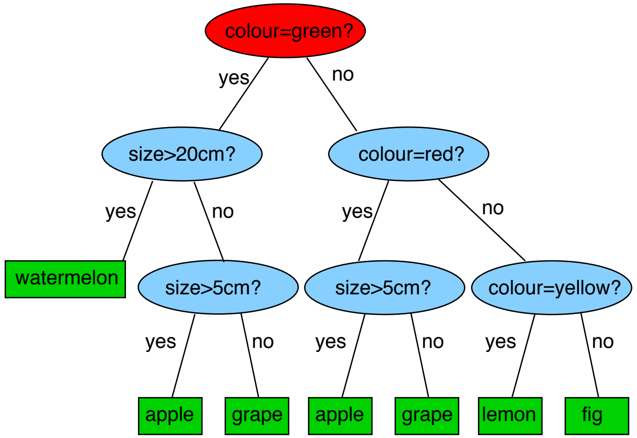
University of Cambridge
Engineering Part IIB

Paper 4F10: Statistical Pattern Processing

Handout 10: Decision Trees



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Introduction

So far we have only considered situations where the feature vectors have been real valued, or discrete valued. In these cases we have been able to find a natural distance measure between the vectors.

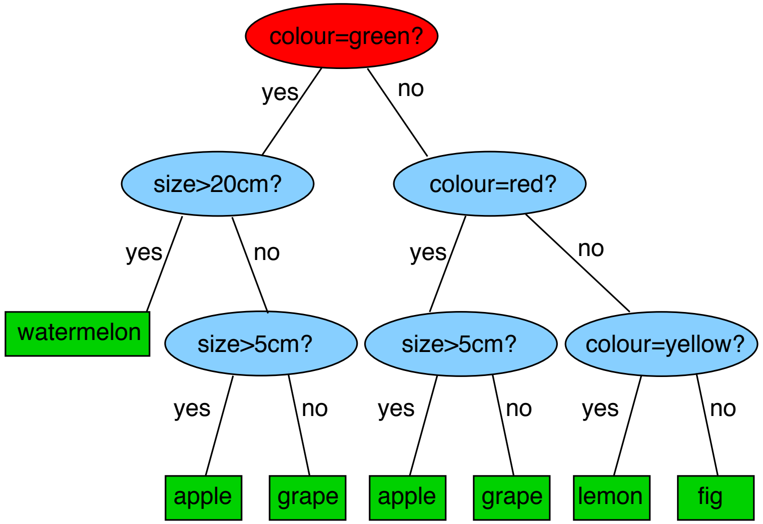
Consider the situation where we have nominal data in addition to the numerical data. For instance descriptions that are discrete and there is no natural concept of ordering. The question is how can such data be used in a classification task. Most importantly how can we use such data to train a classifier.

One approach to handling this problem is to use decision trees, an example of a non-metric classifier - they elegantly handle nominal data. Multiple levels of classifier are used to obtain a final decision. In contrast to the multi-layer perceptrons (another multi-layer classifier) the training of these decision trees is relatively simple and the classification speed is fast.

We will look at the issues behind training and classifying with decision trees. As with the other classifiers supervised training data will be used to train the decision tree.

Example Decision Tree

Consider a simple task to classify fruit according to its colour and size. A reasonable decision tree would be:



The feature-vector, [`red`, 3.0`cm`], is observed, what is the fruit?

1. Does colour=green? NO
2. Does colour=red? YES
3. Is size>5cm? NO

It's a grape!

Decision Tree Construction Issues

Decision tree comprises:

- root node: the top node/question in the tree (red).
- internal nodes: consists of questions (blue)
- terminal nodes (or leaves): consists of a class label (green)

When constructing decision trees a number of issues must be addressed:

1. how many splits should there be at each node (binary?)?
2. what question for root/internal nodes?
   - what order should the questions be asked in?
3. when should a node be declared a leaf?
4. how should a leaf be labelled?

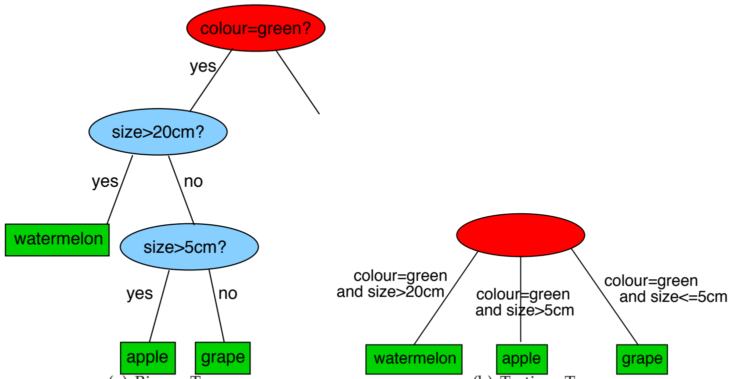
For more general decision trees there are other issues that may be addressed for example handling missing data and pruning trees. These are not considered in this lecture.

Number of Splits

When the question associated with a node is applied the outcome is called a split - it splits the data into subsets. The root node splits the complete training set, subsequent nodes split subsets of the data.

How many splits to have at each node?

Normally the number is determined by an expert. Note every decision and hence every decision tree can be generated just using binary decisions.



(a) Binary Tree (b) Tertiary Tree

Two forms of query exist

- monothetic: `(colour=green?)`
- polythetic: `(size>20cm?)  AND (colour=green?)`

Polythetic queries may be used by can result in a vast number of possible questions.

Question Selection

The basic training paradigm for designing a binary decision tree automatically from training data is

1. generate a list of questions
2. initialise a root node containing all training data
3. sequence through all questions and for each:
   (a) apply the question to the node training data
   (b) partition the data and compute the purity
   (c) record the question with the highest purity
4. attach the best question to the current node and create two offspring nodes
5. split the data assigning as follows:
   - yes data in the left node
   - no data in the right node
6. recursively apply the above algorithm to each new node

Note that this is a so-called greedy algorithm because it only computes a locally optimal partitioning of the data. The complete tree is not guaranteed to be an optimal classifier.

Purity Measures

The aim of a split is to yield a pure node (nodes only containing one class), or get as close as possible.

To assess the purity of the nodes a node impurity function at a particular node N, $\mathcal{I}(N)$ is defined

$$\mathcal{I}(N) = \phi(P(\omega_1|N), \ldots, P(\omega_K|N))$$

where there are K classification classes.

The function $\phi()$ should have the following properties

- $\phi()$ is a maximum when $P(\omega_i) = 1/K$ for all i
- $\phi()$ is at a minimum when $P(\omega_i) = 1$ and $P(\omega_j) = 0, j \neq i$.
- It is symmetric function (i.e. the order of the class probabilities doesn't matter).

The obvious way to use the purity when constructing the tree is to split the node according to the question that maximises the increase in purity (or minimises the impurity). The drop in impurity for a binary split is

$$\Delta\mathcal{I}(N) = \mathcal{I}(N) - \frac{n_{\mathrm{L}}}{n_{\mathrm{L}} + n_{\mathrm{R}}}\mathcal{I}(N_{\mathrm{L}}) - \frac{n_{\mathrm{R}}}{n_{\mathrm{L}} + n_{\mathrm{R}}}\mathcal{I}(N_{\mathrm{R}})$$

where:

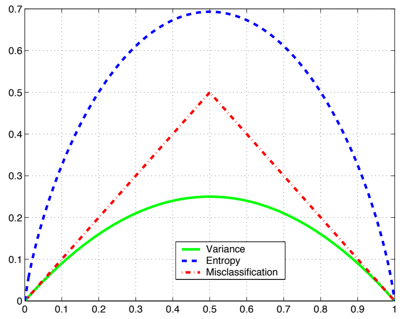
- N_{L} and N_{R} are the left and right descendants;
- n_{L} is the number of the samples in the left descendant;
- n_{R} is the number of the samples in the right descendant;

Purity Measures

There are a number of commonly used measures:

- Entropy measure:
$$\mathcal{I}(N) = -\sum_{i=1}^{K} P(\omega_i|N)\log(P(\omega_i|N))$$
- Variance measure: for a two class problem a simple measure is
$$\mathcal{I}(N) = P(\omega_1|N)P(\omega_2|N)$$
- Gini measure: this is a generalisation of the variance measure to K classes
$$\mathcal{I}(N) = \sum_{i\neq j} P(\omega_i|N)P(\omega_j|N) = 1 - \sum_{i=1}^{K}(P(\omega_i|N))^2$$
- Misclassification measure:
$$\mathcal{I}(N) = 1 - \max_{k}(P(\omega_k|N))$$

The purity measures for a two class problem are shown below.



Non-Binary Purity Increase

We may also want to extend the binary split into a multi-way split. Here we can use the natural extension

$$\Delta\mathcal{I}(N) = \mathcal{I}(N) - \sum_{k=1}^{B} f_k \mathcal{I}(N_k)$$

where f_k is the fraction of the samples in descendant k

$$f_i = \frac{n_i}{\Sigma_{k=1}^{B} n_k}$$

The direct use of this expression to determine the number of splits B has a drawback:

- large B are inherently favoured over small B.

To avoid this problem the split is commonly selected by

$$\Delta_B\mathcal{I}(N) = \frac{\Delta\mathcal{I}(N)}{-\Sigma_{k=1}^{B} f_k \log(f_k)}$$

This is the gain ratio impurity

Using the splitting rules described before results in a greedy algorithm. This means that any split is only locally good. There is no guarantee that a global optimal split will be found, nor that the smallest tree will be obtained.

Question Set Generation

Only consider binary questions with n training samples. The question set generation can be split into two parts.

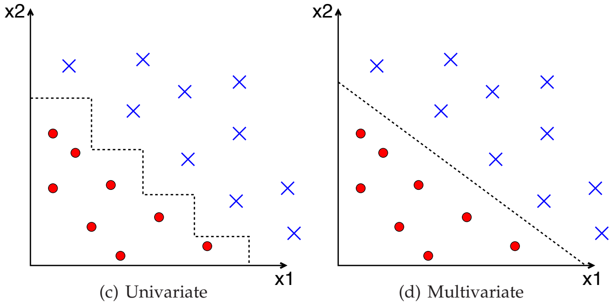
- Nominal data: a set of questions associated with specific nominal attribute needs to be specified, e.g.
  - fruit colour: `(colour=green?)`, `(colour=red?)`

  For many tasks, such as clustering the phonetic context in speech recognition, the exact set of questions is not found to be important, provided a sensible set of questions is used.
- Naturally ordered data: Only considering splits parallel to the axis (combinations are possible) The choice of where to split for a particular dimension is determined by:
  1. sorting the n-samples according to the particular feature selected ;
  2. examining the impurity measure at each of the possible $n-1$ splits;
  3. selecting the split with the lowest impurity;

  Each of the possible d-dimensions should be examined.

Multivariate Numerical Questions

In some situations the proper feature to use to form the decision boundary does not line up with the axis.



(c) Univariate

(d) Multivariate

This has lead to the use of multivariate decision trees. Here decision do not have to be parallel to the axis. The question is how to select the direction of the new split.

This may be viewed as producing a linear hyperplane that correctly partitions the data. This is the same problem as generating a linear decision boundary. We can therefore use for example:

- perceptron criterion;
- logistic regression;
- support vector machines.

There is a problem with this form of rule as the training time may be slow, particularly near the root node.

Declaring a Leaf Node

If the splitting is allowed to carry on we will eventually reach as stage where there is only one sample in each node.

Pure nodes can always be obtained!

However these pure nodes are not useful. It is unlikely that the tree built will generalise to unseen data. The tree has effectively become a lookup-table. There are a number of techniques that may be used to stop the tree growth at an appropriate stage.

- Threshold: the tree is grown until the reduction in the impurity measure fails to exceed some specified minimum. We stop splitting a node N when
$$\Delta\mathcal{I}(N) \leq \beta$$
where β is the minimum threshold. This is a very simple scheme to operate. It allows the tree to stop splitting at different levels.
- MDL: a criterion related to minimum description length (MDL) may also be used. Here we look for a global minimum of
$$\alpha\text{size} + \sum_{\text{leaf nodes}} \mathcal{I}(N)$$
size represents the number of nodes and α is a positive constant. The problem is that a tunable parameter α has been added.

Other generic techniques such as cross-validation and held-out data may also be used.

Labelling Impure Nodes

If the generation of the tree has been very successful then the nodes of the tree will be pure. By that it means that all samples at a terminal node have the same class label. In this case assignment of the terminal nodes to classes is trivial.

However extremely pure trees are not necessarily good. It often indicates that the tree is over tuned to the training data and will not generalise.

For the case of impure nodes they are assigned to the class with the greatest number of samples at that node. This is simply Bayes' decision rule (pick the class with the greatest posterior).

$$\hat{\omega} = \arg\max_i \{P(\omega_i|N)\}$$

where

$$P(\omega_i|N) \approx \frac{n_i}{\sum_{k=1}^{K} n_k}$$

and n_i is the number of the samples assigned to node N that belong to class ω_i.

Classification Trees?

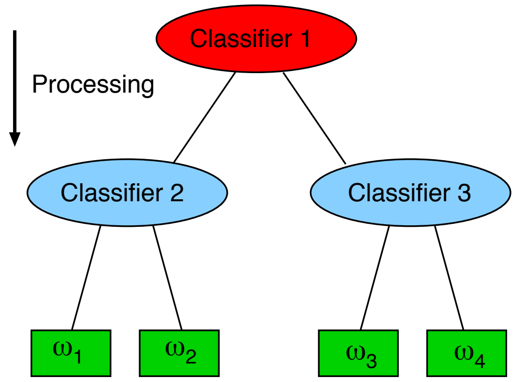
The classification tree approach is recommended when:

1. Complex datasets believed to have non-linear decision boundaries, which may be approximated by a sum of linear boundaries.
2. Data sets with nominal data.
3. There is a need to gain insight into the nature of the data structure. In multi-layer perceptrons it is hard to interpret the meaning of a particular node or layer, due to the high connectivity.
4. Need for ease of implementation. The generation of decision is relatively simple compared to, for example, multi-layer perceptrons.
5. Speed of classification. Classification can be achieved in cost $\mathcal{O}(L)$ where L is the number of levels in the tree. The questions at each level are relatively simple.

Standard forms of classification tree implementations are: CART, ID3, C4.5.

Tree-Based Reduction

Given a tree-structure, it is possible to use this tree-structure as an approach to combine multiple binary classifiers to form a multi-class classifier without the "no-decision" regions of simple voting.



The above Directed Acyclic Graph (DAG) is one approach:

- classification/training works from root node down
- top classifier classifies $\{\omega_1, \omega_2\}$ vs $\{\omega_3, \omega_4\}$
- performance will depend on ordering of classes
- possible to use purity measures previously described

Mistakes at the top-level cannot be corrected by lower levels

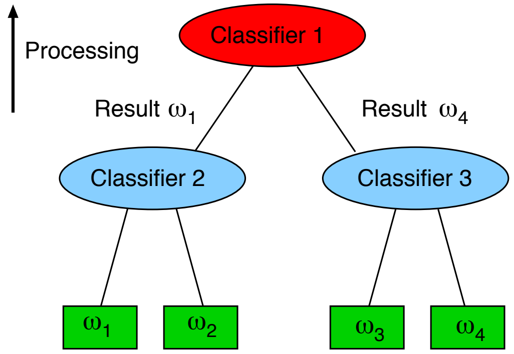
- top-classifier task highly complicated

Adaptive Directed Acyclic Graph

Adaptive DAG classifiers are an alternative process:

- classification works from leaf nodes up
- classifiers decide between results from lower classifiers

Simple "knockout" competition



Above diagram, the actions are for a particular observation:

- Classifier 2 applied to split ω_1 vs ω_2 - yields ω_1
- Classifier 3 applied to split ω_3 vs ω_4 - yields ω_4
- Classifier 1 applied to split ω_1 vs ω_4 to yield final result

Classifier 1 changes depending on the class outputs!

DAG versus ADAG

System	# classifiers	# operations
DAG	$K-1$	$\log_2(K)$
ADAG	$K(K-1)/2$	$K-1$