive or toward the right for a false positive. To assess the accuracy of a model, we can measure the area under the curve. The closer the area is to 0.5, the less accurate the corresponding model is. A model with perfect accuracy will have an area of 1.0.

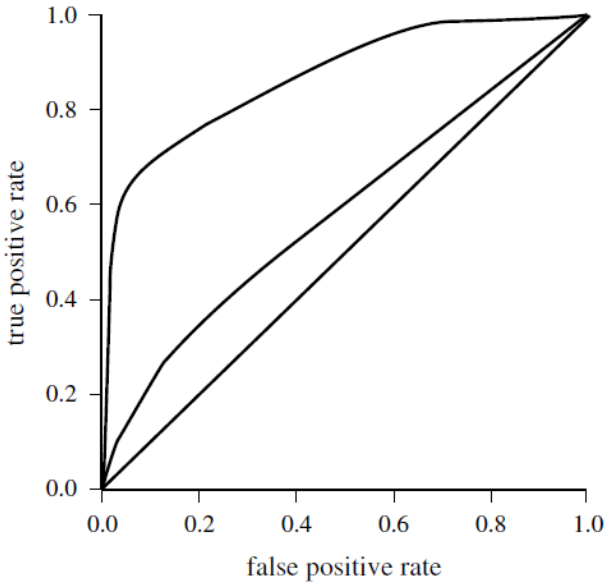


Figure 3 A sample ROC curve

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