Methods for Knowledge Discovery in Data

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Dissertation submitted in partial fulfilment of the requirements for the degree of Doctor Europeo en Informática, presented by

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June, 2004

The more perfect a nature is the fewer means it requires for its operation.

Aristotle's

All exact science is dominated by the idea of approximation

Bertrand Russell

Agradecimientos

Agradezco muy sinceramente la ayuda prestada por mi Director de Tesis, Prof. Dr. Miguel Toro durante todos estos años. Su contribución ha sido fundamental en la formalización de los algoritmos de este trabajo.

Agradezco a Erika y Andrea, cuyo amor ha sido la energía elemental que ayudó a mantener este barco contra viento y marea. Sin ellas este trabajo no habría podido ser.

Agradezco a mis padres, que me dieron los materiales esenciales para la culminación exitosa de esta fase de mi vida, y que aquí y Allá se están todavía preguntando en que cosas he andado metido todo este tiempo.

Agradezco a amigos y colegas que me han ayudado. A los colegas R. Martínez de la U. de Sevilla , H. Shahbazkia y Fernando Lobo de la U. de Algarve, por la gentileza que tuvieron de leer el manuscrito original y hacerme valiosas críticas. A G. Oliveira e A. Jones por su corrección del manuscrito en Inglés. A J. Lima, por su ayuda en la revisión de algunos algoritmos. A T. Boski, por su aliento permanente. A F. Saravia y a María Pía Labbé por su entusiasta apoyo desde mi distante y querido Chile.

Una palabra especial de agradecimiento a los colegas del Departamento de Lenguajes y Sistemas de la Universidad de Sevilla. Me han tratado de tal modo, que en todo momento me he sentido allí como en mi tierra.

Parte del tiempo de trabajo de esta tesis, ha sido hecho con el apoyo del programa de acción 5.2 PRODEP financiado por la Unión Europea.

Abstract

This thesis contributes to the development of tools for Supervised Learning, and in particular for the purposes of classification and prediction, a problem of interest to everyone working with data.

After analysing some of the most typical problems found in instance-based and decision trees methods, we develop some algorithmic extensions to some of the most critical areas found in the process of Data Mining when these methods are used.

We begin by studying sampling data and the benefits of stratified data composition in the training and test evaluations sets. We study next the characteristics and degree of relevance of attributes, a problem of paramount importance in data mining. We do this by means of identifying the discriminatory power of attributes with respect to classes. Selecting most relevant attributes increases algorithm complexity, which is exponential in the number of attributes. For this reason, verifying every other possible subset of candidate attributes is sometimes out of question. In this respect, we provide a low-complexity algorithm to help discover which attributes are relevant and which are not [Serendero et al., 2003]. This technique forms an integral part of the classification algorithm, and it could be utilised by rule induction algorithms using trees, as well as instance-based methods using distance metrics for the application of the principle of proximity.

In most instance-based methods, vector records relate to a class as a whole, i.e., each record considered on its integrity relates to one class. The same idea is present in decision trees, and for that reason classes appear only at tree leaves. On the contrary, our algorithm relates class membership to cell *prefixes*, allowing a complete and new approximation of sub-cell component elements to class membership. This concept is a fundamental part of our algorithm.

Most instance based methods, and in particular, *k-NN* methods deal with the problem of searching similar records to some unseen object in the data hyperspace based on distance metrics. Selecting “close” neighbour objects from the hyperspace can be a computationally expensive process. We contribute in this respect by offering a search mechanism based on a tree structure with a low complexity cost and where the distance calculation considers first attributes that are more relevant.

Selecting best neighbours of representative patterns not only depends on the proximity of similar objects. We define several selection criteria weighted according with data characteristics, thus adapting the algorithm to different data.

For all experiments, we present a comparison of results from two different sources, namely results from the literature and results obtained in our own hardware using a relatively new benchmark tool. This way is possible to keep equal testing conditions, a condition difficult to find in figures from the literature.

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1 Introduction

The most important goal of handling data and performing computation is the discovery of knowledge. We store data about a certain process and retrieve later that information in order to use it in a meaningful way. To put it in the words of R. W. Hamming, *the purpose of computing is insight, not numbers.* [Hamming, 1973]

Getting insight from small or moderate amounts of data was manageable until recently. However, data collection with today's computer technology has had such an increment in volume in the last years that represents an explosion overwhelming all expectations. According to a recent study "*The world produces between 1 and 2 exabytes*[1] *of unique information per year, which is roughly 250 megabytes for every man, woman, and child on earth." …"It's taken the entire history of humanity through 1999 to accumulate 12 exabytes of information. By the middle of 2002 the second dozen exabytes will have been created"*. In the conclusion of the same report, its authors say: "*It is clear that we are all drowning in a sea of information. The challenge is to learn to swim in that sea, rather than drown in it. Better understanding and better tools are desperately needed if we are to take full advantage of the ever-increasing supply of information"*[Lyman, 2000].

These huge amounts of information do not only represent a challenging data warehousing problem. In the last forty years database technology and disk capacity has allowed the easy storage, manipulation and fast retrieval of ever growing volumes of data, which is at the heart of today's information society. However, much of this increased power is wasted because humans are poor at gaining insight from data presented in numerical form. When a database stores measurements, events, dates or simply numbers, queries on that database return facts. Facts however are not exactly knowledge, in the sense of concepts representing generalizations about data relations. These concepts are the ones permitting the learning process to take place, by improving our performance in an environment.

Congruent with the above indicated data production of the last years, the increase in database size as well as the ever growing high dimension of records has dramatically

expressed the idea that besides other relations than the ones defined a priori by database designers, there was knowledge which could be extracted from databases. Moreover, this knowledge would be crucial in the decision-making process.

With this premise in mind, the field has had a tremendous impact primarily on industry wanting to take advantage of this hidden knowledge. The globalisation of information through the Internet and the establishment of the *e-business* have increased the need for tools and methods to elaborate knowledge from data produced massively every second.

At the same time, the size of the problem made also clear that looking for knowledge through tedious manual queries on large databases would have to be replaced by advance computer algorithms running on faster hardware, as the sole possible solution.

It is within the goal of addressing these challenging issues that has taken place the development of the area of *Knowledge Discovery* (KDD). Although inherently associated with the area of databases for they contain the raw material for the elaboration of knowledge, KDD is at the confluence of other research areas as well, such as statistics, machine learning, pattern recognition, neural networks, rough and fuzzy sets among others.

KDD is all of them and none of them. It is all of them, because the discipline jointly uses techniques from several of these areas in order to attack the old problem of finding patterns in data. It is none of them, because it is something more than the simple joint utilization of these techniques developing its own methods, data structures and algorithms. The reason for this development came as a realization that in solving problems, which involve thousands of high dimensional records, no single method could be expected to work well in the face of such diversity of data.

The term *Knowledge Discovery* appeared around 1989 and was defined as:

"...The nontrivial process of identifying valid, novel, potentially useful, and ultimately understandable patterns in data" [Frawley et al., 1991].

However, the name popularising the field has been *Data Mining*, mostly used in the economic and financial spheres. Later, the name was extended to *Knowledge Discovery*

[1] An exabyte is a billion gigabytes or 10^{18} bytes.

in Databases or KDD [Fayyad et al., 1995] to refer to the whole process, reserving the name *Data Mining* only for the central inductive task[2].

For these late authors, KDD is:

"The process of using the database along with any required selection, pre-processing, sub-sampling, and transformations of it; to apply data mining methods (algorithms) to enumerate patterns from it; and to evaluate the products of data mining to identify the subset of the enumerated patterns deemed 'knowledge'".

In general, there are three main steps in the Knowledge Discovery process. First, target data needs to be selected whether at a raw state or already in database format. At this pre-processing stage, data is normalized and clean. A decision needs to be made on what to do with records exhibiting missing data or data that seems to be in error. It is also required at this stage to deal with the various types which data can present, in particular its domain size, ordering, boundary values, etc.

Second, a phase recognized as Data Mining, which is the central inductive process of pattern extraction. Inductive means obtaining knowledge through the inference of a new theory from a set of observations, which is the experience. At this stage and depending on the method been used, global or local hypotheses are created capturing the existing relations in patterns of data under analysis.

Third, knowledge can be extracted from the obtained patterns. However, the resulting information is not always in an easily interpretable form. For this reason, pattern information and relations found must be put in a textual, graphical or visual form which is more intelligible, such that can be understood and therefore useful to the expert domain. Still the users of the data mining process must use the resulting knowledge. They have to determine whether the accuracy of the results, the understandability of the extracted knowledge, the time span to produce results and its practicality is useful or not for them, establishing new goals. Generally, at this stage, the process reiterates again to approximate to new objectives such as improving results, simplifying already obtained knowledge or improving its visual representation.

[2] In the context of this work we used indistinctively both expressions.

In all these three phases, the interaction between the domain expert and the programmer is required several times. Data and its meaning is not known by the programmer. It is the domain expert experience and knowledge, which facilitates the work of the programmer. For knowledge always can use previous knowledge about a domain to generate a picture closer to reality. Furthermore, algorithm development and resulting performance are data dependent. Therefore, choosing existing or designing new algorithms requires the programmer expertise. In many cases, the parameters used to produce hypotheses about data need to be changed dynamically as a function of data and the algorithm itself. Interaction between the expert of the domain and the programmer is again required. Finally, yet important, at the very end of one iteration cycle within this process, is the decision of the data owner to accept or not the results produced and offered by the programmer.

1.1 Motivation for this thesis. Some background

This thesis is about Data Mining and its related field Machine Learning (ML), itself a sub-field of Artificial Intelligence. ML is the scientific field studying how machines can learn, which is one of the components of intelligence. [Langley, 1996] proposes the following definition of learning:

"Learning is the improvement of performance in some environment through the acquisition of knowledge resulting from experience in that environment"

Both ML and Data Mining depend heavily on inductive reasoning, i.e. the reasoning from particular observations available to the researcher leading to general concepts or rules.

Example 1 The following are examples of inductive reasoning and learning:

A tennis player trying to hit a forehand shot, will spend hundreds of shots learning how to hit the ball in order to send it through the net at the desire height, speed and direction, in order to place it far from the reach of his/her opponent. After 1000 shots, he/she will have (hopefully) learned how to hit the ball appropriately. The knowledge extracted from all those patterns describing the ball trajectory and place of impact, will be then used the following time a similar shot is hit.

Someone concerned with the lack of water for human needs could measure over a period of a year the amount of water wasted in a typical family home. This is the experience. After observing many patterns of water consumption, this information could be processed to demonstrate that 60% of that water contains only soap, 20% contains other polluters and the remainder 20% contains other organic matter. This is the knowledge. Using this knowledge in order to build houses with simple filter systems to recycle a scarce resource such as water would mean that we have learned something.

In the context of this work, we deal only with the first subtask of the learning process, namely the methods to acquire knowledge including the first two phases of knowledge discovery referred to above.

Knowledge has to be extracted from data. Most of the time, we found data on its original raw state, normally requiring a pre-process phase in order to be useful. Data has to be clean, ordered, complete and consistent. Let us accept for the time being, that data is ready to be processed. Records (examples, observations, objects) are usually presented to the programmer as a sequence of vectors formed by Attribute values of various data types. They represent the independent variables, with various degrees of correlations between them. These attributes can be associated or not with a given label or class, representing the dependent variable. Thus, a typical representation is the following:

$$r = \langle A_1 \mid a_1, A_2 \mid a_2, .., A_i \mid a_i, .., A_n \mid a_n, c \rangle \qquad \textbf{(1.1)}$$

We find an ordered sequence of the pair *Attribute/value* and optionally a corresponding class, a symbol representing one among a finite discrete set of values.

Depending on the presence or absence of the class, two classical problems constitute a central goal in Data Mining. If the class is present in the available data, the goal can be class prediction. If there is no input of classes, the goal will be clustering: to find natural groupings or clusters of records in order to characterize data.

In the first case, learning from examples with or without a known class is called Supervised Learning in Machine Learning taxonomy. Its goal is to obtain relevant data patterns from available examples. These in turn will be used to generate general or local hypotheses representing knowledge. This knowledge is used later to predict the class for new unseen data. This process, which organizes data into a number of predetermined categories, is called Classification. Classification is an uncertain task by nature, aiming at making an educated guess about the value of the dependent variable class, based on the value of the independent variables represented by attribute values. When the submitted examples do not exhibit class membership, and the original database has some natural cluster structure, a clustering algorithm must be first run, in order to make explicit to each example its associated class label. The classification algorithm can be executed after this.

When no prior data is available for learning, we are in the world of Unsupervised Learning or Learning from Observation. The system must discover by itself its class membership. To do that, it must first characterize common properties and behaviour of examples forming clusters of records. The idea is to create groups of records with the smallest possible differences among their members and the largest possible differences between groups. This task has no prediction to make but to discover and report to the user about the most informative patterns found in the dataset under analysis. For this reason, it is also known as Data Description.

It is within the framework of Supervised Learning that we have developed a Classification tool, which is described in the following sections.

1.2 Instance-based and Decision Tree methods

Out of the many Supervised Learning methods used by Data Mining to create knowledge from data, we have concentrated our attention into two of the most popular inductive techniques: Decision Trees and Instance-Based methods. In the rest of this chapter, we briefly describe both methods and some of their difficulties. We will finish

by proposing a method that uses a) the generation of local hypotheses according to nearby neighbours used by instance-based methods, and b) a tree structure as decision trees do, although in our case is not the tree making any class membership decision, but helping in the whole process.

Decision trees have been used since the 1960s for classification [Hunt, 1966] and [Moret, 1982]. They did not receive much attention within statistics until the publication of the pioneering work on CART [Breiman, 1984]. Independently Quinlan popularised the use of trees in Machine Learning with his ID3 and C4.5 family of algorithms [Quinlan, 1983, 1987, 1993]. According with [Smyth, 2001] early work on trees uses statistics emphasizing parameter estimation and tree selection aspects of the problem, more recent work on trees in data mining has emphasized data management issues [Gehrke et al., 1999].

Decision trees perform classification by executing sequential tests on each of the attributes of a new instance against known records whose patterns are used to create the Decision Tree. While the tree's nodes represent attribute value thresholds, the leaves represent the attached classes to these patterns. The new instance to be classified advances in the tree by executing attribute value comparisons at each node, with branching based on that decision. The process is reiterated until a leaf node is reached, assigning its class to the new instance.

The attraction of these tools comes from the fact that data semantics becomes intuitively clear for domain experts. Much of the work on trees has been concentrated on univariate decision trees, where each node tests the value of a single attribute. [Breiman, 1984], [Quinlan, 1986, 1993]. The test done at each node in this type of decision trees, divides the data into hyperactive planes, which are parallel to the axis in the attribute space.

Instance-based learning, (also known as case-based, nearest-neighbour or lazy learning) [Aha, 1991], [Aha, 1992], [Domingos, 1996], belongs to the inductive learning paradigm as is the case with Decision Trees. However, contrary to these, there is not a unique hypothesis generated before the classification phase. Rather, training examples are simply stored and local hypotheses are generated later at classification time for each new unseen object. The local generated hypothesis utilizes the mathematical abstraction of distance used to implement the *Principle of Similarity*

applied to objects. Consequently, the class of a new object can be disclosed by finding an earlier object of known class, which is not perfectly symmetric but *"similar"* to it.

Similarity can be understood using the mathematical concept of distance. To say that two objects are *similar* is the same as saying that the two objects are *near* to each other. To say *"near"* also means that we are interested in finding existing records, which do not necessarily produce exact matches with the unknown instance. Instead of using the nearest example [Duda, 1973], this paradigm uses the *k* nearest neighbours for classification (*k-NN*). There are two main methods for making predictions using *k-NN*: *majority voting* and *similarity score summing*. In majority voting, a class gets only one vote for each record of that class in the set of *k* top ranking nearest neighbours. The most similar class is assumed as the one with the highest vote score. In the second case, each class gets a score equal to the sum of the similarity scores of records of that class in the *k* top-ranking neighbours. The most similar class is the one with the highest similarity score sum.

Methodologically, the Instance-Based approach represents the opposite when compared with Decision Trees because there is no explicit generalization of some general function. Rather, for each new case a specific function is locally constructed implicitly from the similarity measure above. On the other hand, Decision Trees methodology is a model approach. It creates a general explicit function drawn from the available examples, which is used in all new cases to determine class membership.

These two methods present several problems, related to attributes characteristics, algorithm complexity and accuracy in prediction.

1.2.3.1 Problems with Decision Trees

Some problems with Decision Trees described in the literature are among others:

- They offer a unique hypothesis to interpret every other possible input, which not always fits the real class distribution of examples in the data space [Quinlan, 1993].
- In univariate trees, tests carried on each attribute are based on a certain threshold value calculated after some information gain criterion, which makes them sensible to inconsistent data as well as small changes in data [Murthy, 1996].

- The input order of attributes heavily determines the predictive skill of the classification algorithm. Choosing the right attribute subset and its order can be computationally expensive [Aha et al., 1994].
- The presence of irrelevant attributes increases the computational cost and can mislead distance metric calculations [Indk, 2000]. In datasets with high dimension, not only they do face higher computational cost problems, the interpretation becomes cumbersome to the expert domain as well.

1.2.3.2 Problems with Instance-based methods

- They are "lazy" in the sense of storing data and not doing much with it until a new instance is presented for classification [Cios, 1998].
- The cost of classifying new instances can be high [Mitchell, 1997]. The running time and/or space requirements grow exponentially with the dimension [Indyk, 1999].
- They can be very sensitive to irrelevant attributes [Domingos, 1996].
- They represent instances as points in the Euclidean space, a dimension reduction problem that constitutes a challenge on itself.
- In k-NN methods, choosing the right value for k is not an easy task. A high value increases computational complexity. A small value makes them very sensible to noise data [Riquelme, 2001].

Still both of these methods face general problems common to other methods such as irrelevant attributes, noise sensibility, *overfitting* and symbolic attributes. We will refer to each one of these later.

Furthermore, it is a known fact that no induction algorithm is better than other in all data domains [Mitchell, 1980], [Brodley, 1995]. For these reasons efforts have been done in order to unify some classification methods as done for instance with RISE, which tries to combine strengths and weaknesses of instance-based and rule based methods [Domingos, 1996]. In [Quinlan, 1993], instance-based and model-based methods are combined for classification; the method uses training data to provide both, local information (in the form of prototypes) and a global model. Another attempt uses a multi-strategy combining two or more paradigms in a single algorithm [Michalski,

1994] and still an even longer process is proposed by [Schaffer, 1994] to use several induction paradigms in turn, using cross-validation to choose the best performer.

1.3 Objectives

The point of departure for our approach has been an old programming statement by [Dijsktra, 1972]. Essentially, it says that in developing a new algorithm, much of its simplicity and accuracy will be obtained if we use the right structure for it. The more powerful and appropriate is the data structure for a given problem, the better the algorithm required to manage the data.

A second idea comes from the well-known Minimum Description Length (MDL) principle, which roughly state that the best theory for a body of data is the one that minimizes the size of the theory and the necessary volume of information required to specify the exceptions relative to the theory. In other words, use the smallest amount of information in order to develop a full concept. [Rissanen, 1978]

With these central ideas in mind our goal was to develop a classification tool able to:

- Take advantage of the model-based and instance-based approaches as well as the general principles, to construct a combined simple, low complexity classification algorithm.
- Pre-process available data storing not only training data from a sample but additional information in order to avoid putting the burden on computation at running time.
- Offer a fast searching method for a nearest neighbour approach.
- To develop a predictor within the statistical framework of a data sample stored in a permanent structure, to deal with scalability problems.
- To use a tree structure able to avoid the Boolean decision threshold values typical of univariate[3] decision trees.
- To provide for a simple attribute selection and ordering schema able to deal to a certain extend with the problem of irrelevant attributes.

[3] Node tree holding one attribute.

- To dynamically use decision parameters for class membership assignment of new instances, adapting the algorithm to different data domains.

1.4 Contributions of this thesis

The main contributions of this thesis are (in no particular order of importance):

- The successful combination of elements from the model and instance-based paradigms into a simple, low-computational and coherent classification algorithm [Serendero et al., 2001]. This performs equally well with various types of data, numeric or symbolic and with relative dimensional size datasets by using a stratified sample technique.
- The development of a *sub-cell* concept and its relationship with labels is essential in our framework. A sub-cell corresponds to the *prefix* of a *cell*, which we define as a vector formed by *n* attributes representing a hypercube in the data space. Sub-cells allow a very precise identification of various types of areas regarding class distribution in the data space, thus contributing to help with a cell's class membership. We have no knowledge to this date of this concept being used before for this purpose. Beside the fundamental use in our algorithm, this concept eventually would allow the development of easy clustering techniques, which constitutes one of the traditional goals of scientists analysing data. Using sub-cells would be also beneficial in the application of the technique known as *tree pruning*. This could be achieved by keeping in the data structure prefixes only associated with just one class. The remaining portion of cell vectors known as its *suffix,* could be *'pruned"* , thus reducing feature dimensions, tree size and algorithm complexity as a direct consequence.
- Related to the previous point, is the development of an alternative search method in the hyperspace looking for nearest neighbours. This method is better than standard k-NN methods in terms of error classification rate as well as execution time. Using a simple distance mechanism working on restricted data spaces, it takes advantage of the triangle inequality principle for pruning most of the tree from unnecessary search. The net result is a sub-linear

complexity algorithm, for nearest neighbour search, thus improving the algorithm's complexity, a key problem with these methods.

- The dynamic and combined utilization of weighted decision parameters in the selection of a best neighbour allows the algorithm to follow closely the specific characteristics of a given dataset. Decision parameter weights are obtained from an evaluation set depending on its classification skills. This approach represents a step forward into the solution of the known problem that any classification tool does not perform equally well in all data domains.
- *Relevant* and *irrelevant* attributes are identified using a simple low-computational mechanism [Serendero et al., 2003]. All values corresponding to each attribute are projected into a one-dimension projection using the attribute's previously discretized intervals. Using the concept of *semi-exclusive intervals* for a user-defined threshold value, sub-cell frequencies are used to help with the determination of relevant and irrelevant attributes.
- The use of a permanent *trie* structure to hold training data vectors (that we call *cells*) represents a class spatial map, which keeps within reasonable boundaries search times.

1.5 Structure of this text

The following is the structure of this text: In Section 2 we describe the State of the Art of Supervised Learning methods, in particular the method used as a basis for this thesis: instance-based methods. Considering the use of a tree structure, which holds training data, we elaborate on the various types of search using these types of structures in inductive methods.

Section 3 is the core of this thesis. We give a general overview of the algorithm and provide most of the basic definitions used throughout this thesis. We also include a description of the search mechanism of most representative patterns, as well as present the basic assumptions about input data.

In Section 4 we describe data pre-processing main tasks carried out before tree growth, namely sampling, and the basic ideas behind the method used for ordering attributes. This section also includes data discretization and the effect of modifying the size of intervals in attribute's partitions.

In Section 5 we briefly describe all datasets used in our experiments and present all results done while testing our classification tool. These results comes from two different sources, namely the bibliography as well as results originated running a popular benchmark tool in our own software. We discuss these results ending the section with general conclusions.

In Section 6, we define and explain the use of *decision parameters,* which help to select most representative patterns, a process which is at the heart of the classification algorithm. Weights for each decision parameter are previously calculated by running the algorithm using as input a subset of the training examples known as evaluation set. Together these weighted parameters are used in the final selection process of the best example when classifying new instances through a merit function. The section supplies some figures on the contribution of these decision parameters and explains the implementation of required functions.

In Section 7 we explain the actual implementation of Trie-Class, including data structures, tree building, a comparison of our search method with others, and a required dictionary file and other supporting files used to capture attribute class distributions. In Section 8 we offer some general conclusions. A Bibliography and Appendixes completes this thesis.

1 Introduction

2 State-of-the-Art

Characterizing the state-of-the-art in Data Mining is not an easy endeavour, as this fast growing area of knowledge receives contributions from many different communities such as machine learning, statistics, databases, visualization and graphics, optimisation, computational mathematics and the theory of algorithms. In front of this rainbow of different views, as we show later, there is the additional difficulty in choosing objectively what to report as the most rapidly growing sub-areas, most remarkable success stories as well as the prominent future trends of research. For all this, the choice is subjective and reflects our personal views on what seems to be the most important aspects of the state-of-the-art in Data Mining at this stage.

"The main reason for this fast developing pace of Data Mining in the research, engineering and business communities is the explosion of digitalized data in the past decade or so, and at the same time, the fact that the number of scientists, engineers, and analysts available to analyse it has been rather static". This comment was done at a workshop meeting leading scientists in the field in 1999 and it seems to be valid today [Grossman, 1999]. To recall what was said in the introductory section, the world produces between 1 and 2 exabytes of unique information per year [Lyman, 2000]. Moreover, the speed at which this information spreads around the world will also skyrocket. The coming generation Internet will connect sites at OC-3 (155 Mbits/sec) [Grossman, 1999]. In October 2002 the wireless Internet service provider Monet Mobile Networks launched the first wireless broadband Internet service in the USA that lets users surf the Web via laptop, handheld and desktop computers at speeds more than 10 times faster than dial-up modems. This service is based on Qualcomm Inc.' s CDMA2000 1xEV-DO wireless technology for data, and offers peak speeds of 2.4 megabits per second compared to the previous version' s peak speed of 144 kilobits per second [Forbes, 2002]. Around the same time, a USA Congress Commission was reporting 7.4 million users of high-speed lines in that country at speeds exceeding 200 Kbits/sec during the second half of 2001[FCC, 2002].

The consequence to this bottleneck of huge masses of information requiring to be analysed represents an enormous pressure on the data mining community in general to

produce better, larger scale, and more automatic and reliable tools to extract knowledge from this data.

2.1 Active areas of research and new challenges and directions

The scope of research topics in Data Mining is very broad, challenging scientists working on various communities.

In 1997 [Dietterich, 1997] did a survey on the area of machine learning and suggests four current directions for the field as a reflex of the previous five years of research. His main selected topics where: (a) ensembles of classifiers, (b) methods for scaling up supervised learning algorithms, (c) reinforcement learning, and (d) learning complex stochastic models. He did still mention other active topics such as learning relations expressed as Horn clause programs, area also known as Inductive Logic Programming, the visualization of learned knowledge, neural networks methods, algorithms for dealing with overfitting, noise and *outliers*[4] in data and easy-to-understand classification algorithms.

All of these areas where included later in a broader report on Data Mining from 1998, produced at a state-of-the-art workshop done at the Centre for Automated Learning and Discovery at Carnegie Mellon University (CONALD), which brought together an interdisciplinary group of scientists including approximately 250 participants [Thrun, 1998]. In their final report they were able to recognize eleven active areas of promising research, which in our opinion give the broader picture of present research in Data Mining. For this reason, in the following lines we enumerate and briefly describe each one of them.

2.1.1 Active learning (AI)/experimental design (ED)

Known by these two names depending on whether the area is referred from the Artificial Intelligence of Statistics community, the area addresses the question of how to explore, i.e., choosing which experiment to run during learning. This is done under the assumption that during learning, there is an opportunity to influence data collection.

[4] In statistics, an outlier refer as the case that does not follow the same model as the rest of the data. [Weisberg, 1985]

Business-customer relations and robot training are two examples of choosing correctly the learning data.

2.1.2. Cumulative learning

Many learning problems relate to a continuum of data growing incrementally, which can change patterns in non-obvious ways. The problem is that often, data complexity and volume and the statistical algorithm used for analysis makes almost prohibitive daily evaluation over the entire existing data starting from scratch. For instance customer behaviour can represent roughly steady patterns over a period of time, changing afterwards under influences such as fashion changes, social concerns or just new government regulations.

2.1.3. Multitask learning

The main question posed in this area is whether we can devise effective multi-task learning algorithms, which generalize more accurately through transferring knowledge across learning tasks. This situation is the result of several domains characterized by families of highly related (but not identical) learning problems. Consumer behaviour on specific industry products shows similar attitudes. People's different diseases share similar symptoms, making it a promising possibility of transferring knowledge on people patterns across domains.

2.1.4. Learning from labelled and unlabeled data

The problem addressed in this area, is the fact that we do not always dispose of labelled data. Trying to filter e-commerce data and typifying customers on the fly in a busy Internet site is an expensive process. Can we afford to try labelling all customers? Is it possible to devise algorithms that exploit unlabeled data when learning a new concept?

2.1.5 Relational learning

It refers to the fact that in many learning environments, instances are not presented as an already arranged vector of attributes in a static form. Rather, the relation exists

between whole entities sitting in different files, as is the case with intelligent relational databases. And it is this relation the one that is important for learning new knowledge.

For instance, being able to cross information of people among their jobs, their assets and bank situation together with their tax profile is crucial in tax evasion applications. Devising algorithms of the same relational nature of the data structure is here the challenge.

2.1.6 Learning from huge datasets

Large data renders impossible the use of algorithms that require reading data files several times. For instance, astronomical web traffic and grocery data are among other areas where this situation forces to devise algorithms that can scale up extremely large databases.

2.1.7 Learning from extremely small datasets

This is the opposite situation to the one describe above. Some datasets are just too small for current learning algorithms. Robotics and face recognition problems are examples of application areas with a very limited number of training cases. How can learning be done in these situations, other than resorting to prior knowledge?

2.1.8 Learning with prior knowledge

This is one of the solutions referring to the problem above described of working with scarce training data. Specially, when there is available solid prior knowledge about certain pattern behaviours. The question is then how to incorporate this prior knowledge in statistical methods, and how to devise flexible tools that ease the insertion of this knowledge, sometimes uncertain and abstract.

2.1.9 Learning from mixed media data

Existing algorithms cope in general with just a few types of data. The fast development of multimedia databases poses the challenge of learning from image, acoustic, numerical and nominal data together. Algorithms in this area will have to be able to integrate all these within the learning process, solving first the design problem of

whether to learn separately for each data type as a first step, or handling all these different types on a feature level.

2.1.10 Learning causal relationships

How do we know that a person's obesity, which represents a massive problem in rich countries today, is not due to the consumption of diet colas or the absence of sugar in their daily diet?

How do we separate correlation from causality? The challenge in this respect is in the development of algorithms able to learn causality, the necessary assumptions to be made and the implications they have.

2.1.11 Visualization and interactive data mining

Visualization of data patterns takes an important part in the learning process of many domains. The owner of data participates interactively in the data mining process, observing partial results, rearranging data and reprocessing again until finding desired patterns. The problem is that high-dimensional data as well as some type of data such as text are hard for human visualization. So the problem is how can we devise algorithms able to look at these large and sometimes obscure datasets and how to incorporate in the learning cycle the knowledge of the expert "taking a look" at data?

2.2 General trends

In 1999 a workshop took place on mining large distributed data, bringing together scientists working on information and data management, algebra and number theory, and statistics and probabilities [Grossman, 1999]. Their goal was to discuss the current state-of-the-art of data mining and data intensive computing, as well as opportunities and challenges for the future. The focus of their discussion was on mining large, massive, and distributed data sets.

After confirming the explosion in the amount of digital data and the rather static growth of scientists, engineers and analysts available to work on this data, they conclude that the way to bridge the gap required the solution of the following fundamental new research problems: (a) developing algorithms and systems to mine

large, massive and high dimensional data sets; (b) developing algorithms and systems to mine new types of data; (c) developing algorithms, protocols, and other infrastructure to mine distributed data; (d) improving the easy of use of data mining systems; and (e) developing appropriate privacy and security models for data mining. With the exception of the last topic, there is an agreement on all others as areas of interest in new research.

Perhaps more interesting in this report is a chapter in advances on new applications, which is always a strong force for the discipline of Data Mining to advance. The list of these new applications at the time of the report are included in the following categories: (a) Business & E-commerce Data; (b) Scientific, Engineering & Health Care Data; and (c) Web Data. Several applications from each of these categories were reported: Business Transactions, Electronic Commerce, Genomic Data, Sensor Data, Simulation Data, Health Care Data, Multimedia Documents and The Data Web. These topics coincide with those indicated by [Witten, 1999] on his book. The book's chapter "Looking forward" largely refers to these same topics.

One simple way of verifying actual trends observed in Data Mining research is to look at research production presented on most recent international congresses of renowned prestige in the field. Obviously there is the risk of bias at various levels when using this method. First, one has to determine what constitutes a leading congress. Another area of potential bias is represented by the fact that a congress organizing committee uses its own criteria to define the areas of research that are important at present time. Still another element of bias is the classification of articles as full papers, short presentations or posters. In some cases, a crowded area of research reaching already the maximum number of articles defined by the organizing committee would end up classifying as a poster an article that in a normal situation would have been accepted. In view of these difficulties, one has to be careful when drawing conclusions from such an exercise. Nevertheless this method still allows us to see which research areas capture most attention, provided that we assume that organizing committees selection criteria represent a good sample of trends in the entire field. This is what we have done, selecting as input four international congresses [ICDM 2002], ICML-2002], [KDD 2002] and [ECML/2002] grouping together research topics roughly corresponding to coincident sub-areas. Table 2.1 shows a quantified volume of articles accepted by area of research in decreasing order. They are classified in one of two

categories: full articles and posters/short presentations. We did assume that these last two were more the less equivalent, material still not mature enough but important to publish.

Table 2.1 Accepted papers in Data Mining and Machine Learning in four International Congresses during 2002.

Articles by Area of research	Number and Type		
	Full	Short	Total
Statistical Methods	27	6	33
Clustering & Similarity	19	9	28
Graphs, Trees & Hierarchical structures	20	5	25
Text Classification	21	4	25
Rule Learning	16	6	22
Reinforcement Learning	22	0	22
Ensembles of Classifiers	20	1	21
Streams, Time series/Temporal Data	15	4	19
Support Vector Machines (SVM)	18	1	19
Theoretical Foundations	17	2	19
Web Mining	11	6	17
Frequent patterns/item sets/Sequential patterns	11	2	13
Sampling & Feature Selection	6	4	10
Classification / Evaluation	5	5	10
Intrusion Detection and Security	6	2	8
Bio informatics	6	2	8
Other	1	7	8
E-business. Market & cost. Analysis	2	5	7
Relational Learning	5	1	6
Visualization	2	2	4
Active Learning	3	0	3
Neural Networks	1	2	3
Medical Applications	3	0	3
Applications of Learning	3	0	3
ILP	3	0	3
Cost-sensitive learning	3	0	3
Outlier detection	1	2	3
Distributed Data Mining	0	2	2
Learning from examples	0	2	2
High Performance D.M.	0	1	1
Performance Evaluation	0	1	1
		Total	351

We have grouped these publications following the structure adopted in the congresses themselves, putting together those that seem reasonably similar. This grouping still

presents an additional bias, as some publications could perfectly be classified into two or more groups. To avoid this, we did follow the grouping use by congresses.

Although these figures do not allow us to declare that these are the trends in research at present time, due to the difficulties in classifying this material and the inherent bias in their selection, they are still useful to visualize the big picture. The first one is to confirm that the traditionally developed areas in Data Mining and Machine Learning such as statistical methods (with a strong emphasis on Bayesian methods among them), clustering, decision trees, and rule learning are still leading the volume of activity. Secondly, there are other areas that show also growing activity such as text mining, ensemble of classifiers, time series, Support Vector Machines and Web mining. These trends cannot be a surprise as they were announced five years ago as reported earlier in this section.

Coincident with these general trends, a recent article on the state-of-the-art by [Flach, 2001] identified similar trends after reviewing around a dozen books in the area of Machine Learning. These include: a trend towards combining approaches that were hitherto regarded as distinct and were studied by separate research communities; a trend towards a more prominent role of representation; and a tighter integration of machine learning techniques with techniques from application areas such as Bio informatics.

2.3 Different Perspectives of Data Mining

The richness and fast evolving of the Data Mining discipline not only comes from its large variety of research areas of interest as reported in the previous section. Depending whether you look at Data Mining from the database, the statistical or machine learning perspectives, it exists in the field three strong and different perspectives of development and paradigms.

In a recent work by [Zhou, 2003] in his own words he goes "mining" on Data Mining books. The author analyses three leading and popular authors in the field [Han et al., 2001], [Witten et al., 2000] and [Hand, 2001] whose academic books on Data Mining take respectively the three perspectives mentioned above. The observed differences are put in evidence from the very definition of Data Mining from each of these authors. In the Han and Kamber book [Han et al., 2001] data mining is defined as:

"The process of di scovering interesting knowledge from large amounts of data stored either in databases, data warehouses, or other information repositories".

In Witten and Frank's book [Witten et al., 2000], Data Mining is defined as:

"The extraction of implicit, previous ly unknown, and potentially useful information from data" ([9], pp. xix)

In D. Hand book [Hand et al., 2001], the authors define it as:

"The analysis of (often large) observational data sets to find unsuspected relationships and to summarize the data in novel ways that are both understandable and useful to the data owner"([6], pp.1).

Others such as [Zhou, 2003] put next in evidence other differences among these views, such as the concept of Knowledge Discovery in Databases (KDD) and the whole theme of the chapters covered in all three books to finally suggest (rather than conclude as put it by the author) that:

"…thus from the difference in the coverage of these books, it could be perceived that the database, machine learning and statistics perspectives of data mining put particular emphases on efficiency, effectiveness and validity, respectively" (Ibid, page 4).

To our understanding, there are perhaps less differences between the Database and Machine Learning perspectives when compared against the Statistics view of the problem. The reason for this is that both approaches emphasize algorithms and data structures, bringing together the objectives of efficiency and effectiveness. In fact, machine learning and database scientists share a common core of computer science courses, which naturally bring close their views to solutions on data mining problems. On the other hand, they both lack a strong background on statistics, a deficiency that only interdisciplinary approaches can help solving. The difference between computer scientists and statisticians is precisely the subject of [Smyth, 2001] which devotes an

entire chapter of a recent book dedicated to scientific and engineering applications [Grossman, 2001]. Beginning with a common understanding among statisticians that *"data mining is not much more than the scaling up of conventional statistical methods to massive data sets",* this author explain which are the popular techniques in data mining that have their roots in applied statistics. Among them, nearest neighbours, naïve Bayes and logistic regression for prediction models, and *k*-means and mixture models using expectation-maximization for clustering and segmentation. The one exception to this rule is association rules [Agrawal et al, 1993], a technique that have no clear "ancestors" in the statistics literature, although the author immediately declares that is arguably that how many real-world data mining applications rely on association rules for their success. Nevertheless, while there is some truth in this view of data mining as an extension of applied statistics, this author clearly states that while there is some truth in this viewpoint, "*a more accurate reflection of the state of affairs is that data mining (and more generally computer science) has indeed introduced a number of new ideas within the general realm of data analysis, ideas that are quite novel and distinct from any prior work in statistics"* [Smyth, 2001].

There is one very important aspect that should be emphasized. For a data miner to understand the fundamental role of Statistics in data analysis, requires at the very least some minimal exposure to statistical concepts. Rather than learning a set of specific detailed models it is probably more important to appreciate the general mindset of statistical thinking. For instance, computer scientists are quite aware of the problems posed by very large datasets for analysis, and their efforts will concentrate on structures offline, parallel processing and other software and hardware resources to face the problem, rather than focusing their attention in the theory of sampling for instance and the search of a solution to develop their models with less but more representative data of the problem at hand. To over simplify this point, tell for instance to a computer scientist that the problem is to mine people's opinion on the next national election. They will be thinking on how to hold and structure million of voters as part of the problem to solve. On the contrary, the statistician will focus on the sample size and quality in terms of people's view representation. This is the sensibility lacking in many computer scientists.

This lack of understanding from many computer scientists and engineers working in data mining comes from a limited exposure to statistical ideas in their undergraduate

curriculum, although engineers are better prepared with this respect than computer scientists. [Lam, 2000]. After analysing several success stories of the joint efforts by data miners and statisticians working together, Smyth concludes correctly in our opinion that for data miners the message is clear:

"S*tatistics is an essential and valuable component for any data mining exercise. The future success of Data Mining will depend critically on our ability to integrate techniques for modelling and inference from statistics into the mainstream of data mining practice"* [Smith, 2001].

The figures from table 2.1 seem to confirm this assertion.

2.4 Similarity searching in tries

Searching constitutes a fundamental problem not only in Data Mining techniques but also in computer science as a whole. Most computer programs search for specific data in order to execute their algorithms. For this reason, a good indicator of the state-of-the-art in Machine Learning and Data Mining techniques using distance metrics is to take the pulse to these algorithms. In this chapter we review a unifying view to these techniques, in relation to our own search mechanism.

The search operation can be applied to structured (database) data or to unstructured repositories of information, developed in the evolution of information and communication technologies. For this last type of scenario, required search algorithms can no longer be those of exact search applied in structured data, where the answer represented by a key formed by a number or string, is identical to the one given in the query. Traditional database query languages were built around this principle. With the evolvement of unstructured data though, the concept of *"similarity searching" or "pro ximity searching*" has been developed. This is to say, searching for objects or elements which are similar or closer to a given query element. Within this framework searching in *tries* or *multi-way* trees takes advantage of its structure. In the rest of this section we explain the general concept and related algorithms in this area.

2.4.1 Similarity searching metric spaces

The fundamental idea of the *principle of similarity* is that while symmetry is a measure of indistinguishability[5], similarity is a continuous measure of imperfect symmetry [Lin, 2001]. Consequently the class of a new object can be disclosed by finding an earlier object of known class, which is not perfectly symmetric but *"similar"* to it. The degree of similarity between two objects is implemented using the mathematical abstraction of distance.

A work representing a vast survey on search algorithms demonstrate that all existing algorithms for proximity searching consist in building a set of *equivalence classes*, discarding some classes, and searching exhaustively the rest [Chavez, 2001]. Some applications where this concept appears are among others: unstructured text retrieval, query by content in multimedia objects as well as in structured databases, computational biology and our own area, pattern recognition and function approximation. For all these methods and applications two main techniques seems to cover the entire spectrum, namely *pivoting* and *Voronoi partitions* [Aurenhammer, 1991].

2.4.2 Some concepts for a metric space

A non-negative function *d (x, y)* describing the distance between neighbouring points constitutes a metric. A metric space is then a set possessing a metric. In general, a metric space is formed by a set $\mathbb{S}$ of valid objects with a global distance function (the metric *d*) which, for every point $x, y \in \mathbb{S}$ gives the distance between them as a nonnegative real number *d (x, y).* A finite subset of set $\mathbb{S}$ that we could call $\mathbb{X}$ with size $n = |\mathbb{X}|$ is the search of objects where we search. Then function *d (x, y)* can also be express as d: $\mathbb{S} \times \mathbb{S} \rightarrow \mathbb{R}$. The smaller the distance *d (x, y),* the closer *x* is from *y*.

For a metric to be considered as such, it must satisfy:

[5] Impossible to differentiate or tell apart.

$$
\begin{aligned}
&\text{(I)} \quad \forall \mathbf{x,y} \in \mathbf{S},\ \mathbf{d(x,y)} \geq \mathbf{0} && \textbf{positiveness} \\
&\text{(II)} \quad \forall \mathbf{x,y} \in \mathbf{S},\ \mathbf{d(x,y)} = \mathbf{d(y,x)} && \textbf{symmetry} \\
&\text{(III)} \quad \forall \mathbf{x} \in \mathbf{S},\ \mathbf{d(x,x)} = \mathbf{0} && \textbf{reflexivity} \\
&\text{(IV)} \quad \forall \mathbf{x,y} \in \mathbf{S},\quad \mathbf{x} \neq \mathbf{y} \Rightarrow \mathbf{d(y,x)} > \mathbf{0} && \textbf{strict positiveness} \\
&\text{(V)} \quad \forall \mathbf{x,y,z} \in \mathbf{S},\ \mathbf{d(x,y)} \leq \mathbf{d(x,z)} + \mathbf{d(z,y)} && \textbf{triangular inequality}
\end{aligned}
\qquad \textbf{(2.1)}
$$

If the distance does not satisfy the strict positiveness property IV, then the space is called a *pseudo-metric*. Also, in some cases property II does not hold. It then receives the name of *quasi-metric*. This is the case if for instance you are taking corners in a city as objects, and you want to measure travelling distances for a car. The existence of one-way streets would make the distance asymmetric.

The above axioms express intuitive notions about the concept of distance: distances between different objects are positive and the distance between x and y is the same as the distance between y and x. The triangle inequality means roughly that the distance from x to z to y is never shorter than going directly from x to y. As we show later, this property is crucial in some search algorithms using trie structures.

Some typical distance functions used in distance calculations are shown in the following table. Among them, most used ones belong to the Minkowski family of distances also known as the *L metric*.

$$\text{Euclidean distance: } d(x,y) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2} \qquad \textbf{(2.2)}$$

$$\text{Manhattan or City-block } d(x,y) = \sum_{i=1}^{m} |x_i - y_i| \qquad \textbf{(2.3)}$$

$$\text{Chebychev distance [Michalsky, 1981]: } d(x,y) = \max_{i=1}^{m} |x_i - y_i| \qquad \textbf{(2.4)}$$

The above distances belong to the Minkowski [Batchelor, 1978] family of distances L_m, which can be express as:

$$d(x,y)=\left(\sum_{i=1}^{m}\left|x_i-y_i\right|^r\right)^{1/r} \quad \textbf{(2.5)}$$

Other distances are,

Canberra distance: [Michalsky, 1981]

$$d(x,y)=\sum_{i=1}^{m}\left|\frac{x_i-y_i}{x_i+y_i}\right| \quad \textbf{(2.6)}$$

Quadratic distance [Michalsky, 1981]:

$$d(x,y)=(x-y)^T Q(x-y)=\sum_{j=1}^{m}\left(\sum_{i=1}^{m}(x_i-y_i)q_{ji}\right)(x_j-y_j) \quad \textbf{(2.7)}$$

Where Q is a problem-specific positive definite *m x n* weight matrix.

Mahalanobis distance [Nadler, 1993]:

$$d(x,y)=\left[\det \mathrm{V}\right]^{1/m}(x-y)^T V^{-1}(x-y) \quad \textbf{(2.8)}$$

V is the covariance matrix of $A_1..A_m$ and A_j is the vector of values for attribute *j* occurring in the training set instances 1..n

Correlation distance [Michalsky, 1981] :

$$d(x,y)=\frac{\sum_{i=1}^{m}(x_i-\overline{x_i})(y_i-\overline{y_i})}{\sqrt{\sum_{i=1}^{m}(x_i-\overline{x_i})^2\sum_{i=1}^{m}(y_i-\overline{y_i})^2}} \quad \textbf{(2.9)}$$

where $\overline{x_i}=\overline{y_i}$ and is the average value for attribute *i* occurring in the training set.

Chi-square distance:

$$d(x,y)=\sum_{i=1}^{m}\frac{1}{sum_i}\left(\frac{x_i}{size_x}-\frac{y_i}{size_y}\right)^2 \quad \textbf{(2.10)}$$

sum_i is the sum of all values for attribute *i* occurring in the training set, and $size_x$ is the sum of all values in the vector *x.*

Kendall's Rank Correlation:

$$d(x,y) = (x-y)^T Q (x-y) = 1 - \frac{2}{n(n-1)} \sum_{i=1}^{m} \sum_{j=1}^{i-1} sign(x_i - x_j)\, sign(y_i - y_j) \qquad \textbf{(2.11)}$$

In all Equation above distance functions *x* and *y* are vectors of *m* attribute values.

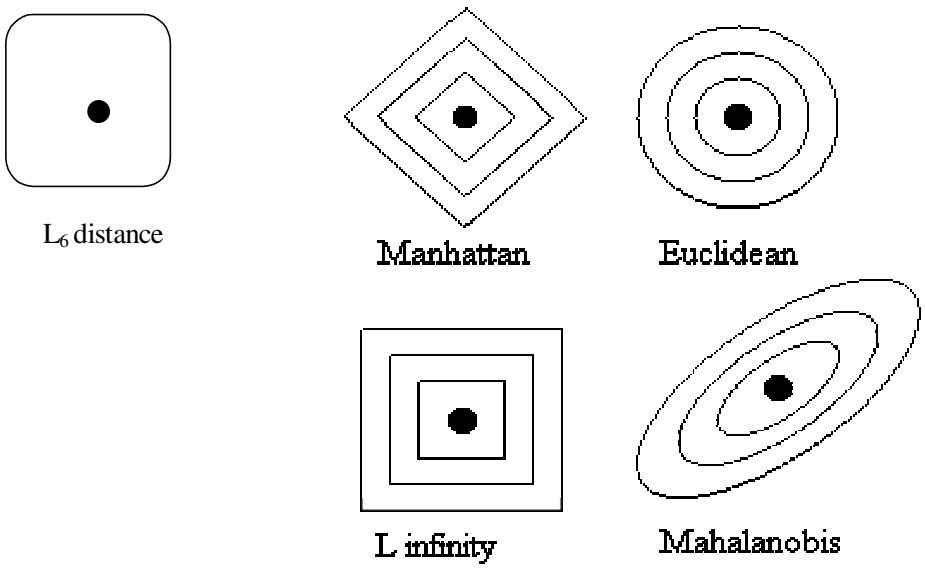

Fig. 2.1 Different contours for constant Manhattan, Euclidean, L_6, L_∞ infinity and Mahalanobis metrics in 2D space.

Fig. 2.1 shows graphically in two dimensions some of the *L* family of distances. When $r = 1$, it correspond to the Manhattan or City-block distance. For $r = 2$ corresponds to the Euclidean distance. When the value of r tends to infinity ∞, it corresponds to the Chebychev distance or max distance.

In many applications the metric space in a vector space, where the objects are k-dimensional points and where the similarity is interpreted geometrically. Also known as *k-dimensional vector space,* this is a particular metric space where objects have *k* real-valued coordinates $(x_1, x2,\ldots,x_k)$. Having the chance of using geometric and coordinate information gives to this metric a certain advantage over general metric spaces, which do not dispose of this information. Among the most popular search structures for vector

spaces are *kd-trees* [Bentley, 1975], *R-trees* [Guttman, 1984], *Quad-trees* [Samet, 1984], *X-trees* [Berchtold, 1996] and others.

2.4.3 Types of search

Typically most similarity methods use three types of query within their metric spaces:

1) ***Range query***, where *d (q, r)* for a query of all elements *x* within a certain distance *r* from *q*, $\{u \in \mathrm{X} / d(q,u) \leq r\}$. A plethora of tree algorithms can be included into this group, whether they work on discrete or continuous distance functions. A not exhaustive list includes: BKT (Burhkard-Keller Tree) [Burkhard, 1973], FQT (Fixed-Queries Tree)[Baeza-Yates, 1994], MT (Metric Tree) [Uhlmann, 1991), SM (Slim Tree) [Traina, 2000], VPT (Vantage Point Trees) [Yianilos, 1993], BST (Bisector Trees) [Kalantari, 1983], VT (Voronoi Tree) [Dehne, 1987], M-tree [Ciaccia, 1997]. And still some of them that can be extended to m-ary trees such as: MVPT (Multi-Vantage-Point Tree) [Bozkaya, 1997] and GNAT (Geometric Near-neighbour Access Tree) [Brin, 1995].

2) ***Nearest Neighbour query*****,** or *NN*. Here to goal is to retrieve the closest elements to query *q* in $\mathbb{X}$, which is;

$$\{u \in \mathrm{X} / \forall v \in \mathrm{X}, d(q,u) \leq d(q,v)\}.$$

3) ***k-Nearest Neighbour query*** (*k-NN*). Similar to the query in (b), but referred to the *k* closest objects to *q* in $\mathbb{X}$. This is, retrieve a set $\mathrm{B} \subseteq \mathbb{X}$ such that |B| = *k* and $\forall u \in B, v \in S - B, d(q,u) \leq d(q,v)$.

The last two groups are called in general *NN* queries or *k-NN* queries (case (b) been assimilated when k equals 1). Most of the existing solutions for *NN* queries uses range-searching techniques and can be found in most of the tree structures listed under that query type above.

In all the above types of queries the number of distance evaluations performed gives the algorithm complexity. At one extreme, all these queries can evaluate all distances for all objects. In many cases this is impossible to achieve in a reasonable span of time.

For this reason, most of the time search algorithms pre process an index structure for data storage, with the goal of saving distance computations when answering similarity queries. Sometimes there is a high cost in building this structure although this is balanced with less distance calculations at query time and hence, lower algorithmic complexity. Some results for *IBk*, the Weka implementation of an instance-based learner are presented in Section 7 as a comparison with our own classifier.

2.4.4 Equivalence relations

Search algorithms using an index structure partition the set $\mathbb{X}$ into subsets providing a mapping between data and their classes. At query time some of these are selected to determine the location of relevant elements; those elements are inspected to provide the required answer.

In most algorithms this partitioning of the data space generates equivalence relations between objects in a partition, where partitions, given a set $\mathbb{S}$, are denoted as partition $\varphi(\mathbb{S}) = \{\varphi_1, \varphi_2 \ldots\}$. This relation, denoted by ~, is a subset of the cross product $\mathbb{S} \times \mathbb{S}$, the set of ordered pairs of $\mathbb{S}$. Two objects $x, y \in \mathbb{S}$ are said to be related, denoted by $x \sim y$, if they belong to the same partition. This relation is equivalent if it satisfies for all $x, y \in \mathbb{S}$ the properties of reflexivity ($x \sim x$), symmetry ($x \sim y \Leftrightarrow y \sim x$) and transitivity ($x \sim y \wedge y \sim z \Rightarrow x \sim z$). Every partition $\varphi(\mathbb{S})$ induces an equivalence relation and conversely, every equivalence relation induces a partition. Hence, an element φ_i of a partition is called an equivalent class. According with [Chavez, 2001]:

All existing indexing algorithms for proximity searching consist in building an equivalence relation, so that at search time some classes are discarded and the others are exhaustively searched. (p.27)

A large class of algorithms to build the equivalence relations are based on *pivoting,* which consist in defining a number of representative objects or "pivots" and doing distance calculation between any object and a given pivot. These receive different names in the literature: *points* [Arya, 1998], *vantage points* [Yianilos, 1993], *key* [Bergman, 1999]. The equivalence relation is defined in terms of distance calculations

between the objects and the pivots: two elements are equivalent if their distance to all pivots is the same.

Instead of using "pivots", another large class of algorithms use a different type of equivalence relation based on "groups", meaning the proximity to a set of elements. This algorithms use the Voronoi equivalence relation based on groups $\{g_1, g_2,\ldots,g_m\}$ is:

$$x \sim (g_i)\ y \Leftrightarrow closest\ (x, \{g_i\} = closest\ (y, \{g_i\})$$

where $closest\ (x, S) = \{w \in S,\ \forall w' \in S,\ d\ (z, w) \leq d\ (z, w')\}$.

The associated partition is the Voronoi partition [Aurenhammer, 1991]. In other words, in these class of algorithms, the space is divided with one partition for each group g_i and the class of c_i is that of the points that have c_i as their closest centre.

2.5 Searching in tries

Most trie structures use for searching one of the two mechanisms described in the previous subsection, namely *pivoting* or Voronoi *"centers".* Next, we give the general context for searching in tries and talk about some of these algorithms in no particular order.

Tries are perhaps most widely used in text processing applications, such as string matching, approximation string matching and compression schemes [Andersson et al., 1994], as well as in algorithms with genetic sequences, data structures of dynamic hashing tables, remote sensing imagery, etc [Aoe et al., 1996; Bergman, 1994; Alber et al., 2001]

Often, when searching in databases, people are often interested in close but not necessarily exact matches. The problem consist in finding "approximate" matches, such as spell checking, fingerprint analysis, voice recognition, image understanding and DNA sequences. These processes use some distance measure to compare how close or far are objects among themselves. For this reason they are in general computationally expensive. Therefore, the need for sub linear search is mandatory, hopefully using a mechanism where most of the database is never directly examined.

Close objects in tries can be searched using a distance metric satisfying the mathematical equivalent of the *triangle inequality,* first introduced by [Burckhard et al., 1973] avoiding complex comparisons to each object in the database. Suppose that given

objects *x, y, z* from a dataset *R*, an integer *k*, and some distance metric *d*, it is required to find all objects in the database with a distance from *x* of not more than *k.* The triangle inequality states that:

$$\forall x, y, z \in R,\ d(x, y) \geq |\, d(x, z) - d(y, z)| \qquad \textbf{(2.12)}$$

If we assume now a node *p* at level *l* in the trie with value *D*, every object at leaves descendant from *p* has a distance *d* from the key object *keyl.* Thus, if $|D - d(x, keyl)| > k$, then we know from the triangle inequality above that *d(x, s')* is greater than *k* for all objects *s'* which are descendants of *p.* Thus search node can be pruned at *p.*

Taken advantage of this property several search algorithms using tries defined some set of *key* objects or *central* objects from the universal set, being representative for some data clusters in the data space. Then, as the case for instance of the *Triangulation Trie* in [Berman, 1994], the trie becomes a representation of the distances from the objects in the database to this set of *keys*. In some remote sensing image problems the straightforward application of the triangle inequality theorem allows the search algorithm to discard a substantial number of images to compare in the feature space [Alber et al., 2001].

In [Berman, 1994] a Triangulation Trie is defined using only a distance measure as a tool. The only requirement being that this satisfies the triangle inequality property, in order for the algorithm compares distances only for a selected object's subset. The construction of the trie is done first choosing a set of keys from the universal set, that can be chosen according to some arbitrary convenient criteria. This is important because the performance of searches in the trie depends on the choice of these keys. For each object in the database is created a vector consisting of the ordered set of distances to the key objects. These vectors are input into the trie. Hence, the trie is a compact representation of the distances from the objects in the database to this set of "keys".

In [Heinz, 2002], a Burst trie is proposed for searching string text, in which strings are maintained in order for faster access. Because tries and ternary search trees [Bentley, 1997], [Clement, 2001] are fast but space-intensive, the proposed structure compress data into so-called *containers* linked to a regular trie called *access trie.* Searching involves using the first few characters of a query string to identify a particular container. A list structure or a binary search tree can be used to give form to containers,

so search within its boundaries is fast. When the container becomes inefficient, it is burst, that is, replaced by a trie node and a set of child containers holding each one half of the previously contained strings.

The concept of *containers* is similar to the previous idea of *super nodes* developed in [Berchtold, 1996] on the structure called the *X-tree*. Observing the problem with the R*-tree [Beckmann, 1990] consisting in the overlap of the bounding boxes in the directory, which increases with higher dimensions, the authors proposed a split algorithm minimizing overlap by the use of *super nodes* for high dimensional spaces. Overlap is the percentage of the volume of data that is covered by more than one directory hyper rectangle. This is correlated to the query performance since in processing queries, overlap of directory nodes results in the necessity to follow multiple paths, thus increasing search time.

More formally, the overlap of an *R-tree* node containing hyper rectangles $\{R_1,R_2,\ldots,R_n\}$ is defined as:

$$overlap = \frac{\left\| \bigcup_{i,\, j \in \{1..n\}, i \neq j} (R_i \cap R_j) \right\|}{\left\| \bigcup_{i,\, j \in \{1..n\}} R_i \right\|}. \qquad \textbf{(2.13)}$$

‖A‖ denotes the volume covered by A.

The *X-tree* consists of three different types of nodes: data nodes, normal directory nodes and super nodes. Super nodes are large directory nodes of variable size (such as multiple of the usual block size). The basic goal of these super nodes is to avoid splits in the directory that result in an inefficient structure.

The *LC-trie* or *level-compressed trie* is introduced in [Andersson, 1993, 1994] corresponding to a compact version of the standard trie data structure. The central idea in this structure is that the highest complete levels of a trie can be replaced-without losing any relevant information- by a single node of degree m^i, the replacement being made top-down. If it is assumed that the input consists of independent random strings from a Bernoulli-type process [Flajolet, 1983], the expected search cost in an LC-trie is $O(\log \log n)$, which is significantly better than $O(\log n)$, achieved by the conventional trie.

2.6 Data Mining and Statistical Sampling

Inductive learning supposes the prior existence of a dataset with records of known class. Depending on the size of the target population the study of a sample from this population is sometimes required. Sampling is the subject of this sub-section.

Let us begin by agreeing with [Smyth, 1999] on his assertion that the appreciation of the fundamental role of statistics in data analysis and in general about statistical ideas is an aspect often overlook by computer scientists simply by their lack of understanding. This is due in part by the fact that most courses in computer science give little room for anything other than a cursory introduction to statistics. This does not mean that our approach belongs to the stream of statistical data mining, neither that we share the view of some statisticians that might argue that data mining is not much more than the scaling up of conventions statistical methods to massive data sets. Indeed Data Mining has introduced its own ideas for data analysis, which are quite novel and distinct from any prior work on statistics.

2.6.1 Random sampling

Simply stated, in statistical terms a *random sample* is a set of items that have been drawn from a population in such a way that each time an item was selected, every item in the population had an equal opportunity to appear in the sample This implies that (1) measurements taken on different items (or trials) are unrelated to one another and (2) the joint distribution of all variables remains the same for all items [Johnson, 1998].

Choosing a sample, and more specifically a statistical sample as define above is crucial for instance-based methods. This is particularly true today, in the presence of huge terabyte databases representing the size of available data we are planning to work with. It would take long hours if not days to execute the training phase without selecting just a small subset for this purpose. For this reason sampling is a good solution. But the results of the algorithm obtained from a sample must be representative for the whole population. With this in mind the goal consist in selecting a sample from the population, such that the performance of the mining algorithm is probably close to what it would be if we run it on the entire database [John, 1996]. At the very least, the selected records to form the sample should fulfil the requirements of a statistical simple random sample

(SRS): *"A SRS of size n is taken when every possible subset of n units in the populatio n has the same chance of being the sample"* [Lohr, 1999]. This sample set sometimes called "evaluation" set (often confused in the literature with the "test" set), is used in the generation of the model function and permits also carrying out the evaluation of the mining algorithm.

The final goal of evaluation is to measure the accuracy of the algorithm, which is the probability of correct classification of previously unseen randomly selected records. These records, only used for this purpose throughout the entire mining process are known as the *test set,* and they do not form part of the working sample. Sample records form the evaluation set, generally called the *training set*, which is mined to "*learn"* about data patterns, thus allowing the development of the classification algorithm. To preserve the validity of the estimation, these two sets must be mutually exclusive during the whole classification process.

Out of the many possible existing bias in selecting sample records, we had two main concerns in creating the sample. First, the sample should have the characteristics of a SRS. Second, we want a sample that incorporates *class distribution* knowledge existing in the whole population database. The reason for this is obviously related to the final goal of building a class predictive model.

When not available, information on class distribution can be collected from the evaluation set, calculating simple probabilities for each class. In some other cases prior knowledge from the expert domain exists, as is the case with several of available datasets from the UCI data repository [Murphy, 1994].

It is desirable that the final accuracy of a classifier be estimated using a method with low variance and bias. For this reason, several accuracy estimation methods exist: Holdout or Sub-sampling, k-fold Cross-validation, Leave-one-out, Stratification, Bootstrap [Kohavi, 1995], [Efron et al., 1993], [Mitchell, 1997].

2.6.1.1 Holdout method

The holdout method sometimes called *test sample estimation*, divide data into two mutually exclusive subsets called a *training set* and a *test set*, or *holdout set*. It is common to designate 2/3 of the data as the training set and the remaining 1/3 as the test

set. The training set is used in the "learning" process while the test set serves t o measure the quality of the induced classifier.

Formally, let $\mathcal{X} = \mathcal{T} \times \mathcal{L}$ be the space of labelled records and $R = \{r_1, r2,...,r_n\}$ a dataset, where $r_i = <v_i \in \mathcal{T}, c_i \in \mathcal{L}>$. An inducer I maps a given dataset R into a classifier $\mathcal{C}$ and this in turn maps an unknown record v $\in \mathcal{T}$ to a class label $c \in \mathcal{L}$. The accuracy of classifier $\mathcal{C}$ is the probability of correctly classifying a randomly selected record:

$Acc = P(\mathcal{C}(r) = c)$ for a randomly selected instance $<r, c> \in \mathcal{X}$.

Further let R_h be the holdout set, which is a subset of R of size h, and let $\mathcal{R}t = R / R_h$. The holdout estimated accuracy is defined as:

$$Acc_h = \frac{1}{h} \sum_{(v_i, c_i) \in R_h} \varphi\left(C(R_t, v_i), c_i\right), \qquad \textbf{(2.14)}$$

where $\varphi(i, j)$=1 if i = 0, and 0 otherwise [Kohavi, 1995].

2.6.1.2 Cross-validation method

Cross validation is a method aiming to estimate the error of a given hypothesis generated by a concept-learning algorithm (classifier). The method specifically refers to generalization error, which is the error on data that has not been seen during training. The method is called sometimes *k-fold-cross-validation* or *rotation estimation* to indicate that the *inducer* is trained and tested *k* times.

Given a set of training data and a concept learner this is how cross validation estimates the accuracy of the hypothesis gained by running the learning algorithm on the data set:

Randomly divide the training data in *k* mutually exclusive sub-sets, called the "*folds*" R_1, R_2, R_3, R_k of approximately equal size. For each one of the *k* folds $t = \{1,2,k\}$ the classifier is trained using R/ R_t and tested on R_t. The resulting cross-validation accuracy estimation is the average of the *k* times the classifier is tested.

Formally, let $R_{(i)}$ be the test set that include record $r_i = <v_i, c>$. Also let $I(R, v)$ be the label assigned to an unlabelled instance *v* by the classifier build by inducer *I* on dataset *R*. Then the accuracy of a cross-validation estimate is given by:

$$Acc_h = \frac{1}{h} \sum_{(v_i, c_i) \in R} \varphi\left(I(R / R_{(i)}, v_i), c_i\right). \quad \textbf{(2.15)}$$

2.6.1.3 Leave one out method

A special case of cross validation is the so-called *leave one out* method, where *k* is chosen as the cardinality of the training set. In other words, for each given example another run of learning is performed using all training data except for this example and the correctness of the classification of the single example left out is checked.

For efficiency reasons *leave one out* is unusual in practice, although in general it will be closest to the real error. Instead, k=10 is a frequently chosen compromise between computational effort and quality of estimation results.

2.6.1.4 Bootstrap method

Bootstrap was introduced by [Efron et al., 1993], and consists in given an evaluation file of size *n*, to create a so-called *bootstrap sample* by sampling *n* records uniformly from data with replacement. This is the training set. All other records form the test set. Since the sample is obtained with replacement, the probability of not being part of this list is $(1 - 1/n)^n \approx e^{-1} \approx 0.368$, and the expected number of distinct objects from the original dataset appearing in the test set is $0.632n$. For instance, consider a dataset $R = \{1,2,3,4,5,6,7,8,9,10,11,12\}$. Randomly sampling *n* instances with replacement would produce the following *training set* $D = \{1,2,10,7,10,5,6,10,5,1\}$. The remaining instances would form the *test set* $T = \{3,4,8,9\}$.

3 The Trie-Class Algorithm. Basic definitions

In this Section we provide a general overview of the Trie-Class algorithm and most of the basic definitions and functions used throughout this thesis, including some examples. We also explain in detail the search mechanism used to extract nearest neighbours and compare its classification skills with a regular *k-NN* algorithm.

3.1 General overview of the algorithm

Our approach to induction is partially based on the instance-based methodology or Nearest Neighbours (*NN*) [Cover, 1967; Salzberg, 1990; Aha, 1991], sometimes also known as case-based reasoning (CBR) [Aha, 1998]. In general, the basic notions of *NN* and instance-based methods are the storage of learning data, the use of some metric to carry out similarity computations by means of calculating distances, and some indexing scheme to help the searching mechanism. A distinctive characteristic of *NN* and CBR in particular is its "*lazy"* approach to problem solving. According to [Aha, 1998] *pure lazy* problem solvers exhibit three typical behaviours:

- They *defer* processing the input until they receive a query request. They just store input examples.
- They are *data-driven*, meaning that they respond to requests by combining information from the stored data and,
- They *discard* any temporary intermediate results created during problem solving.

NN methods also present a more *eager* approach, resembling to a certain extent some model-based approaches in that they retain their inputs into an intensional[6] data structure, reply to queries using this structure and keep it for future requests.

Combining elements that characterize these methods along with ideas from Decision Trees our approach uses a tree structure as an index to store cells from training data in order to *'learn"* , permitting at the same time a very fast search of "*similar*" instances. In a second *thinking* phase, queries on unseen instances are answered using training instances as model. Two of these instances will be selected from the data structure,

[6] Including the rules that describe the inner structure of objects

using a non-Euclidean distance on an attribute-by-attribute basis without normalization. Later, we use different criteria to select one of them as the best available pattern representation of the new unseen instance, as will be explained in Section 6.

3.2 Basic definitions

Notation $\{r \in R, c \in L \mid exp1(r,c) \bullet exp2(r,c)\}$ stand for the set of values of exp2 when *r* and *c* take values in *R* and *L*, and exp1 is true. If exp2(r,c) = *r* then the expression is reduced to $\{r \in R \mid exp1(r)\}$.

Definition 1. Let's consider the closed universe formed by a data file *R* composed of a finite set of *N* records *r*.

$$R = \{r_1, r_2, .., r_N\} . \quad (\mathbf{3.1})$$

In Supervised Machine Learning we find data containing a set of instances, each one described by a vector of attributes and a class label. Attributes are considered to be *predictor* or relevant attributes. They are used as independent variables to induce a certain classification hypothesis, which in turn is used to predict the class of an instance, considered the dependent variable. Therefore, much of this thesis is referred to attributes (or features as they are also called), its characteristics, types and values, and the way they can be used to generate the description of the concept, which is at the centre of the learning process.

Definition 2. In any given record *r* we find a finite set of A_i attributes belonging to set *S,*

$$S = \{A_1, A_2, .. A_i, .., A_n\}, \text{ a nonempty set.} \quad (\mathbf{3.2})$$

Definition 3. Each record *r* is formed by the Cartesian product of *n* attribute values $A_1|a_1 \; x \; A_2|a_2 \; x ... x \; A_n|a_n$ and a class label *c*. Each attribute A_i has its corresponding value a_i, which belongs to domain T_i, such that:

$$r = \langle a_1, a_2, .., a_n, c \rangle, i \in (1..n), a_i \in T_i, c \in L \,. \quad \textbf{(3.3)}$$

Definition 4. Every record *r* is associated with one of *c* class labels belonging to a set *L*.[7]

$$L = \{c_1, c_2, .., c_l\} \,. \quad \textbf{(3.4)}$$

Definition 5. Each class label *c* belonging to records *r* is obtained by the following function:

$$label(r) = c \text{ if } r = <a, c> \,. \quad \textbf{(3.5)}$$

3.3 Definitions on cell discretization

In many Data Mining applications large amounts of data as well as large instance vector dimensions demand some form of data reduction. This is particularly true for methods based on instances or Nearest Neighbours. One of the aspects of the problem attacked by Trie-Class, is to reduce the dimension of each feature by reducing the number of possible values an attribute can take. This goal can be reached by applying discretization to data domains, particularly interesting in attributes exhibiting continue-value types. At the same time, discretization is required in order to work with metric spaces and distance calculations. Discretization has the disadvantage of a potential information loss, allowing two different attribute values to coexist within a given interval thus increasing entropy, a measure of the degree of purity of a given interval with respect to the class. However, the advantage of reducing the search space, a fundamental problem facing almost all algorithms in Data Mining, many times is not harmful for real-world applications [Weiss et al., 1998]. In Trie-Class, discretization is applied to numeric attributes whether discrete or continuous. In the case of nominal attributes, simply each nominal value is assigned a partition of its own.

[7] In this thesis we use indistinctively the words class label, class or just label.

Definition 6. The domain of each attribute A_i can be partitioned into a finite number of user-defined intervals within domain T_i. The number of these intervals can range from 1 to s_i. We assume the existence of function $ord_i()$, which converts the value of an attribute into its corresponding discrete value v_i, which is an ordinal representing the interval value:

$$v_i = ord_i(a_i),\ v_i = (0..s_i),\ a_i \in Ti\ . \tag{3.6}$$

We call value v_i a cell component, which along with other components form cell p as shown later in Equation (3.10).

Definition 7. Let M_i and m_i, be the maximum and minimum attribute values within domain Ti, where w_i is the size of each interval s_i. The number of intervals s_i is simply the ratio of the number of elements in the attribute domain over w_i, a real number.

$$s_i = \left\lceil \frac{(M_i - m_i) + 1}{w_i} \right\rceil, w_i > 0\ . \tag{3.7}$$

Definition 8. Each numerical attribute value a_i fits into an interval represented by the discrete cell component v_i, which is computed using the following floor function:

$$v_i = ord_i(a_i) = \left\lfloor \frac{a_i - m_i}{M_i - m_i} \times s_i \right\rfloor\ . \tag{3.8}$$

If $a_i = m_i$, then the value of v_i will fit into interval zero.

Definition 9. For categorical or symbolic attributes, attribute a_i has its corresponding interval value simply calculated as:

$$v_i = ord_i(a_i)\ . \tag{3.9}$$

If a priori knowledge domain information exists on the actual order of symbolic attributes, then v_i represents the corresponding order number, which in Trie-Class is set

in a dictionary file (described in Section 7). If the interval value calculation for a symbolic attribute does not represent a problem, the same is not true when we want to calculate de distance between these types of values. This is the topic of Section 4.2.

Notice that the number of intervals s_i is not the same for all attributes. They depend on values M_i and m_i, as well as the interval size. These parameters are user-defined. In our implementation, they are declared in the dictionary file. Although not implemented, parameter s_i, could be automatically computed by the system given the simple mechanism we use for domain partitioning as explain above.

Example 3.1

Imagine that a certain record *r* exhibit the value for attribute $a_i = 9$. Let's assume that the domain for this attribute is formed by discrete values ranging from $m_i = 1$ to $M_i = 10$; with $w_i = 2$. Applying Equation (3.7) we obtain $s_i = 5$. Then, applying function $ord_i()$ from Equation (3.8) we would obtain $v_i = ord_i(9) = 4$. Every v_i value will fit into one of s_i intervals belonging to the partition of attribute A_i. In this case, interval number 4 corresponds to the fifth interval, as they begin with interval 0.

If we convert all attribute values from a record into its corresponding interval values v_i we obtain cell *p*.

Definition 10. All v_i elements together form a *cell* vector *p* containing *n* component element values v_i. We call *P* the set of all cells *p* obtained from set *R*.

$$p = \langle v_1, v_2, .., v_i, .., v_n \rangle, \forall p \in P, \forall v_i \in (0..s_{i-1}) \ . \qquad (\mathbf{3.10})$$

Example 3.2

Imagine that we have the following record vector containing five attribute/value pairs: $r = <a_1=9, a_2=3, a_3=5, a_4=6, a_5=1>$.

As in the previous example the values for the following variables are: m_i =1, M_i =10, w_i = 2 and s_i = 5. Applying functions $ord_i()$ from Equation (3.8) to each attribute value a_i and arranging according with Equation (3.10) we convert record r into cell p:

$$p = < v_1 = 4,\ v_2 = 1,\ v_3 = 2,\ v_4 = 2,\ v_5 = 0 >$$

Some specific cells used in this thesis are p^x, p^1, p^2, etc. Cell p^x is a new cell from an instance of unknown class. Cells p^1 and p^2 are cells belonging to the training set with known class.

Definition 11. A multi-attribute-value vector cell p is obtained from its corresponding instance vector r from Equation (3.3) using function $cel(r)$ such that:

$$p = cel(r) \text{ with } p = <v_1,..,v_n>,\ v_i = ord_i\left(a_i\left(r\right)\right),\ i = (1..n) \qquad \textbf{(3.11)}$$

Most classification algorithms and in particular *k-NN* algorithms consider instance vectors relating to a given label as a whole. In Trie-Class we develop the idea of *sub-cell* or *prefix* (as known in text data), which can be associated with one or more classes. In this way, it is possible an "earlier" class membership identification using just a subset of the entire cell, which allows data compression for concept description, a desired goal for the attribute selection problem. Sub-cells are define as follows:

Definition 12. In every cell p we find n sub-cells q_i, which correspond to its prefix:

$$q_i = \left\langle v_1, v_2, .., v_i \right\rangle,\ i = (1..n). \text{ So } p = \left\langle q_i, u \right\rangle \qquad \textbf{(3.12)}$$

where u is the suffix portion. Therefore, we find sub-cells containing 1, 2,..n component elements, where the last of them, called q_n is identical to the full cell p.

The number of records in the dataset exhibiting cell vector p are returned by calling function *freq(p):*

$$freq(p) = \#\left\{r \in R \mid cel(r) = p\right\}. \qquad \textbf{(3.13)}$$

Function *freq* can be equally applied to any sub-cell q_i:

$$freq(q_i) = \#\{r \in R \mid cel(r) = \langle q_i, u \rangle\} \tag{3.14}$$

Definition 13. We define function *kfreq()* as the total number of records where its i[th] value falls into interval *k*.

$$kfreq(i,k) = \#\{r \in R \mid \mathrm{v}_i = k\} \text{ with } v_i = ord(a_i(r)) \ . \tag{3.15}$$

Hereafter we will just write v_i to indicate the full expression $v_i = ord(a_i(r))$.

A restricted variation of the previous function includes the additional argument *c* meaning that a restriction is imposed to objects in interval *k*: they must belong to class *c*. Next function measures the number of sub-cells in a given interval relating to just one label.

Definition 14. Function *lfreq()* produce as result the number of records in a dataset where its v_i cell component is *k* and its label is *c*:

$$lfreq(i,k,c) = \#\{r \in R \mid \mathrm{v}_i = k \wedge label(r) = c\} \tag{3.16}$$

Definition 15. We define function *labels(p)* as the set of labels found in the subset of records with cell *p*.

$$labels(p) = \{r \in R, c \in L \mid cel(r) = p \wedge label(r) = c \bullet c\} \tag{3.17}$$

Definition 16. The number of class labels attached to a given cell *p* is given by the following function:

$$nlabels(p) = \#labels(p) \tag{3.18}$$

the same function can be applied to sub-cells:

$$nlabels(q_i) = \#labels\left(q_i\right) \tag{3.19}$$

In most evaluation sets *R* there is a predominant class label, meaning that most records hold that class. In the literature this is known as "*default rule*" [Domingos, 1996; Brodley, 1996].We call this *'majority class* "as explained in Section 6.

Definition 17. The *class frequency* of a given class correspond to the number or records in a dataset associated with that class.

$$cfreq(c) = \#\{r \in R \mid label(r) = c\} \tag{3.20}$$

Using the previous function we define function *lmaj()* as the function that returns the *majority class*, which is the predominant class in a set *R*.

We now turn our attention to a characteristic aspect of sub-cells, namely its degree of relationship to one or more classes. The intuition here is that we are interested in sub-cells formed by a minimum number of cell component elements relating to one class only. This idea comes from a fundamental concept in Information Theory known as the Minimum Description Length (MDL) principle [Risannen, 1978].

Roughly speaking, the MDL principle states that the "best" theory t o induce from training data is the one that minimizes the complexity of the theory and the length of the data encoded with respect to the theory. In terms of the sub-cells defined by Trie-Class, the shorter the number of attributes in a sub-cell sequence identifying just one class, the strongest this sub-cell is in terms of concept description. We call this the *strength of a cell* and we measure it using the following function.

Definition 18. The *strength* of a cell corresponds to the size of some sub-cell q_i, at the i^{th} component element where it becomes associated with just one label:

$$strength(p) = \#\{1 \le i \le n \mid nlabels(q_i) = 1\} \tag{3.21}$$

Vector cells with greater strength represents vectors located in larger homogeneous areas of the n^{th} dimensional space. Therefore, a strong cell means that more of its v_i values belong to the subset of values associated with a given class. For this reason we

are interested in strong cells as their predictive capability has more confidence when compared with others of less strength.

3.4 Exclusiveness as a measure of attribute relevance

Using some of the functions from the previous subsection, we define now some additional concepts, helping to define the criterion used to determine how relevant a given attribute is.

Whether the discretization method takes or not into account an instance's class membership, all intervals present some class distribution. Our interest is to discover class distribution information within sub-cells, in order to get the kind of information that might be hidden due to a non-supervised discretization process like ours. If intervals belonging to some attribute exhibit a class distribution where one of the existing classes is predominant in relative terms compared with the others, then we are in the presence of *semi-exclusive attributes,* which we define next.

Definition 19. Attribute A_i is said to be *semi-exclusive* for interval *k*, if function *semk()* is true. Parameter φ is a user-defined value representing the fraction of records in interval *k* with class *c*. Function *semk()* is defined as:

$$semk(i,k,\varphi) = \exists c \in L \bullet ((lfreq(i,k,c) / kfreq(i,k)) \geq \varphi) \qquad (\mathbf{3.22})$$

If function *semk()* is true when φ equals 1, then we have an *exclusive interval*, i.e. all v_i values in interval *k* belongs to the same class. In the literature these intervals are known as *primary* [Turney, 1996], [Kohavi et al., 1997] or *pure* intervals [Holte, R., 1993]. The opposite is the concept of *maximum impurity*, indicating that all classes are equally represented on each interval of a given partition [Brodley, 1995]. Modifying the value of φ allows function *semk()* to return true in more or less homogeneous class regions of the instance space. This would be the case for instance of a dataset with four classes with one of them say c_j representing 60% of the class distribution in a given interval *k*. Setting the value of parameter φ to 1 in function *semk()* would provided no information for the region covering that interval. Setting the value of $\varphi = 60$ instead,

function *semk()* would return true allowing to visualize the predominance of class c_j, thus allowing using this information regarding the class at the sub-cell level.

Finding how many of these semi-exclusive intervals exist in whole cells is calculated using the function from next Definition 20:

Definition 20. The degree of exclusiveness of a cell *p* corresponds to the fraction *i* of its *n* cell component values falling into intervals conforming to the *semi-exclusive* property. This property is calculated with the following function:

$$semp(p,\varphi) = \#\{i \in (1..n) \mid \text{semk}(i, v_i, \varphi) \bullet i\} / n \qquad \textbf{(3.23)}$$

We are interested in the fraction of intervals belonging to a given cell complying with the *semi-exclusive* property when this refers to the same class, so we can have consistent information. Used this way, the presence of one or more intervals of this type increases the probability for the cell to be associated with a given class. Hence, cells having intervals exhibiting this property constitute important class pattern predictors.

Definition 21. If all discrete v_i values belonging to attribute $A_i \in R$ are projected into its corresponding intervals, then the *degree of relevance of attribute* A_i with value a_i denoted with symbol δ_i, correspond to the fraction of records falling into those intervals where function *semk()* is true with respect to the total number of records in *R*.

$$\delta_i = \#\{r \in R \mid k = ord_i(a_i(r)) \ \wedge \ semk(i,k,\varphi) \bullet r\} / N \qquad \textbf{(3.24)}$$

Parameter *N* represents the total number of records in set *R*..

Large values for δ means a more relevant attribute when compared with others. The opposite represents irrelevant attributes. The next example illustrates this.

Example 3.3

Let's calculate the value of parameter δ for two attributes, A_1 and A_2, each having domain s_i partitioned in ten equal sized intervals as in Fig. 3.1. The dataset has two classes: *A* and *B*. Frequencies for each interval are shown in the row labelled "*freq*".

Notice that in this case it does not matter which is the predominant class in the set of semi-exclusive intervals included in the calculation of parameter δ as it is the case with function *semp()*. This is so because it is perfectly possible for the same attribute to have different values that can be associated with different classes. This is precisely what matters for attribute relevance. How many values determine cell class membership.

Projecting attribute A_1 values into intervals v_i , with $\varphi = 0.75$

v_i	0	1	2	3	4	5	6	7	8	9	Total	δ
freq	77	32	62	49	79	20	12	23	11	43	408	54/408=0.132
Class	*	*	*	*	*	*	*	*	A	A	54	

Projecting attribute A_2 values into intervals v_i , with $\varphi = 0.75$

v_i	0	1	2	3	4	5	6	7	8	9	Total	δ
freq	227	23	35	17	17	14	12	13	5	45	408	112/408=0.274
class	*	A	*	*	B	B	*	B	*	B	112	

Note: An asterisk means intervals where function *semk()* is false. Shadow areas represent intervals where *semk()* is true with $\varphi = 0.75$.

Fig. 3.1 Attribute values projection in one-dimension to depict its relevance

3.5 Attribute selection

Trie-Class uses a tree structure to hold cell patterns as a mean of speeding up searching most similar objects. As search begins in the root of the tree, the input order of attributes is fundamental if we want most similar instances to remain close to each other in the data hyperspace. For this reason determining the order of attributes is a pre-processing phase executed before tree insertion. (Tree build is explained in Section 7).

Definition 22. The predictive skill of attributes is a measure of its degree of relevance as defined in Equation (3.24). According with this relevance attributes can be ranked in decreasing order of relevance.

$$\beta = \langle \delta_1, \delta_2, .., \delta_i, .., \delta_n \rangle, \delta_i \mid \geq \mid \delta_{i+1} \mid i \in (1..n). \qquad (\mathbf{3.25})$$

Attributes where its relevance $\delta_i = 0$, are orderly pushed to the list's end. These are candidates for elimination ("pruning"), which can be done to improve algorithm

complexity at the expense of some loss in accuracy as shown in Section 4.. An example of a dataset features ordered by its degree of relevance is shown next in Example 3.4.

Example 3.4

Let's consider the Cancer-Wisconsin dataset from Section (5.1.3). It contains nine working numeric attributes representing patient data for cancer diagnosis. Applying formula from Equation (3.24) for each attribute in this dataset, we obtain the following δ values shown in Table 3.1 below. They are ranked by its degree of relevance.

Table 3.1 Attributes degree of relevance values in Cancer dataset

Nº	Attribute name	Frequency	δ_i
1	Uniformity of Cell Size	89	0.218
2	Uniformity of Cell Shape	69	0.169
3	Marginal Adhesion	59	0.145
4	Normal Nucleoli	58	0.142
5	Clump Thickness	54	0.132
6	Bland Chromatin	34	0.083
7	Mitosis	22	0.054
8	Single Epithelial Cell Size	16	0.039
9	Bare Nuclei	9	0.022

We show results later in Section 4 showing how classification accuracy changes with changes in accuracy using only relevant attributes.

3.6 Shape definitions

The similarity hypothesis sustains that what defines a class is that its members are similar to each other and not similar to member of other classes. Therefore, object similarity is determined using distance calculation between corresponding attribute values using functions such as Euclidean or Manhattan.

We are now interested in exploring additional information that might be useful to describe the similarity concept. One such case is constituted by the information concerning intra-attribute relationships within a cell. One of these is the relationship between consecutive attributes belonging to the same cell, which can be represented using the *slope* representation between these two points.

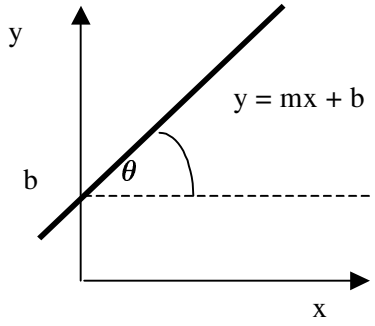

Fig. 3.2 Slope intersection form of a line

For a given line in the xy-plane making angle θ with the x-axis, the slope m is a constant given by $m \equiv \frac{\Delta y}{\Delta x} = \tan\theta$, where $\triangle x$ and $\triangle y$ are changes in the two coordinates over some distance. In general, a slope represents a quantity, which gives the inclination of a curve or line with respect to another curve or line such as the one in Fig. 3.2.

We could graphically represent the *shape* form of a given n-dimensional cell p drawing in two-dimensions all segment lines between pairs of consecutive attributes. We do this by converting each a cell component element into a point. We use the actual attribute value as the y-coordinate and we assign the attribute's order number as the x-coordinate. Hence, we could draw all segment lines between the discrete points $(1,v_1)$, $(2,v_2),..,(n,v_n)$. As we keep constant $\triangle x$ each segment, segment $\triangle y = (y_i - y_{i-1})$ corresponds to a slope between consecutive cell values. An example of such shape representation can be seen in Figure 3.3. In total we would have n-1 line segments to represent a given shape.

Designing a shape retrieval method involves other than shape representation, the definition of some similarity measure and the way these shapes will be accessed or retrieved. [Mehrotra, et al., 1995]. To answer this we first define the space H as the space of all h shapes. Within this space shape similarities are found using some distance

$d(h_1,h_2)$ in order to compare two shapes. Within this framework we propose the following definitions:

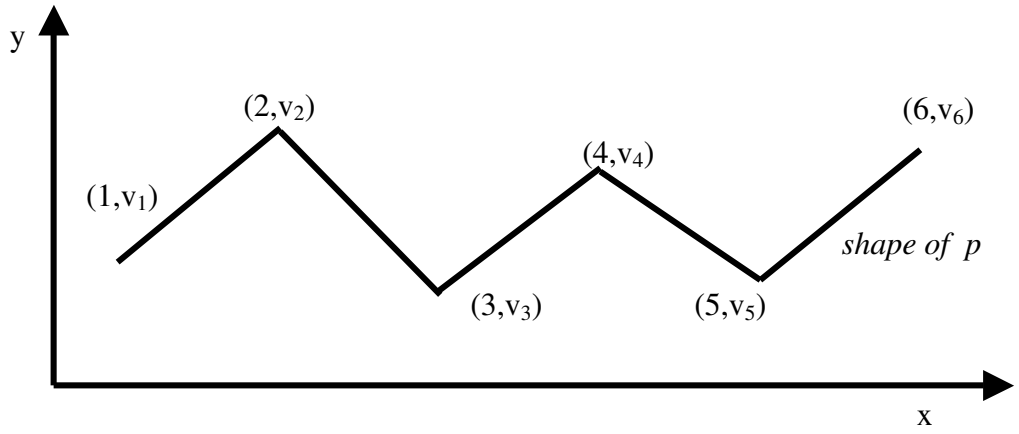

Fig. 3.3 A two-dimensional representation of a cell

Definition 23. The *shape of a cell* is defined as the sequence of its *m* slope components between consecutive values:

$$h =< m_1, m_2, .., m_i, .., m_{n-1} >,\ \mathrm{m}_i = (v_{i+1} - v_i),\ h \in H,\ \text{with}\ p =< v_1, .., v_n > \qquad (\mathbf{3.26})$$

This newly created shape vector contains positive and negative slope values and is one dimension shorter than the cell vector from which is built. The new space *H* represents a space change with respect to space R^n. As can be easily seen this space is not metric as some of its properties are not satisfied, namely, positiveness and symmetry. Within this space we can use a distance measure to determine how close or similar two shapes are from each other. We do that using the following function.

Definition 24. The *shape similarity* between two cells, corresponds to the distance between its corresponding shapes:

$$sp(p', p) = d(h', h) \qquad (\mathbf{3.27})$$

Distance $d(h', h)$ can be any of the standard distances belonging to the Minkowski family explained earlier in Section 2.4.2.

Using shape distances to represent cell similarities can help identifying *shape patterns* in a shape data space. If similar shapes relate to the same class, then this information can enrich the similarity concept.

The degree of shape similarity between two shapes is affected by the actual value of each slope and the slope sign itself, which indicates the relationship between two consecutive attribute values. We illustrate in example 3.5 shape construction and a similarity function.

Example 3.5

Imagine a dataset containing five cells $p^1,p^2,..,p^5$, belonging to some training set, each one formed by seven cell components. Cell values are indicated in Table 3.2.

Table 3.2 Cell vectors and their component values

	Cell component values						
Cells	v_1	v_2	v_3	v_4	v_5	v_6	v_7
p^1	3	6	4	9	4	1	9
p^2	17	10	14	9	9	11	6
p^3	1	19	13	23	10	2	3
p^4	12	9	7	4	8	15	19
p^5	15	5	13	8	7	13	4
p^x	19	9	15	8	9	12	5

The task consists in classifying a new cell p^x from the test set using the shape similarity function. Let's first convert all cell vectors from Table 3.2 into shape vectors applying the shape formula in (3.26). We obtain the shapes and its values indicated in Table 3.3.

Table 3.3 Shape vectors corresponding to cells from Table 3.2

	$(v_{i+1}-v_i)$					
h_1	3	-2	5	-5	-3	8
h_2	-7	4	-5	0	2	-5
h_3	18	-6	10	-13	-8	1
h_4	-3	-2	-3	4	7	4
h_5	-10	8	-5	-1	6	-9
h^x	-10	6	-7	1	3	-7

If we draw the two-dimensional representation of these *h* vectors, we have the figure shown next in Fig. 3.4

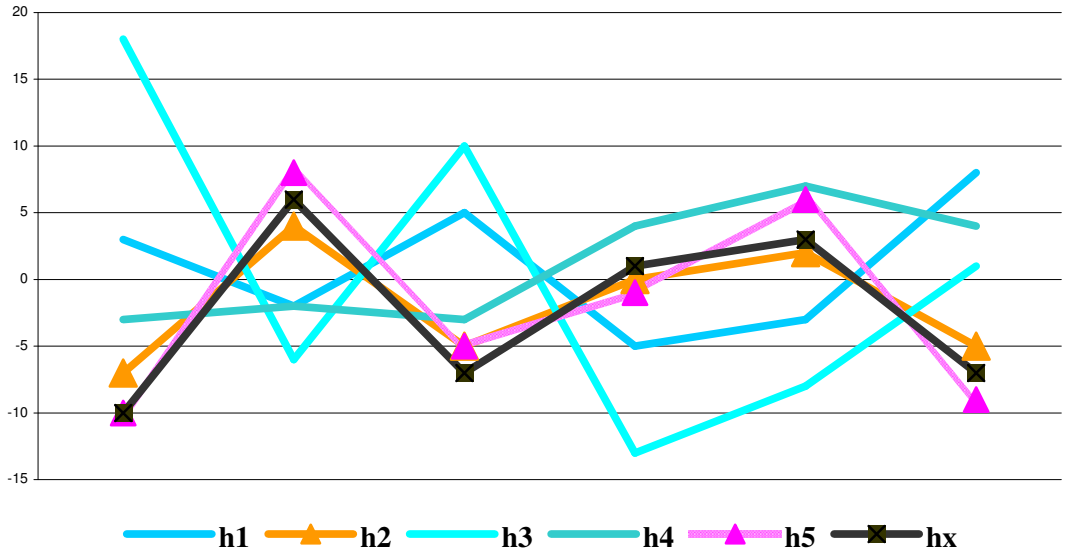

Fig. 3.4 Shape representation of six cell vectors

In this graphical representation, the y-coordinate corresponds to the *m* values and the x-coordinate corresponds to the corresponding m_i order number within shape *h*.

Next, apply the shape similarity function from Equation (3.27) to calculate distances between each shape and h^x using values from Table 3.3 above. Using the Manhattan distance we obtain the following results with the *sp* value shown in the last column on Table 3.4.

Table 3.4 Shape distances and similarity function values

			$\lvert m^x - m \rvert$				$sp(h^x, h_i)$
$d(h^x,h_1)$	13	8	12	6	6	15	60
$d(h^x,h_2)$	3	2	2	1	1	2	11
$d(h^x,h_3)$	28	12	17	14	11	8	90
$d(h^x,h_4)$	7	8	4	3	4	11	37
$d(h^x,h_5)$	0	2	2	2	3	2	11

As visually observed in the graphic of Fig. 3.4, the smallest *sp* values correspond to those were shapes h_2 and h_5 are involved, (represented by segments with small triangles

on its ends) meaning that the distances amongst these shapes are the smallest ones with respect to h^x.

Obviously distance measures between shapes applied in the new shape space, although similar, do not yield the same results as the corresponding cell distances applied in the original record space. This can be seen in next Table 3.5, where we show the result of applying Euclidean and Manhattan distances to cells from Table 3.2, and its comparison with shape distances after changing space values. As it was in Example 3.4, all distance calculations are from p^x to all other points.

Table 3.5 Distance comparison using selected criteria

Total distance values by criterion			
	Manhattan	Euclidean	Shapes
$d(p^x,p_1)$	51	549	60
$d(p^x,p_2)$	7	9	11
$d(p^x,p_3)$	58	758	90
$d(p^x,p_4)$	37	335	37
$d(p^x,p_5)$	14	42	11

As observed, in relative terms distance from p^2 to p^x is the smallest for the Euclidean and Manhattan distances. As for the shape distance, distances to p^2 and p^5 are equally the smallest from p^x as confirmed by its graphical shapes from Fig. 3.4. Using shapes as a classification criterion yields good results as indicated later in Table 6.2 from Section 6. As will be seen, its class prediction capabilities are better that those of using a standard distance for the same purpose, when applied to contending pre-selected close neighbour cells p^1 and p^2. We have no formal demonstration at this point for the reason for this. Intuitively we believe that additional inter-attribute relationship information, besides attribute value information makes this difference.

3.7 Searching for nearest cells

In this section we introduce the search mechanism done by Trie-Class to extract close neighbours with respect to some unknown instance. This is the first approach we use to determine similarity. A second approach will be done afterwards, where these pre-

selected cell patterns are carefully inspected through the use of Decision Parameters explained in Section 6.

Eventually, the number of close neighbours selected could be any. We have chosen to implement our algorithm for just two of them, and we have kept this number in view of our results.

The method we propose here to find nearest neighbours does not use the standard family of distances used by regular *k-NN* methods. It corresponds to a *"greedy"* search method in general, as the best solution at each point is taken using only available information at each node of the tree structure. To illustrate this, lets assume the existence of a new query cell p^x with format as in Equation (3.10). Lets call p^+ the ideal closest object to p^x in the entire dataset. The algorithm's task consists in extracting the closest cell to p^+ and as a result the algorithm will obtain a cell we call p^1

In the original *NN* algorithm this is done using a "brute force" method or some type of index, applying to them the Euclidean distance from p^x to considered objects. In our case distance calculation proceeds attribute by attribute, restricting the allowable search space for a given attribute based on previous attribute values. The allowable search space keeps cell component values in order, so the closest elements to p^x_i are searched starting at p^x_{i-1} and p^x_{i+1} respectively. The search proceeds to both "sides" of p^x_i looking for the closest element. As soon as one of these values is closer to p^x_i it is selected. Trie-Class uses a tree structure, which exactly allows doing this.

If we call cells p^1 and p^2 the two "closest" objects to p^x found in a space with those characteristics, then it will be always true that:

$$d(p^+, p^x) \leq d(p^1, p^x) \text{ and } d(p^+, p^x) \leq d(p^2, p^x)$$

We argue later in Section 7 that objects p^1 and p^2 are more rapidly extracted using this structure when compared with regular *NN* methods, and also that they are better class predictors. In the next subsections we explain the way this is done introducing a general search algorithm for a closest cell, which is the same independently of the number of cell patterns that might be extracted.

3.7.1 Selecting closest pattern

The algorithm extracts close cells one by one. In our case it first get cell p^1. To do this initially dispose of the entire set P as its search data space. The extraction of cell p^1 progress adding one more cell component at a time, where these cell components are the ones found closer to its corresponding p^x elements. As the search progresses, smaller and smaller subsets of P constitute the allowable search space to obtain the next cell component element. For each one of these P_i spaces its dimension and location is given by the values forming the corresponding sub-cell q^i. We explain next the way this space is defined.

The extraction of any cell is done attribute by attribute, with the algorithm proceeding incrementally. Any sub-cell q_i is of the form $q_i = <q_{i-1}, k>$ where k is the next cell component element. Starting with $i = 1$, assuming an empty sub-cell $q_0 = <\varnothing>$ and knowing element q_{i-1}, the problem consist in finding some interval k^1 representing the next cell component, which is the closest value to the unknown element k^x. The found element k^1 must satisfy the following property:

$$\forall k \in K\left(q_{i-1}^1\right) \bullet \left(\left|k^1 - k^x\right|\right) \leq \left(\left|k - k^x\right|\right) \tag{3.28}$$

Where the set $K(q^i)$ is defined by:

$$K\left(q^i\right) = \left\{k \mid < q^i, k > \in P_i\right\} \tag{3.29}$$

Cell component k^1 is the closest element to k^x among the elements in $K(q)$ and P_i correspond to its search space. As each new cell component element k^i is added, the search space for next element k^{1+1} is further restricted to the space defined by the previous sub-cell q_i which is P_i. So the search space of the last element gets confined to space P_n, thus avoiding the search of most of the total data space.

Notice that as it happens with decision trees, the selection of each new k element divides the space into axis-parallel hyper planes.

From the class viewpoint, as long as the search process does not reach the last cell component member, or sub-cell q_i is not associated with just one class, the selection of

the next k element does not impose a class restriction. What matters is to find each time the closest cell component element to the corresponding query element.

What happens if two k values are equidistant from k^x?

In this case frequencies are used as the first option to break this tie. Including frequency as part of the search criterion mechanism aims to avoid *outliers*[8]. It also helps avoiding *overfitting,* defined as the case of a hypothesis that fits the training data and exists another hypothesis that fits less well the same data which performs better over the entire distribution of instances [Mitchell, 1997].

Therefore, the algorithm chooses the k value where $freq(q^1)$ is maximum including the new potential element k. A larger frequency in this context is interpreted as an indication of a close distance, as done in some *k-NN* algorithms [Dasarathy, 1991].

After cell p^1 has been selected the algorithm proceeds searching for cell p^2. The search mechanism is the same as the one already described, except that this time set $K(q)$ has an additional restriction: all objects considered must belong to a class which must be different from the one in p^1.

Originally, cell p^1 with class say c_1 was extracted from some set R. As the class associated with p^1 cannot be in any other subsequent cell extracted p^2, p^3,.., p^n, we remove from the original set R all cells having class c_1. We call R_1 this new subset, which correspond to the complimentary search space where cell p^2 will be extracted. No cells with the class of the already extracted p^1 form part of this space. Follows that if subsequent cells were extracted after extracting p^2, the restricted space would become R_2, R_3,..,R_m, reducing each time the allowable search space, where R_m is the data space corresponding to the search space for cell pattern p^{m+1}.

This entire operation is equivalent to have training records belonging to the same class inserted in different trees and executing sequentially the search on each tree.

The following definition represent the above described search process.

Definition 25.

We define function *neighbours()* as the function that returns two cells p^1 and p^2 representing the closest neighbours found with respect to some unknown cell p^x using the search process already described.

$$(p^1, p^2) = neighbours(p^x) \quad \textbf{(3.30)}$$

It is worth noticing the fact that restricting search spaces starting from the first attribute is equivalent to give more eliminatory power to more relevant attributes. Search spaces allowed for less relevant attributes are restricted. As a *greedy* search selects the best path based solely on tree node information, more precise solutions could be lost. And in this sense, relevant attributes do not have more weight in this process but just the power to eliminate some options.

3.7.2 Using look-ahead to solve ties in cell pattern selection

It is known that greedy search produces sub-optimal solutions [Goodman et al., 1988]. In view of cheap available computing power, is worth trying to improve these solutions without much extra algorithmic complexity. For this reason, if frequencies in candidate cell component elements are also equal, the algorithm applies a *'look ahead'* mechanism. This consists in looking for next closest element k^{i+1} on each conflicting sub-cell with k^i as the next potential component. The process is repeated until is found some component is closer to the respective k^x_j component, or until the end of the cell is reached. When such element is found along this path, the algorithm chose it as the new component element, along with all k values in the path all the way up to the conflicting parent component k^i.

Using this type of limited look-ahead search although it produces an increase on algorithmic complexity, it is controlled by the fact that it is only applied as a last resource to solve tie situations. However, in datasets with larger intervals where chances of equal sub-cells increase, execution times will increase. In general, our results show that limited look-ahead as the one used here produced acceptable execution times.

As a last resort, if ties persist and the last cell component has been reached, the algorithm chooses arbitrarily one of the conflicting k values as the new component. At the end of this process, any selected full cell close to p^x is associated with just one class.

Trie-Class never fails to find an identical full cell to p^x, if such cell exists in the training file as the search process for the next bigger and smaller values with respect to

[8] See subsection 3.9.1

p^x for each attribute begins with this value. In this special case, if cell p^1 equals p^x, the search algorithm stops looking for other close cells. It simply assigns the class of the identical pattern found to p^x. This also means that running against training records, Trie-Class classifies without errors.

3.7.3 The search algorithm in practice

Example 3.6

Lets assume the existence of a dataset with the following five cell patterns:

Table 3.6 Original search space *P* containing 5 cells and a new query

cell	v^1	v^2	v^3	v^4	v^5	v^6	v^7	class
p^2	3	1	1	1	3	2	1	A
p^1	3	1	1	2	1	1	3	A
p^4	3	1	1	2	5	6	9	B
p^5	3	5	3	4	1	2	1	A
p^3	8	5	4	7	9	6	3	B
p^x	4	3	2	5	3	1	5	?

The last row contains the unknown cell p^x. In order to search for the closest cell to p^x, the algorithm proceeds as follows:

Set $q^1 = <\varnothing>$
Search for the closest value to $p^x{}_1 = 4$. The algorithm finds values 3 and 8. Value 3 is selected after comparison. Incorporate value, so $q^1 = <3>$.
Next, look for next elements closest to $p^x{}_2 = 3$. Elements 1 and 5 are found, which are equidistant. So we use the *frequency* criterion. Sub-cell <3,1> has larger frequency than sub-cell <3,5>. Therefore, insert new cell component giving $q^1 = <3,1>$
Repeat the process looking for closer element to target $p^x{}_3 = 2$ among v^3 values.
The only available option is again 1. After insertion we have $q^1 = <3,1,1>$.
The closest elements to $q^x{}_4 = 5$ is 2 so $q^1 = <3,1,1,2>$.
At this stage there are two possible candidate elements: $p^1{}_5 = 1$ and $p^4{}_5 = 5$. Both are equidistant from $q^x{}_5 = 3$ (a distance of 2 units). Which one to chose?
As frequency is equal in both conflicting sub-cells apply *look ahead* technique.
Then look into each of corresponding 6th elements, $p^1{}_6 = 1$ and $p^4{}_6 = 6$.
Calculate distances between them and chose the closest one. As $d(p^x{}_6, p^1{}_6) = 0$ then this element is chosen and also its parent. So now $q^1 = <3,1,1,2,1,1>$.

Get the last element. There is only one member available $p^1{}_7 = 3$. After insertion the final sub-cell extracted is $q^1 = <3,1,1,2,1,1,3>$, which corresponds to the full cell p^1. Finally, As the class of cell p^1 = A, this will be assigned to the new cell p^x.

Fig. 3.5 Searching for close neighbours

Table 3.7 in next Section compares the efficiency in classification between cell pattern p^1 against the equivalent *k-NN* version implemented by the Weka benchmark [Witten, et al., 2000].

3.8 Extraction of p^1 is an efficient alternative to regular *k-NN* methods.

We have already explained *k-NN* methods for classification of new objects of unknown class. We have also explained in Section 3.7.1 the alternative method of extraction of a close pattern represented by the extraction of cell p^1. We believe this alternative method is faster and at least as good as the regular *k-NN* methods, when these use only one close neighbour as pattern model for classification. To support our argument we present next a table to compare classification error rates and execution time when using for classification cell pattern p^1 and the pattern extracted using *IBk*, the k-nearest neighbour implementation done by Weka. This classifier use the Euclidean distance, which is normalized in order to equally treat attributes with different domains, thus controlling the influence they would have in the final distance value. Normalization is done using the known formula:

$$a_i = \frac{v_i - \min(v_i)}{\max(v_i) - \min(v_i)}$$

Variable v_i is the value of attribute *i,* and the maximum and minimum are taken over all instances in the training set [Witten et al., 2000]. Recall that in Equation (3.8) we do a similar normalization at the time we fit the value of an attribute into its corresponding interval. Algorithm *IBk* applies distances to symbolic or nominal attributes according with the Heterogeneous Euclidean Overlap Metric (HEOM) described in Section 4.2.

For the sake of our comparison, all tests with *IBk* were done using one nearest neighbour (k = 1) so no weight requires to be done with distances. As the time taken to

classify a test instance increases linearly with the number of training instances that are kept in the classifier, sometimes is required to restrict this number, which in Weka is done by setting up a window size option.

In our case this option has not been used. Instead, and for both algorithms we do a dataset split of 60% of records for training and 40% for test.

Table 3.7 Classification error rates comparing p^1 and *IBk* algorithm

Dataset			% Error		Difference	Time (s)[9]		Difference
Nº	recs.test	Name	p^1 Trie-Class	IBk Weka	%	p^1 Trie-Class	IBk	seconds
1	17637	Adult	18.3	21.2	2.9	309	4080	3771
2	360	Annealing	2.3	1.4	-0.9	45	4	-41
3	280	Breast-cancer-W	5.5	4.6	-0.9	1	1	0
4	144	Dermatology	7.5	6.3	-1.2	2	1	-1
5	308	Pima Diabetes	24.0	29.5	5.5	2	1	-1
6	21556	Forest cover	24.9	11.7	-13.2	2400	6600	4200
7	122	Heart disease Cl.	30	22.1	-7.9	1	1	0
8	108	Heart Statlog	22.4	27.8	5.4	1	1	0
9	1509	Hypothyroid	1.0	9.7	8.74	30	60	30
10	60	Iris	2.4	5.0	2.6	1	1	0
11	4397	Pendigits	2.3	0.8	-1.5	120	348	228
12	1774	Satimage	12.0	18.4	6.4	25	33	8
13	400	German credit	27.4	27.5	0.1	3	3	0
Average gain of p^1 in error rates and execution time					6.0			8194

All execution times are expressed in seconds[10]. In the case of *IBk* figures comes from the tool itself. As can be seen in Table 3.7, on thirteen datasets Trie-Class is on average 6% better and it took over two hours less time to execute than *IBk*. Error figures for *IBk* are less good if we compared with those obtained doing 10-fold cross-validation from Table 5.15. As the execution time goes up, Trie-Class executes better than *IBk*. Initially Trie-Class is better in 7 out of 13 cases, which represents 54% of cases. When execution time goes over 15 seconds, Trie-Class is better in 71% of cases and this percentage further increases to 75% for the case of datasets where the running time took more than 25 seconds. In other words, as complexity goes up, Trie-Class almost constant search procedure shows its value. In datasets Adult, Forest cover and Pendigits, execution time

[9] Wall clock time measured as running time in a standard PC with a single process running.

took over 2 minutes. In all of them *IBk* takes at least 3 times more execution time than Trie-Class.

Trie-Class classification error increases using only p^1 as the sole criterion for classification when compared with figures using the full algorithm, as will be show in Table 5.15 on Section 5.

3.9 General assumptions on some basic Principles

In this thesis, we adopt assumptions on data, which follow some general accepted principles. We enumerate and briefly explain each one of them.

3.9.1 Data consistency

A basic assumption in this thesis is that the overwhelming majority of instances in *N* are consistent, i.e. each unique cell vector gets associated with only one class, which is a standard assumption as found in [Everitt, 1981;Titterington, 1985; Cios, 1998; Quinlan, 1996].

All training cells where *nlabels(p)* > 1 represent two or more cells with identical cell component values, but with different class. Therefore these cell patterns provide no information class-wise. The cause for this might be that at least one of these cells constitute *noise*, which corresponds to instances for which either the class label is incorrect, some number of the attribute values are incorrect or a combination of the two [Brodley, 1995]. In some other cases *noise* data can correspond to a type of data called *outliers*, data items lying very far from the main body of the data [Kaski, 1997].

In any case, conflicting cells still are located within the same area in the n^{th}-dimensional data space. This brings us back to the basic assumption of the nearest neighbour paradigm: instances that are close to each other will have similar posterior class probabilities [Dasarathy, 1991]. For this reason, in these cases Trie-Class eliminate from the search the identical conflicting cells looking for the next close cell pattern in the same area.

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[10] Trie-Class is implemented in C, not in Java as Weka, So part of time differences can be attached to this factor.

3.9.2 Partition granularity

As we will explain in Section 4, Trie-Class pre-process data before tree building, in such a way that independently of the data type of attributes, their values are discretized. Discretization is the process by which the domain of a continuous attribute is partitioned into a finite number of intervals. This discretization is done using Equations (3.7), (3.8) and (3.9).

In general, small numeric attributes domain, whether discrete or continuous are not discretized at all and the corresponding unit of the domain is used as a default partition, as in Trie-Class this is more a data structure requirement rather than a step in the classification process itself.

In any case, for any cell $p \in P$ we assume that the granularity of all partitions generated by the discretization process is such, that allows every cell in the training set to have a known label, making function $nlabels(p) = 1$.

3.9.3 Class membership, Patterns and the Continuity Principle

Which is the spatial class distribution of object in Supervised Learning?

Are similar classes distributed into continuous areas in that space or rather they are scattered throughout that space at random?

Intuitively, one might think that class distribution in real data tend to be characterized by continuity, meaning that there exists some correlation between attribute values and its mapping to classes, and therefore there are data areas of continuous class distribution. Many classification algorithms compress the feature space based on the certainty that just a few attributes bear the key to class membership. If this is the case, then class distribution indeed presents spatial continuity.

We apply this principle to rather small regions of the dimensional R space covered by cells of the same class. If a new cell of unknown class falls into one of these regions, and existing training cells of the same class are located at distances representing upper and lower boundary values with respect to the unknown object, then we assume that its class is the same as the one hold by cells in that neighbour area.

In Trie-Class specifically we apply this principle to sub-cells q as defined in Equation (3.12).

For instance, lets suppose the existence of sub-cells: $<q_{i-1}, k_1> \in P$ and $<q_{i-1}, k_2> \in P$

Applying function labels from Equation (3.17) to sub-cells we obtain:

$labels(<q_{i-1}, k_1>) = \{c\}$ and $labels(<q_{i-1}, k_2>) = \{c\}$ then, for a new interval $k \in [k1,k2]$ $labels(<q_{i-1}, k>) = \{c\}$

Thus, in interval k sub-cells will also exhibit class c. This criterion is applied in Trie-Class for all spatial areas with no available pattern information provided that cells with the same class bound those regions. In that sense, every other possible new query cell p^x is always approximated to some of the existing classes in the dataset.

4 Pre-processing Data Before Mining

The task of extracting knowledge cannot even begin without preparing data to fulfil the requirements of a particular mining algorithm.

Preparation time taken before mining data represents a considerable portion of the whole knowledge extraction process. This fact is often overlooked by researchers fighting for a split second of execution time, forgetting the hours if not days spent in the preparation of data. For a given algorithm, the number of tasks involved in pre-processing data is independent of the size of the database. In any case, the farther apart the data format is with respect to the needs of the algorithm, the longer the time it takes to complete pre-processing it.

Preparation time must not only be considered as the manipulation of data itself, but as their overall comprehension and meaning. Before anything else we have to know about data characteristics and its representation, including type of variables and their meaning, the type of noise and missing data which we might expect, information about the classes and its distribution, the frequency of updates and the cost of misclassification among others. But most important of all, we definitely have to know the purpose of the data owner, and the exact notion of the problem he/she wants to solve. This is fundamental, if we are planning to make any sense out of data.

In the rest of this section, we explain the data preparation needed prior to tree construction and execution including sample selection, attribute value discretization, the treatment of categorical attributes, attribute selection and the effects of changing interval size after discretization.

4.1 Converting records into discretized patterns

Attribute values belong to one of several data types: qualitative or non-numerical (symbolic, linguistic), quantitative or numerical (continuous, discrete). Because our classification algorithm and the ranking of attributes are based in a nominal space, all continuous attributes are first discretized. This is done, based on the information taken from a user-supplied dictionary file[11].

11 For a layout of the dictionary, see Annex I.

Discretization is the process of partitioning the domain of a continuous attribute into a finite number of intervals [Lebowitz, 1985].

There are three criteria to classify discretization methods: global vs. local, supervised vs. unsupervised, and static vs. dynamic [Dougherty, 1995]. Numerous discretization methods used to induce one-level decision trees and instance-based methods utilize the class label in the partitioning of the data space [Payne, 1998]. Others use domain specific information [Lebowitz, 1985; Aha, 1995]. Still in some other cases the discretization process consider the number of instances in the interval [Cattlet, 1991]. We use the *Equal Interval Width* (EIW) single feature discretization method (sometimes called *binning*) [Wong et al., 1987], which do not make use of instance classes in the discretization process. For this reason sometimes it is called unsupervised discretization method.

Intervals are represented by discrete integers using the symbol $s_{i,}$ which corresponds to the number of intervals within a given domain. Function *ord()* described in (3.8) does this conversion. Notice that when *ai* and m_i are equal, v_i equals zero, which corresponds to the first possible interval value. The number of intervals obtained on each partition, are given by Equation in (3.7). For attributes represented by rational numbers the corresponding interval value is calculated according to Equation (3.8). For categorical attributes this simply corresponds to its ordinal value, as described in Equation (3.9).

If *a priori* knowledge on domain information exists on the actual order of symbolic attributes, as done in some discretization methods [Kerber, 1992], then the interval value represents the corresponding order number, which is set in the dictionary (see Appendix I). Next section specifically deals with symbolic attributes. If this information does not exist, one has to be careful of not imposing any order on these values. In [Brodley, 1995a], when a feature has more than two observed values, then each feature-value pair can be mapped to a prepositional feature, which becomes true if and only if the feature has the particular value in the instance. We explain in Section 4.2 the distance between two unordered symbolic values done in Trie-Class.

It could be argued that using binning as discretization method causes us to lose information about the class distribution in the n^{th} dimensional space. This effect is even more negative, in methods where discretization is done with the purpose of identifying class membership, using the so-called *impurity or goodness measures*. [Murthy et al.,

1994]. The goal of most of these methods is to use discretization as an important component of the classification model. Some examples of these methods are *Gini Index* criterion [Breiman et al., 1984], *Minimum Description Length* [Rissanen, 1978], *information gain* [Quinlan, 1986], *ChiMerge* system [Kerber, 1992], *recursive entropy discretization* [Fayyad et al., 1993], *Max minority* [Heath et al., 1993], *maximal marginal entropy* [Chmielewski et al, 1994], S*tatDisc* [Richeldi et al., 1995].

Although inferior to the entropy family of methods as shown in [Fayyad et al., 1993], the difference in performance between equal width discretization and some of these methods is small [Dougherty et al., 1995].

Other than the simplicity and lower computational cost of this method our goal with discretization has to do with storing training records in an index of manageable size, in order to increase searching efficiency, as long as the number of partitions is representative of the concept description. Partitioning attribute domains into s_i intervals helps reducing tree size as well as in some cases allowing concept generalization. The well-known loss of information problem derived from discretization is attenuated in our case. The most important information for each sub-cell individually considered is its class. With this respect, the only negative effect of this is class overlapping, which has the net effect of postponing class membership in sub-cells as they increase their size of component members.

As additional help to attenuate some loss of information due to discretization, we keep class distribution information for *semi exclusive* values in a specific file as explained later on Section 7.

It has also being related the equal width binning mechanism to a higher sensibility to outliers [Dougherty, 1995]. To help with this, semi-exclusive intervals can be tuned setting parameter φ in Equation (3.22) to a somewhat larger threshold value.

4.2 The special case of categorical attributes

Many Machine Learning and Pattern Recognition methods require that input take the form of numeric values. As Trie-Class uses a distance calculation for the extraction of near neighbours to some unknown cell p^x, the presence of *symbolic* attribute types represent a problem of its own. Symbolic values are values representing concepts that cannot be ordered, and therefore, there is not an obvious distance between them. This is

the case for instance for the letters of the alphabet, or concepts such as "*red*", *"white"* and *"blue"* (provided we do not consider their wave length values of course). Near neighbours methods resort to special metric schemes to solve the similarity problem in these cases, a problem central to pattern matching.

Many methods have been proposed in the literature to overcome this problem, such as the Value Difference Metric (VDM) from [Stanfill, 1986], counting the features that match as in [Towel, 1990], the PEBLS system that incorporate MVDM, a modified version of VDM in [Cost, 1993]; the basic idea of the later being that two values of the same attribute are similar if they give similar likelihood for all possible classifications. Also, the Heterogeneous Euclidean Overlap Metric (HEOM) which basically attributes binary values to distances depending whether two values of the same attribute are equal or not equal, the Minimum Risk Metric (MRM) which directly minimizes the risk of misclassification using conditional probabilities [Blanzieri, 1999].

In many cases applications symbolic attributes appear along with continuous attributes. For this reason it is used a heterogeneous distance function, as is the case with the software IB1, IB2 and IB3 [Aha et al., 1991; 1992] as well as the one used in [Giraud-Carrier et al., 1995]. This function defines the distance between two values *x* and *y* of a given attribute *a* as:

$$d_a(x,y) = \begin{cases} 1, & \textit{if x or y is unknown, else} \\ \textit{overlap(x,y) if a is nominal, else} \\ \textit{rn\_diff}_a(x,y) \end{cases} \qquad \textbf{(4.1)}$$

When any of the attributes is unknown a maximal distance of 1 is returned.

The *overlap* function is defined as:

$$\textit{overlap}(x,y) = \begin{cases} 0, & \textit{if } x = y \\ 1, \textit{otherwise} \end{cases} \qquad \textbf{(4.2)}$$

and the range-normalized difference *rn_diff* is defined as:

$$rn\_diff_a(x,y) = \frac{|x-y|}{max_a - \min_a} \quad \textbf{(4.3)}$$

Where max_a and min_a are the maximum and minimum values respectively observed in the training set for attribute a. The normalization serves to scale the attribute down to the point where differences are most of the time less than one.

Overall, Trie-Class uses a heterogeneous distance calculation. The first one explained in Section 3.7 search cell patterns close to the unknown cell p^x. The second one used within the context of decision parameters, use a straightforward distance calculation when comparing two already pre-selected cell patterns, which will be shown in Section 6.1.2.

For the case of symbolic attributes, Trie-Class uses a simple distance calculation. It is based on conditional probabilities in order to determine the distance between categorical attributes. As it was explained in Section 3.7, for the ith attribute belonging to the unknown sub-cell $q^x = <q^x_{i-1}, q^x_i>$, the problem consist in determining whether element q^x_i is closer to element k^1 or element k^2 both belonging to the set of sub-cells $p = <q_{i-1}, k>$.

If q^x presents the same value of some existing element k, then distance is zero and element k is selected. If not, Trie-Class uses the distance computation that we explain next.

Definition 26. The distance between two categorical attributes v^x and v^i given the class c of v^i, depends on the probability of class c given value v^x.

$$d(v^x, v^i) = \begin{cases} 0, \ if\ v^x = v^i, else \\ 1 - P\left(c_i \mid v^x\right) \mid label\left(v^i\right) = c\ , c_i, c \in L, v^x, v^i \in s_i \end{cases} \quad \textbf{(4.4)}$$

Expression P(c | v) expresses the conditional probability of class c given value v^x and it is calculated as the prior probability of c times the joint probability of c and v:

$$P(c,v) = P(c) \bullet P(c \cap v) \quad \textbf{(4.5)}$$

The meaning of this distance calculation is simple: the larger the probability that v^x is associated to the class of v^i, the shorter the distance between them. When this

probability is zero, the distance is a maximum, i.e., equal to one. If the probability is the maximum then distance is zero.

As can be seen, this distance depends on the Prior Probability of a given class, represented as $P(c)$, and the joint probability of value v^x and the class associated with value v^i.

When comparing distances $d(q^x, k^1|c_1)$ and $d(q^x, k^2|c_2)$ where c_1 and c_2 represent the known classes of k^1 and k^2, the distance calculation is indirectly calculated and restricted only to the correlation of q^x against classes c_1 and c_2.

The intuition behind this is simple. When choosing the next closest element for sub-pattern q^x, the only reference is the class associated with each of the two contending members. Therefore, the "closest" neighbour will be the one where its class correspond to the class that q^x also better relates.

When the label associated with v^i is unknown and $labels(q^i) > 1$, Trie-Class resort to one of the options of the general search case, which were described in Section 3.7. In all other cases the algorithm uses Equation (4.1). This mechanism works better than the simple overlap idea of Equation (4.4).

We tested for this effect datasets *Adult, Annealing, German credit* and *Census,* which contain an important number of symbolic attributes. Classification performance when considering distance as decision parameter did improve on average over 2.5% when compared with the simple overlap distance for the same datasets.

Next we show a simple example of distance calculation for symbolic attributes as done by Trie-Class.

Example 4.1

Suppose a dataset formed by multidimensional attribute vectors, and attribute A_i is symbolic and its domain set consisting of A_i = {v_1= "*blue", v* $_2$ = *"red", v* $_3$ = *"yellow"* }. The set of available classes in this dataset is L = {c_1 = "A", c_2 = "B", c_3 = "C"}. Table 4.1 below shows prior class probabilities hypotheses and also joint probabilities for each class given the value. These data was compiled using training set data.

Imagine we are given a new query value for sub-cell q_x = (v_3 = *yellow, c = ?*) with unknown class. Using the search process Trie-Class comes up with two possibilities as

the nearest sub-cells: $q_1 = (v_1 = blue, c_1)$, and $q_2 = (v_2 = red, c_2)$. The problem consist to know whether value *yellow* is closer to value *blue* or *red*, i.e., whether distance $d_1(v_3,v_1)$ is greater or smaller than distance $d_2(v_3,v_2)$.

Table 4.1 Class distributions by value for a symbolic attribute

Categorical values		Class hypotheses			
		c_1	c_2	c_3	
Prior class hypotheses	$P(c)$	0.50	0.30	0.20	1.0
v_1=blue		0.40	0.30	0.25	
v_2=red	$P(c \cap v)$	0.24	0.04	0.45	
v_3=yellow		0.36	0.66	0.30	
Class probability		1.00	1.00	1.00	

Using values from Table 4.1 and applying Equation (4.1) we obtain the following results:

$$d_1(v_3, v_1) = (1 - 0.18) = 0.820 \text{ and } d_2(v_3, v_2) = (1 - 0.198) = 0.802.$$

So $d_1(v_3, v_1) > d_2(v_3, v_2)$, value *yellow* is closer to value *red* than to value *blue*. Thus, there is a greater likelihood that the class corresponding to value *yellow* is c_2, which is the class associated with value *red*.

4.3 Feature reduction and elimination

Data Mining techniques face the challenge represented by the so-called *dimensionality* problem. Often, data is represented by datasets containing N instances each of them formed by n features or attributes. Sometimes know as multivariate data, it can be thought of as a $(N \times n)$ data matrix. The dimensionality n plays a significant role in multivariate modelling. In text classification problems, web traffic, commercial supermarket transactions or clustering of gene expression data, n can be as large as 10^3 or 10^4 dimensions and the amount of data needed according to density estimation theory scales exponentially in n. This is the so-called "*curse of dimensionality*" problem. Fortunately, transaction data is typically sparse, meaning that only a small percentage of the entries in the $N \times n$ matrix are nonzero. Taking advantage of this, the idea of using subsets of items or *itemsets* has been developed in market basket analysis, which

represent "*information nuggets*" in large high-dimensional transaction datasets. Finding frequent *itemsets* from a sparse set of transaction data is one solution for the problem as studied by [Agrawal, 1993] and more recently in [Han, 2001].

Not only the number of attributes poses a formidable complexity problem but also the fact that, not all attributes contribute equally to solve classification problems.

Within this context, two well-known problems arise when using decision tree structures and instance-based algorithms for supervised learning, which are of interest to us. Firstly, the attribute's input order heavily determines the predicting skills of the algorithm. The reason for this is that some attributes have more discrimination power than others predicting the right class for the unknown instance. Choosing the wrong order of attributes could move values apart in the hyperspace that otherwise would be closer. For instance imagine than in a tree, the fifth attribute is the one with a larger statistical correlation with a given class in the dataset under analysis. Two records with identical values for attribute five, but having different values in the previous four attributes would end quite distantly from each other in the hyperspace, misleading the classification algorithm. For this reason, at input time when building the tree we want attributes ordered by their discriminatory power with respect to class labels, as done for instance in some rule induction algorithms [Quinlan, 1986] [Cover, 1967], [De Mántaras, 1991].

Secondly, the presence of irrelevant attributes increases computational cost and can mislead distance metrics calculations [Indyk, 2000]. This is particularly true for nearest neighbour algorithms, which determine the class label of an unknown instance using the geometric concept of proximity, which involves the notion of distance between points in a n-dimensional space [Lee et al., 1984]. As the position of the instance is defined by the value of its attributes, if these are not relevant, then the basic assumption is violated.

Based on these, attributes are characterized as *relevant* or *irrelevant*, in terms of their degree of contribution to the classification hypothesis [Kohavi, 1997; Lebowitz, 1985][12].

The complexity of feature selection algorithms is related among other factors to the number and quality of attributes. Searching most relevant attributes cannot be exhaustive in many cases. The dimension of datasets is exponential in the number of

[12] These authors still identify *redundant* attributes, a situation which we do not address here.

attributes. Hence, verifying every other possible combination of best attributes is, in many cases, out of the question [Lesh, 1998].

In this section we present a low computational and simple empirical algorithm for the supervised learning task in order to:

- Establish a criterion to decide which attributes are relevant.
- Choose the best attribute input order for processing.
- To diminish classification algorithm complexity, as well as increasing or at least preserving its predictive skills.

4.3.1 Ordering attributes

In general, our method ranks attributes by its capacity of predicting classes as in [Gennari et al., 1989]. We measure this capability without directly taking directly into consideration other attributes from the original sequence. Indirectly, inter-attribute relationship exists; attribute values are not independent from the value of other attributes in a given pattern, as is the case in most real life cell vectors.

We postulate that this capacity of influencing class prediction increases, when a given attribute interval shows a significant frequency of values fully or predominantly associated with one class as defined in Equation (3.22). In this sense, we soften the Boolean definition found in [Kohavi et al., 1997].

How and how much significant the frequency of these type of patterns in a given interval should be, and the way it could be used as a measure for attribute relevance is the topic of the next sub-section.

4.3.2 Looking at sub-cells from the "clearest" viewpoint

Our objective is to find the most useful discriminative attributes with the purpose of improving the classifier prediction accuracy [Guyon, 2001]. This heuristic criterion has been used successfully before [Liu et al., 2000].

We have already stated in Section 3 that strong sub-cells with small values for i (shorter sub-cells) where $nlabels(q_i) = 1$, represent large areas of the data space related to one class. If a new instance to be classified falls into one of these areas, its chances of correct classification increase. Most of its neighbours will share the same label. For this

reason, we are interested in looking at the entire data space from the viewpoint of attributes with larger number of examples where classes are *"visible"* directly from them. Using this simple criterion would avoid endless combination of possibilities as done in traditional attribute selection methods [Miller, 1990; Brodley et al., 1995; Kohavi et al., 1997] among others.

In any dataset *R*, visibility relates to the problem of looking at the data space from the viewpoint that allows a better view to existing classes. Take for instance the well-known example of looking at four numbered tennis balls suspended in a three-dimensional space as shown in Fig. 4.1. Suppose that the objective of the viewer is to be able to distinguish the tennis ball numbers. Looking at that space from different angles represented by the three bulb lights in Fig. 4.1, more or less ball numbers are distinguish. *All solutions lie in the hyperspace. Our problem consists in finding them*[13]. We consider being more *relevant* attributes allowing a better *view* of larger number of sub-cells in terms of class membership. On Fig. 4.1, the view from "A" is the only one that allows full visibility of the 4 ball numbers. This is the most interesting view if the goal was to discover as much ball numbers as we could.

The shortest sub-cell contains only one component element is $q_1 = <p_1, c>$. If it does relate to one class only, it means that larger areas of the hyperspace relate also to one class label. And by the principle of continuity the probability of correctly classifying new instances falling into these intervals also increase.

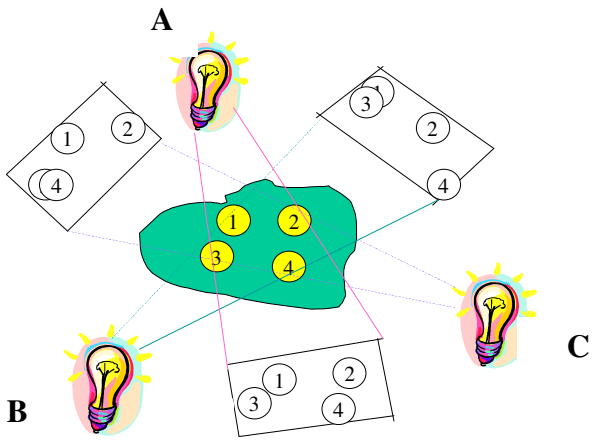


Fig. 4.1 Different views on the same set of solutions

To identify better views on the data space from the viewpoint of an attribute all of its values are projected into a one-dimensional discretized space, as was shown in Fig. 3.1. This corresponds to build the root node of a multi-way tree using one attribute. This resembles the *1R* classification system [Holte, 1993] although in this system the ranking of features is based directly on error rates using each individual attribute as the sole classification hypothesis. In our case we are interested in the total number of sub-cells components found in *semi-exclusive intervals* define in Equation (3.22), for a given attribute A_i and φ values. Attributes showing more individual cells in *semi-exclusive intervals* are also more *relevant* as calculated by variable δ defined in Equation (3.24). The intuition behind this is that trees formed using these attributes in top levels will produce larger data areas associated with one class, helping to define early class membership in the data hyperspace. Based on this, we can set attribute relevance as a measure allowing attribute comparison as explained in the next section.

To avoid the effect of *outliers,* in the form of few cells laying in one interval related to one class, a minimum number of records in one semi-exclusive interval can be set as a constrain in Equation (3.22). For instance, [Holte, 1993] used 3 and 6 as minimum existing values on his tests.

4.3.3 Reducing attribute numbers

Ranking attributes is done according with attributes relevance as we already explained in Section 3.5. As we will show in our results (Section 5), doing this improves the predictive accuracy of the classification algorithm.

Reducing the number of irrelevant attributes drastically reduces the running time of a learning algorithm and yields a more general concept, easier to understand by the domain expert. This reduction though, cannot be done without a cost. The trade-off is done at the expense of losing some predictive accuracy. With this constrain in mind, our goal is *to find a minimum subset of attributes S' such that when the classification algorithm is applied accepting some error ε, we can obtain a new predictive accuracy* T' as expressed in Equation (4.6) on next page.

[13] Thanks to Prof. Rafael Martinez from US/LSI for this remark.

$$S' \subset S, \text{ that satisfies } T' \leq T + \varepsilon . \quad \textbf{(4.6)}$$

This new set S' obtained from original list β in Equation (3.25) will include only *relevant* attributes discarding all others provided the accepted error ε is respected. The classification algorithm rebuilds the tree using the new sequence in S'. At running time, and using some user-user-defined error over the existing prediction value T a new T' value is obtained. Error ε is a function of cost and quality [Brodley, 1995]. If Equation (4.6) is satisfied and $(T' - T) \leq \varepsilon$, then S' is adopted as the new set of attributes. Otherwise, threshold value φ should be reduced and list β rebuilt. As a result this will increase the number of attributes in subset S' and hopefully will also increase prediction accuracy T' diminishing ε.

Tables 4.2 and 4.3 show the effect of both attribute ordering and reduction and the corresponding gain or loss in accuracy. In column (A) of Table 4.2 we show the new order of attributes for each dataset after applying our ordering process. Relevant

Table 4.2 Average attribute reductions after compression

Nº	Number Attrib.	Dataset	N. º Records		(A) New Attribute Order Number represents original ordinal number (**Bold face** = attribute is *relevant*)	(B) Relevant Attributes (%)
			Training	Test		
1	24	Hypothyroid	1598	1063	**18,23,21,1,20,22,7,5,13,24**,19,17,16,15,14, 12,11,10,9,8,6,4,3	41.7
2	24	Dermatology	218	140	**20,22,27,29,6,12,8,25,33,34,24,15,10,31,26**, **30,14,23,7,**32,28,21,19,18,17,16,13,11,9,5,4, 3,2,1	57.6
3	33	Adult	28468	15060	**3,9,14,2,4,5,7,8,13,6**,1,10,11,12	71.4
4	13	Diabetes	462	306	**5,6,2,7,4,8**,3,1	75.0
5	12	Forest covert	15120	565892	**1,10,5,6,4,12,8,7,9,3**,11,2	83.3
6	12	Pendigits	7494	3498	**6,12,3,7,11,4,2,15,5,14,16,8,1,10**,9,13	87.5
7	16	Cancer–W.	407	273	**7,2,1,8,3,9,4,6,5**	100.0
Average number of relevant attributes after reduction						73.8

attributes are indicated in bold. The reduction rate in the number of attributes is shown in column (B). On average, over a quarter of the number of attributes are found to be irrelevant and could be eliminated, thus decreasing algorithm complexity and consequently execution time and storage.

Next in Table 4.3 we show a clear improvement in classification accuracy results after attribute ordering. The table shows error rates produced when using the original order of attributes (A), results when attributes are ordered (B) and results for the case when only relevant attributes were used (C).

We observe a decrease in error rate in all seven cases. The average decrease in error rate of 4.3% in Table 4.3 is similar to results for different datasets where this technique was applied previously reported in [Serendero et al., 2001].

As for attribute reduction, although not conclusive due to experiment size, variation in error rate is 3% greater after attribute reduction (C-B). This fact seems related to the intensity of attribute *'pruning* '' (see Table 4.2).

Nevertheless, in 43% of cases, reducing the number of attributes increases predictive accuracy, meaning that our algorithm to determine attribute relevance works well. Attributes at the list's end are indeed irrelevant for predictive purposes

In general, these figures confirm that gain in predictive accuracy is significant and steady when applied to different data domains. It also confirms the generally accepted need for ordering attributes when tree structures and instance-based methods are used.

Table 4.3 Variation in predictive error rate after ordering and reduction in the number of attributes

		Classification Error Rates (%)			Absolute (%) variation due to:	
Nº	Datasets	Original (A)	Ordered (B)	Reduced(C)	Order (B-A)	Reduction (C-B)
1	Forest covert	28.2	20.5	23.9	-7.7	+3.4
2	Dermatology	10.2	4.5	6.5	-5.7	+2.0
3	Diabetes	27.8	22.2	22.5	-5.6	+0.3
4	Pendigits	9.3	5.3	2.0	-4.0	-3.3
5	Cancer –W.	5.5	2.2	1.8	-3.3	+0.4
6	Adult	18.9	16.0	10.6	-2.9	-5.4
7	Hypothyroid	1.6	0.7	1.1	-0.9	-0.4
				Average	-4.3	-3.0

As expected, a large reduction in the number of attributes results in greater error rates although this could be user controlled by reducing attributes up to a maxim error value ε accepted as stated in Equation (4.4). In the face of large datasets with high dimensions where traditional feature reduction methods represent very high computational costs, this method can be a fair solution.

5 Evaluation and Results

In this section, we present experiments to support the claim that Trie-Class compares favourably over a wide variety of induction algorithms tested on various data domains. We performed classification experiments with Trie-Class on several datasets and compared them against other classifiers in terms of accuracy and error figures, as we did in [Serendero et al., 2001 and 2003]. Additionally we use the well-known tool bench "WEKA" [Witten et al., 2000] to test selected typical classifiers running on our own hardware. The selection of classification tools used for testing is rather arbitrary and it was done with the purpose of offering a comparison with the most typical and different techniques.

In presenting our results form these two different sources we use the same datasets. These datasets include from 2 to 10 classes, from 150 to half a million instances of available data and from four up to 56 attributes. All types of data can be found in these datasets, from discrete to symbolic, thus being somehow representative of the many available existing data for research in the public domain. Datasets used for testing Trie-Class come from public domain in the web, mainly from the U.C.I., [Murphy, 1994].

In the rest of this Section, we provide a brief description of datasets used in our experiments, the evaluation method to obtain results and present our results from two different sources.

5.1 Data used in experiments

We next describe briefly each one of the datasets used in our experiments. They were manipulated to fit our algorithm from the original state in which we obtain them from the Web. The explanation that follows was taken from the data owners or researches using the data themselves.

5.1.1 Adult dataset. (Census USA 1994)

B. Becher extracted data for this dataset from the 1984 USA Census Bureau Database. Found at UCI repository this database was given by R. Kohavi and B. Becker, and first quoted by [Kohavi, 1996]. It contains 45,222 instances after removing

unknown values. Around 65% percent of these are used for training and the remaining 35% for testing. There are fourteen (14) attributes, most of them symbolic or categorical and two (2) classes: people earning up to fifty thousand dollars a year or more. The problems consist in determining whether a person earns over USD$50,000 per year. Classes are labelled as '>50K' and '<50H' and their probabil ity distribution is:

Probability for label ' >50K' : 23.93% / 24.78% (without considering unknowns). Probability for label ' <=50K' : 76.07% / 75.22% (without considering unknowns).

5.1.2 Annealing dataset

Donated by David Sterling and Wray Buntine, this database contains 798 instances and 38 Attributes. Out of these, six are continuously valued, three are integer-valued and the remaining twenty-nine are nominal-valued. There is six classes with one of them holding over 80% of records.

This dataset contains many '-' values literally defined by the authors as *'not applicable'*, which are different from '*missing values',* indicated with a '?' Therefore, they can be treated as legal discrete values, which we have done in the case of all twenty-nine symbolic attributes. For a detail of the used dictionary definition, see Appendix II.

There are also many missing attribute values in this dataset. We convert them all to the mean value of each class distribution group.

5.1.3 Breast Cancer (Wisconsin) dataset

This dataset is one of several from the UCI repository [Murphy, 1994], and it was originally obtained from the University of Wisconsin Hospitals, Madison from Dr. W. H. Wolberg [Mangasarian, 1990]. There are originally 699 instances but we have eliminated 16 for missing some attribute values, so only 683 are used. Out of ten attributes, the first one is just a reference number so only nine (9) attributes are used. All of them are numeric with an equal domain value ranging from one to ten. There are two possible class labels: *benignant* or *malignant* and they have a distribution of 458 instances (65.5%) for the *benignant* class and 241 instances representing 34.5% for the *malignant* class.

5.1.4 Dermatology dataset

This database is from the UCI repository,, and was originally owned by Nilsel Ilter and H. Altay Guvenir. The database contains six classes, 366 instances and 34 attributes, one of which is nominal.

The aim is to determine the type of Eryhemato-Squamous Disease. The differential diagnosis of this disease is a real problem in dermatology. They all share the clinical features of Erythema and scaling, with very little differences.

5.1.5 Diabetes (Pima Indian) dataset

This dataset was originally prepared for the use of participants for the 1994 A.A.A.I. Spring Symposium on Artificial Intelligence in Medicine. Original donor is V. Sigillito from the National Institute of Diabetes and Digestive and Kidney Diseases, USA.

There are 768 instances on this dataset where all patients were females at least 21 years old of Pima Indian heritage. Each instance has eight attributes. There are two possible classes. The diagnostic investigates whether the patient shows signs of diabetes according to World Health Organization criteria or not. There are no missing attribute values.

Class Distribution is: No diabetes: 500 (65.1%). Positive for diabetes: 268 (34.9%).

5.1.6 Forest Cover type dataset

Original donors of this database available since 1998 are from the Forest Service and the University of Colorado, USA. Owners are J. A. Blackard and the Colorado State University.

There are 581,012 instances in this database, each representing a 30 x 30 meters square cell of undisturbed forest. Each of these holds 12 attribute measures and 54 columns of data. Ten of these attributes are quantitative variables, four are binary (wilderness areas), and forty represent binary soil type variables.

Natural resource managers responsible for developing ecosystem management strategies require basic descriptive information including inventory data for forested lands to support their decision-making processes. However, managers generally do not have available data from neighbouring lands outside their immediate jurisdiction. One

method of obtaining this information is using predictive models. Thus, the problem consists in recognizing various forest cover types as classes among the eight existing groups: Spruce/Fir, Lodge pole Pine, Ponderosa Pine, Cottonwood/Willow, Aspen, Douglas fir and Krummholz. Class distribution is largely dominated by two of these classes, holding around 80% of the instances among themselves (Spruce-Fir and Lodge pole Pine).

We use a stratified sample of around 56,800 records with splits in 60 and 40% for training and testing datasets as shown in Table 5.1.

5.1.7 Heart disease dataset (Cleveland).

From UCI repository, this database is from 1998 and the donors and responsible for the data collection are:

1. Hungarian Institute of Cardiology. Budapest: A. Janosi, M.D.
2. University Hospital, Zurich, Switzerland: W. Steinbrunn, M.D.
3. University Hospital, Basel, Switzerland: M. Pfisterer, M.D.
4. V.A. Medical Centre, Long Beach and Cleveland Clinic Foundation: R. Detrano, M.D., and Ph.D.

This database contains 303 cases, including 13 attributes (4 cont, 9 nominal). There are seven vectors with missing values. Only two classes used out of the original five (no, degree 1, 2, 3, 4). Class distribution: 164 (54.1%) no, 55+36+35+13 yes (45.9%) with disease degree 1-4. We use all 303 vectors replacing all missing values with the mean value of their class group.

5.1.8 Heart disease Statlog

Donated by R. King among a group of other databases, this particular version of the heart disease dataset contains 270 instances with 13 attributes each, (extracted from a larger group of 75), Among them, there are six real continuous values, three ordered, one ordered and three nominal or symbolic. There are no missing values. Out of the 270 instances, 150 plus 120 observations were selected from the 303 cases of the Cleveland Heart database.

There are two classes to be predicted: Absence or presence of heart disease in patients.

5.1.9 Hypothyroid dataset

This dataset originally used by Quinlan in the case study of his article "Simplifying Decision Trees" (International Journal of Man-Machine Studies (1987) 221-234) contained 3772 learning and 3428 testing examples. There are 21 attributes on each instance, out of which 15 are binary and 6 continuous. There are three possible classes and the problem is to determine whether a patient referred to the clinic is hypothyroid. These classes are: normal (not hypothyroid), hyper function and subnormal functioning. Because 92 percent of the patients are not hyperthyroid, a good classifier must be significantly better than 92%. As we show later in this section, in our case this figure is 99.3%. All binary attribute fields with missing values were conserved as legitimate symbolic values. These correspond to attributes numbers: 2, 5 till 17 and 19th.

5.1.10 Iris dataset

From Fisher, (1936), this is one of the best-known databases to be found in the area of pattern matching. The data set contains three classes of 50 instances each, including four attributes. Each class refers to a type of iris plant. One class is linearly separable from the other two and these are not linearly separable from each other.

5.1.11 Pen-Based Recognition of Handwritten Digits: “pendigits” dataset

Donors of this dataset are E. Alpaydin and F. Alimoglu from the Department of Computer Engineering at Bogazici University, Istanbul, Turkey. There are 10,992 instances in this dataset, each with sixteen (16) attributes and ten (10) classes. The authors have used 7494 instances for training and validation and 3498 instances for test. All 16 attributes are integers in the range 0 to100.

The database consists of a collection of 250 samples from 44 writers. The samples written by 30 writers are used for training, cross-validation and writer dependent testing, and the digits written by the other 14 are used for writer independent testing. A WACOM PL-100V pressure sensitive tablet with an integrated LCD display and a cordless stylus are used to collect handwriting samples. Each writer is asked to write 250 digits in random order inside boxes of 500 by 500 tablet pixel resolution. Written digits are represented as constant length feature vectors.

5.1.12 Satellite image dataset (STATLOG version)

The Statlog databases are a subset of the datasets used in the European Statlog project and the original title of them is: Statlog Databases. Donors are R. D. King and the Department of Statistics and Modelling Science, University of Strathclyde, Glasgow, Scotland.

The databases available here were in used in the European Statlog project, which involves comparing the performances of machine learning, statistical, and neural network algorithms on data sets from real-world industrial areas including medicine, finance, image analysis, and engineering design.

The Landsat Satellite database consists of the multi-spectral values of pixels in 3x3 neighbourhoods in a satellite image, and the classification associated with the central pixel in each neighbourhood. The aim is to predict this classification, given the multi-spectral values. In the sample database, the class of a pixel is codified as number.

There are 6,435 instances in this dataset, where 4435 instances were used for training and the remaining 2000 cases were used for test. There are 36 semi-continuous attributes with numeric values ranging from zero to 255. There are six decision classes: 1, 2, 3, 4, 5 and 7.

The original database was generated from Landsat Multi-Spectral Scanner image data. The sample database was generated taking a small section (82 rows and 100 columns) from the original data. One frame of Landsat MSS imagery consists of four digital images of the same scene in different spectral bands.

The database is a small sub-area of a scene, consisting of 82 x 100 pixels. Each line of data corresponds to a 3x3 square neighbourhood of pixels completely contained within the 82x100 sub-area. Each line contains the pixel values in the four spectral bands (converted to ASCII) of each of the nine pixels in the 3x3 neighbourhood and a number indicating the classification label of the central pixel. In each line of data the four spectral values for the top-left pixel are given first followed by the four spectral values for the top-middle pixel and then those for the top-right pixel, and so on with the pixels read out in sequence left-to-right and top-to-bottom. Thus, the four spectral values for the central pixel are given by attributes 17,18,19 and 20, which are the attributes suggested by the authors to build predictive models.

5.1.13 German credit dataset

This dataset is a donation of Dr. H. Hofmann, from the Institute of Statistics, at the University of Hamburg, Germany. There are 1000 instances on this database. Two datasets are provided. The original dataset contains categorical/symbolic attributes. There exists also a version with numeric attributes for those classifiers that cannot handle categorical attributes. This file has been edited and several indicator variables added to make it suitable for this purpose. Several attributes such as attribute 17 are coded as integers. This was the form used by Statlog. There are 20 attributes (7 numerical and 13 categorical) in the original version, whereas are 24 attributes in the numeric version.

The problem in this dataset consists in correctly classifying bank creditors as *"bad"* or *"good"* . The dataset requires the use of a cost matrix, shown below

	1	2
1	0	1
2	5	0

(1 = Good, 2 = Bad)

The rows represent the actual classification and columns represent the predicted classification. In this dataset, it is worse to class a customer being good when in fact is bad, than to class a customer as bad when it is good.

5.2 The evaluation method used by Trie-Class

The method to evaluate our classification algorithm's predictive accuracy, consists in repeatedly splitting of the evaluation data $\mathcal{R}$ into two mutually exclusive sets: R_h training and R_t test sets in 6/10 and 4/10 proportions respectively *carrying both of them approximately the same class distribution as the one observed for the whole population* (see Fig.5.1).

We do this applying the *stratified sampling* strategy. One first pass over the evaluation data is done to obtain class distribution figures by copying records into subsets of the same class, thus creating as many subsets as classes exist. Out of each one

of these, we randomly pick a subset of records without replacement, which amount according to their class distribution proportion calculated as:

$$Sample_{(i)} = \left\{(R_T/100) \times (Sclass_{(i)}/100) \times N\right\} \quad \textbf{(5.1)}$$

Function S*class (i)* returns the number of instances on a given class subset. The total size of the sample is then given by:

$$TSample = \#\left\{r \in Sample_{(i)}\right\} \quad \textbf{(5.2)}$$

Tsample corresponds to the size of the training set. All complementary records to *TSample* in *N* go into the test set.

This whole process is repeated 10 times. Each time, the classifier is rebuilt from scratch and trained again on a new training set. Estimating accuracy is done using once the new test set as input. Average mean error and standard deviation values are calculated from these runs.

An example of stratified sample is shown in Table 5.1. It corresponds to the forest cover type dataset [Murphy, 1994]. This file contains 581,012 records and seven classes. Out of that total we have taken a sample of around 10% of the global population containing 56,800 records, with approximately the same class distribution.

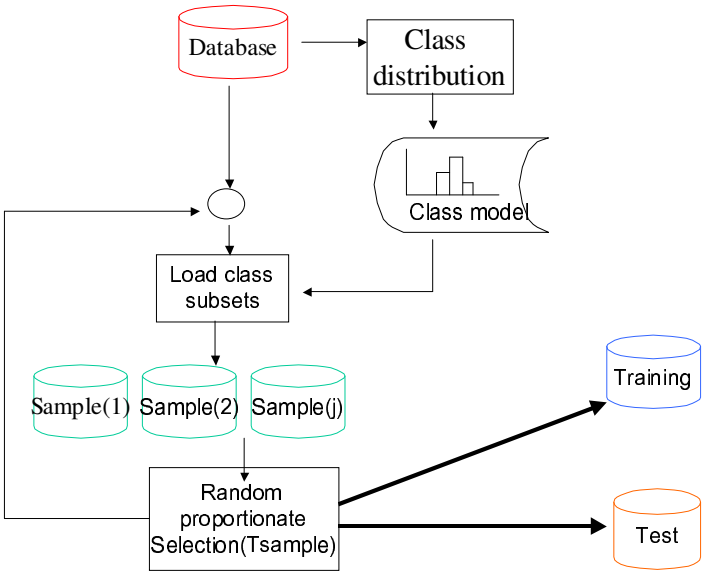


Fig. 5.1. Flowchart for training and test sample subset selection

As shown in Table 5.1, the stratified sample technique preserves identical class distribution in the training file if compared with the distribution in the entire population.

Table 5.1 Stratified sample characteristics in forest covert dataset

Forest covert dataset			Typical training file		Sample size	
Class distribution	Size (recs.)	%	Size	%	Size	%
Spruce fir	211,840	36.5	20,700	36.5	16,642	48.1
Lodgpole Pine	283,301	48.8	27,700	48.8	12,451	36.4
Ponderosa Pine	35,754	6.2	3,521	6.2	1,875	5.5
Cottonwood/Willow	2,747	0.5	284	0.5	176	0.5
Aspen:	9493	1.6	908	1.6	550	1.6
Douglas-fir	17,367	3.0	1,700	3.0	1,039	3.0
Krummholz	20,510	3.5	1,988	3.5	1,178	3.4
TOTAL	581,012		56,800		34,153	

5.3 Comparison of results with other classifiers

As already mentioned, we present our results in two ways depending on their source. For a larger number of classifiers we used figures from the bibliography. The idea in this case is to cover results for a large spectrum of classifiers, which sometimes are difficult if not impossible to obtain and experiment. This method might not be entirely correct from a statistics viewpoint. In fact, we do not control the testing conditions under which these results were obtained, such as possible differences in hardware, the sample selection method, the percentages of data records used for training and testing, the treatment to missing values as well as differences in evaluation methods under which results are presented. For this reason, we present a second set of results obtained after carrying experiments in our own hardware[14], using the well-known benchmark "WEKA" [Witten et al., 2000].

5.3.1 Results using figures from the bibliography

We present next tables with results for classification tools taken from various sources in the bibliography, namely [Murthy, 1994], [Murthy, 1996], [Domingos, 1996],

[14] A PC with a 32-bit architecture, nominal speed of 300Mhz, 128 MB of available RAM running under Windows 98.

[Quinlan, 1998], [NCU, 2000], [Liu, 2000], [Li, 2000], [Riquelme, 2000], [Bologna, 2000], [PMSI, 2001] and [Collobert, 2001].

With respect to these data, we tried to present the best possible results for each classifier found on the available sources. These results are presented in order by their error predictive figure on the test set, indicating the source on the right-hand column. The error rate in accuracy is calculated as the error percentage classifying records from the test set. On each table, the results include our own classifier for comparison purposes. Results were obtained applying a stratified ten-fold cross-validation evaluation using approximately 60% for the training set and 40% for the test set, as described in Section 4.1.6. We indicate the mean value out of the ten runs, including the corresponding standard deviation.

Table 5.2 Adult dataset: Error Rate in predictive models

Method	Error-rate (%)	Reference
FSS-Naïve-Bayes	14.1	UCI
NBTree	14.1	UCI
C4.5-auto	14.5	UCI
IDTM- (Decision table)	14.5	UCI
HOODG	14.8	UCI
C4.5-rules	14.9	UCI
SVM	15.0	Zadrozsny, 2002
C4.5	15.5	UCI
Voted-ID3- (0.6)	15.6	UCI
CN2	16.0	UCI
Naive-Bayes	16.1	UCI
Voted-ID3- (0.8)	16.5	UCI
T2	16.8	UCI
Saxon	17.2	PMSI, 2001
1R	19.5	UCI
NN (3)	20.4	UCI
Trie-Class	10.6 ± 1.2	Ours (1)

(1) Using only the following relevant attributes taken from its original order: 11, 12, 6, 10, and 1 in that order.

Table 5.3 Annealing dataset: Error Rate in predictive models

Method	Error Rate (%)	Reference
PEBLS	1.2±. 8	Domingos, 1996
MsCBA+Boosted C4.5	1.4	Liu, 2000
MsCBA	2.1	Liu, 2000
RISE	2.6±. 9	Domingos, 1996
NB	2.7	Liu, 2000
LB	3.6	Liu, 2000
CBA	3.6	Liu, 2000
Boosted C4.5	4.3	Liu, 2000
RIPPER	4.6	Liu, 2000
C4.5 (AdaBoost Ensemble)	4.9	[Quinlan, 1998]
k-NN, k=1	7.5	Riquelme, 2000
C4.5+NB	7.8	Liu, 2000
Trie-Class	2.3± 0. 3	Ours

Table 5.4 Wisconsin Breast Cancer: Error Rate in predictive models

Method	Error Rate (%)	Reference
FSM	1.7	NCU, 2001
MsCBA+Boosted C4.5	2.2	Liu, 2000
NB	2.4	Liu, 2000
3-NN stand Manhattan	2.9	NCU, 2001
21-NN stand. Euclidean	3.1	NCU, 2001
DIMLP	3.3	Bologna, 2000
OC1	3.8 ± 0.3	Murthy, 1996.
C4.5	4.7 ± 2.0	Murthy, 1996
CART-LC	4.7 ±0.6	Murthy, 1994
CART-AP	5.0 ± 1.6	Murthy, 1994
RIAC (prob. inductive)	5.0	Hamilton et. al.
k-NN (k=7)	25.8	Riquelme, 2000
Trie-Class	1.5 ± 0. 2	Ours

Table 5.5 Dermatology dataset: Error Rate in predictive models

Method	Error Rate (%)	Reference
DIMLP	3.3	Bologna, 2000
C4.5-1	3.9	Bologna, 2000
C4.5-2	4.1	Bologna, 2000
C4.5-3	4.8	Bologna, 2000
MLP	4.9	Bologna, 2000
LDA	34.9	Bologna, 2000
Trie-Class	4.5 ± 0.3	Ours

Table 5.6 Pima Indian Diabetes: Error Rate in predictive models

Method	Error Rate (%)	Reference
MsCBA+C4.5+NB	22.0	Liu, 2000
Logdisc	22.3	NCU, 2001
Incnet	22.4	NCU, 2001
DIPOL92	22.4	NCU, 2001
SMART	23.2	NCU, 2001
GTO DT (5 x CV)	23.2	NCU, 2001
DIMLP	23.3	NCU, 2001
LDA	23.6	NCU, 2001
k-NN, k=7	24.7	Riquelme, 2000
C4.5 (Rel. 8)	25.4 ± 0.3	Quinlan, 1996
Trie-Class	18.5 ±1.6	Ours

Table 5.7 Forest cover: Error Rate in predictive models

Method	Error Rate (%)	Reference
HISURF	13.0(*)	Hegland, 2000
One SVM	16.8	Collobert, 2001
C4.5	29.2	Chou et al., 2000
Neural Network (back prop.)	30.0	J. Blackard
LDA	42.0	J. Blackard
Trie-Class	20.5 ± 2.5	Ours

(*) Result obtained on the evaluation set

In [Garcke, 2002] 93.7% in accuracy is reported for this dataset, but this is done considering 10 attributes, using the evaluation set and for only 1 class: Ponderosa Pine. For this reason, we did not include it.

Table 5.8 Heart disease, Cleveland: Error Rate in predictive models

Method	Error Rate (%)	Reference
MsCBA+Boosted C4.5	10.2	Liu, 2000
IncNet	10.0	NCU, 2001
28-NN, stand, Euclidean, 7features	14.9 ± 0.5	NCU, 2001
Fisher discriminant analysis	15.8	NCU, 2001
LDA	15.5	NCU, 2001
25-NN, stand. Euclidean	16.4 ± 0.5	NCU, 2001
16-NN, stand. Euclidean	16.0 ± 0.6	NCU, 2001
FSM82.4 - 84% on test only	16.0	NCU, 2001
Naïve Bayes	16.6 – 17.5	NCU, 2001
KNN, k=7	17.8	Riquelme, 2000
C4.5 tree	21.5	Liu, 2000
Trie-Class	10.8± 0.2	Ours

A total of 303 records were used for the Heart disease, Cleveland dataset. Four attribute values labelled ”?” from original attribute Nº 12 and 2 from attribute Nº 13 were converted to its mean values.

Table 5.9 Statlog Heart disease: Error Rate in predictive models

Method	Error Rate (%)	Reference
LDA	16.4	Bologna, 2000
Naïve Bayes	16.4	NCU, 2001
TAN	16.7	Li, 2000
DIMLP	16.9	Bologna, 2000
MsCBA+C4.5+NB	17.0	Liu, 2000
MsCBA+C4.5	17.4	Liu, 2000
MLP	17.5	Bologna, 2000
DeEPs	17.8	Li, 2000
MsCBA	18.1	Liu, 2000
KNN, k=11	18.5	Riquelme
CBA	18.5	Liu, 2000
C4.5 tree	21.8	Liu, 2000
IB1c	26.0	NCU, 2001
Trie-Class	18.8±1.7	Ours

Table 5.10 Hypothyroid dataset: Error Rate in predictive models

Method	Error Rate (%)	Reference
C4.5-3	0.4	Bologna, 2000
C4.5-1	0.4	Bologna, 2000
RIPPER	0.8	Liu, 2000
NB	1.5	Liu, 2000
DIMLP	1.6	Bologna, 2000
CBA	1.6	Li, 2000
DeEPs(dynamical α)	1.7	Li, 2000
CN2	1.7 ± 0.5	Domingos, 1996
MLP	2.15	Bologna, 2000
RISE	2.5 ± 0.4	Domingos, 1996
LDA	4.15	Bologna, 2000
Trie-Class	0.7 ± 01	Ours

Table 5.11 Iris dataset: Error Rate in predictive models

Method	Error Rate (%)	Reference
MsCBA + Boosted C4.5	2.7	Liu, 2000
C4.5	3.7	Li, 2000
DeEPs (α = 12)	4.0	Li, 2000
OC1	5.3 ± 3.1	Murthy, 1996
RIPPER	5.3	Liu, 2000
LB	5.3	Liu, 2000
msCBA	5.3	Liu, 2000
CART-LC	6.5 ± 2.9	Murthy, 1996
OC1-AP	7.3 ± 2.4	Murthy, 1996
CART-AP	6.2 ± 3.7	Murthy, 1996
CBA	7.1	Li, 2000
Trie-Class	2.1 ± 0.3	Ours

Table 5.12 Pendigits dataset: Error Rate in predictive models

Method	Error Rate (%)	Reference
DeEPs (α = 12)	1.8	Li, 2000
k-NN (k = 3)	2.2	Murthy, 2001
k-NN (k = 1)	2.3	Murthy, 2001
C4.5 (full)	3.4	Chawla, 2001
Loss-based (L(y) = -y)	7.2	Zadrozsny, 2001
Trie-Class	2.4 ± 0.2	Ours

Table 5.13 Satellite image dataset (STATLOG): Error Rate in predictive models

Method	Error Rate (%)	Reference
k-NN	9.4	NCU, 2001
k-NN, k=2,3, Euclidean	9.7	NCU, 2001
Boosted C4.5	10.3	Liu, 2000
LVQ	10.5	NCU, 2001
DeEPs	11.5	Li, 2000
MsCBA+Boosted C4.5	12.3	Liu, 2000
RBF	12.1	NCU, 2001
TAN	12.8	Li, 2000
Alloc80	13.2	NCU, 2001
LB	13.6	Liu, 2000
C4.5	14.8	Li, 2000
CBA	15.1	Li, 2000
Trie-Class	10.1± 0.4	Ours

Table 5.14 German Credit dataset. Error Rate in predictive models

Method	Error Rate (%)	Reference
CBA	28.5	Liu, 2000
C4.5 tree	28.4	Liu, 2000
MsCBA+Boosted C4.5	24.8	Liu, 2000
RIPPER	27.8	Liu, 2000
LB	24.7	Liu, 2000
NB	25.9	Li, 2000
SORES	32.9	Duntsch, 1998
Naive Bayes	25.3	Friedman, 1996
Trie-Class	25.9 ± 1.5	Ours

5.3.2 Results from experiments done in our own hardware

Results showed in this section were obtained running in our own hardware[15] some selected classifiers using Weka. This is an open-source machine learning workbench implemented in Java developed at the University of Waikato, New Zealand [Witten et al, 2000], which is freely available on the World Wide Web at the following address: (*www.cs.waikato.ac.nz/ml/weka*).

The Weka experiment environment is a comprehensive tool for machine learning and data mining. Mainly directed to classification problems, this software implements old as well as new algorithms using the object-oriented Java programming language, and thus it allows the incorporation of other classification software using its Java class hierarchy. The tool also implements regression, association rules and clustering algorithms. Although is possible to run the environment from the command line, the system includes a GUI that provides the user with more flexibility and easiness of use. Evaluation methods include leave-one-out and cross-validation among others.

We present results for three main classifiers. For all cases, we calculate error rate percentages and standard deviation ($\overline{s}$) against the test set using the 10-fold cross-validation evaluation method. All classifiers were executed against exactly the same datasets previously selected and converted to WEKA format "arff".

[15] A regular PC, Pentium II at 500Mhz, with 255Mb of main memory.

The first classifier for which we show results is *IBk*, a nearest neighbour classifier where we set parameter k = 2, for comparison purposes with our own implementation that extracts also two best close neighbours. Other parameter settings for this and other classifiers are shown in Annex 2. The second one is Weka own improved version of Quinlan's C4.5 called J4.8 which we used with confidence factor of 0.25 and 2 minimum number of objects. Actually, according with its authors, J4.8 implements a later and slightly improved version of C4.5 [Witten et al., 2000]. The third classifiers used is a version of Naive Bayes that we include because this is one of the classical classifiers whose accuracy figures can be used as a reference.

The last classifier used for comparison purposes is SMO, a version of a Support Vector Machine classifier. Because SMO could only handle two-classes datasets, we show only results for datasets where this was the case.

Table 5.15 Comparison in Classifiers accuracy using Weka against Trie-Class

Nº	Datasets Name	#inst,attrib,class	Percentage error and standard deviation in Classifiers Naive Bayes		IBk[1]		J4.8		SMO		Trie-Class	
			Error	$\overline{s}$	Error	$\overline{s}$	Error	$\overline{s}$	Error	$\overline{s}$	Error	$\overline{s}$
1	Adult	45221, 14, 2	17.4	0.52	20.9	0.4	14.7	0.48	15.0	0.69	**10.6**	0.51
2	Annealing	998, 38, 6	13.5	3.45	**0.8**	0.76	1.6	0.94	-	-	2.3	0.30
3	Breast cancer W	699, 9, 2	4.0	2.31	4.7	3.63	5.9	3.13	3.0	2.73	**1.5**	0.20
4	Dermatology	358, 34,6	**2.5**	1.58	4.5	4.21	4.2	1.99	-	-	4.5	1.11
5	Pima Diabetes	768, 8, 2	24.2	3.61	27.9	4.13	25.3	3.0	22.5	4.70	**18.5**	2.60
6	Forest cover [2]	53889, 12, 9	29.8	0.40	**13.3**	0.38	19.4	0.33			20.5	0.51
7	Heart Clev.	303, 13, 2	15.5	6.69	23.8	6.62	21.8	7.82	15.6	5.95	**10.8**	0.22
8	Heart Statlog	270, 13, 2	14.8	7.20	25.6	7.50	25.6	8.81	15.9	7.42	18.8	1.73
9	Hypothyroid	7200, 21, 3	4.8	0.64	8.7	0.79	**0.5**	0.38	-	-	0.7	0.33
10	Iris	150, 4, 3	4.0	4.66	4.8	4.65	4.7	4.50	-	-	**2.1**	0.25
11	Pendigits	10992, 16,10	14.2	1.41	**0.6**	0.30	3.4	0.69	-	-	2.4	0.75
12	Satimage	6435, 36, 6	20.7	1.17	17.7	1.18	15.4	1.36	-	-	**10.1**	1.21
13	German credit	1000, 20, 2	25.1	3.90	27.2	5.77	32.0	4.26	**24.0**	4.48	25.9	1.94

Note: All error results expressed in percentage of instances in error from the test set. Lower error rates for each dataset are indicated in bold face.

(1) For all cases we use the IBk classifier with k =2, resembling our own case..

(2) WEKA did not run on the original full size dataset.

Classification results in Table 5.15 are in general similar to those in the bibliography when comparing error values exhibited by classifiers from both sources and the same datasets. On average, relative percentage differences amount to a mere 4.9%. In addition, classifiers results from both sources show the same relative order of accuracy among themselves when classifying the same dataset. The first of these two aspects can be observed when comparing results obtained for the popular classifier C4.5[16] from these two different sources, as shown in Table 5.16.

Table 5.16 Comparing C 4.5 Error Rates from two sources

Nº	Datasets Name	Origin of error figures		Relative Difference (%)
		Weka (ours)	Bibliography	
1	Adult	14.7	14.5	1.4
2	Annealing	1.6	1.4	12.5
3	Breast cancer W	5.9	4.7	20.3
4	Dermatology	4.2	3.9	7.1
5	Pima Diabetes	25.3	25.4	-0.4
6	Forest cover	19.4	29.2	-50.5 (1)
7	Heart -Cleveland	21.8	21.5	1.4
8	Heart Statlog	25.6	21.8	14.8
9	Hypothyroid	0.5	0.4	20.0
10	Iris	4.7	3.7	21.3
11	Pendigits	3.4	3.4	0.0
12	Satimage	15.4	14.8	3.9
13	German credit	32	28.4	11.3
	Mean relative percentage difference			4.9

(1) This result was obtained training and testing only on 10% of the original file size. As explained before, we could not manage to put Weka to run against its full version.

A third aspect, although secondary is the fact that in all cases but three classifier results from the bibliography are better than results from their counterparts running under Weka. This is normal because we did run C4.5 from Weka using the default options provided and did not tune up its parameter values, as is usually the case with results presented in the bibliography.

Consequently, in this particular case, we believe that it is legitimate to extend the comparison from our own experiments to those of the bibliography for completeness

[16] The commercial implementation receives the name of C5.0

since it does not alter significantly the relationship in terms of accuracy between ours and other classifiers.

We present next in Table 5.17 execution times for the very same cases indicated in table 5.16. This represents a straight and simple measure of algorithm complexity taken to build and to execute these classifiers.

Table 5.17 Classifiers execution total time for each individual fold using Weka.

Dataset	Classifiers Build + execution time in *wall clock* seconds				
Name	SMO	IBk	J4.8	Naive Bayes	Trie-Class
Adult	20602	6304	65.3	167	309
Annealing		3.8	3.92	0.82	45
Breast cancer W	0.35	3.91	0.1	0.04	0.5
Dermatology		0.65	0.19	0.07	0.3
Pima Diabetes	0.77	0.48	0.18	0.02	2
Forest covert		8220	817	50	5220
Heart Cleveland	0.82	0.18	0.07	0.01	0.5
Heart Statlog	0.68	0.18	0.09	0.03	0.5
Hypothyroid		613.8	5.8	0.24	260
Iris		0.1	0.11	0.06	0.5
Pendigits		325	10.21	1.42	45
Satimage		15.9	1.59	0.11	8
German credit	7.49	2.77	3.1	0.044	5

Execution time in Trie-Class is largely better than in traditional Nearest Neighbour algorithms, one of the objectives in creating this tool. Although we observe larger execution time figures compared with J4.8 in nine out of thirteen datasets these times are under 10 seconds.

5.4 Performance Conclusions

Our results shows that on average Trie-Class performs as good as several of the leading classifiers reported here, whether this comparison is done against classifiers running in our test bench or whether we compare with those results from the bibliography. In particular this is true with respect to the landmark classifier C4.5 [Quinlan, 1986] and the instance-based learning *k-NN* algorithm [Aha, 1991].

Table 5.18 Error Rate comparison between Trie-Class, k-NN and two versions of C4.5

Classification error rates (%)

Nº	Dataset	k-NN	C 4.5 Bibliography	J4.8 Weka	Trie-Class
1	Adult	20.9	14.5	14.7	**10.6**
2	Annealing	**0.8**	1.4	1.6	2.3
3	Breast cancer W	4.7	4.7	5.9	**1.5**
4	Dermatology	4.5	**3.9**	4.2	4.5
5	Pima Diabetes	27.9	25.4	25.3	**18.5**
6	Forest cover	**13.3**	29.2	19.4	20.5
7	Heart -Cleveland	23.8	21.5	21.8	**10.8**
8	Heart Statlog	25.6	21.8	25.6	**18.8**
9	Hypothyroid	8.7	**0.4**	0.5	0.7
10	Iris	4.8	3.7	4.7	**2.1**
11	Pendigits	**0.6**	3.4	3.4	2.4
12	Satimage	17.7	14.8	15.4	**10.1**
13	German credit	27.2	28.4	32	**25.9**

Note: we show in bold type smaller error rates.

These differences can be clearly seen when isolating the comparison in classification error rates between Trie-Class and these two other classifiers.

As Table 5.18 shows, in eight out of thirteen cases (61.5%) Trie-Class was superior to *IBk*, C4.5 and J4.8 (Weka's *k-NN* version), independently of the source for these figures.

We believe that modified instance-based methods such as the one proposed in this thesis represent a powerful challenge to other classification methods. The key issues are solving the complexity of the search problem of similar instances by means of appropriate data structures as a first approximation to object similarity, and a dataset dependent set of criteria to inspect selected close patterns. Compared with other *k-NN* methods for instance, ours resolves successfully an important weakness of these methods represented by the search complexity problem and the determination of the value of *k* as stated in a recent work [Riquelme, 2001]. In the extreme case for these methods the distance calculation for all instances in the search space becomes intractable.

About the execution time issue, it seems to exist a generalized view that execution time should be very small in all cases, for a classification algorithm to be considered useful. In our opinion, it is always desirable to have the goal of reducing algorithm complexity and thus execution time. Nevertheless, this goal finally depends on the data

owner defined as the maximum allowed time he/she consider reasonable. A doctor waiting for a Data Mining program to forecast a patient possibility of a serious disease, does not have the same time requirements as a biologist trying to classify some type of diatomaceous. Moreover, one cannot forget that in many cases in real-life situations data preparation and pre-processing takes sometimes hours if not days even before the Data Mining algorithm can start execution. Within this context, to be concerned with few more or less seconds in execution time does not look reasonable, especially if the gain in execution time is done at the expenses of losing accuracy. Because this, we cannot more agree with the statement that: "*Ideally, accuracy should not suffer at the expense of improved performance."* [Brighton et al, 2002].

6 Choosing the best close neighbour

Most *NN* classification algorithms use only the distance between objects as the sole criterion to select the best neighbour object. In the case of the family of *k-NN* algorithms, after *k* closest neighbours are selected, a voting on the majority class of selected close objects is used, with a neighbour vote decreasing with its distance from the test example [Bentley, 1980; Friedman et al., 1977; Dasarathy, 1991]. Algorithms for discrete and real-value functions have been developed as in [Mitchell, 1997] with refinements including the case where the query point exactly match one or more training objects. Also, many other algorithms have been developed to increase the search efficiency of *k-NN* in the sense of choosing a group of objects that best represent the class of the unknown object, as we refer in Section 2. However, most of the time the recurrent criterion for choosing among subset *k* of pre-selected training members is the dominant class.

In Trie-Class we use a mixed method in two phases to select the best hypothesis. As a first phase, we extract two nearest cells from the tree structure holding training records using the search mechanism described in Section 3.7. We call these cells p^1 and p^2 and each one of them is associated to a different class.

The second phase consist in the selection of one of them to assign its class to the unknown cell p^x. On this phase, cells p^1 and p^2 and the query object itself are inspected in order to make a final decision. This is what we explain next.

Trie-Class uses six weighted *decision parameters* (DP) that characterize the selected cells to make its final selection. DP's are weighted before run time according with their predictive skills on a particular dataset. Hence, adapting themselves to the characteristics of the dataset where the classification will be done. After weighted they are applied to contending cell patterns p^1 and p^2 to decide which one of them best represents the new object.

By carrying this second inspection on similar cells including the unknown cell p^x we somehow try to overcome a known problem. The similarity criterion must be applied to a pre-defined set of features and the definition of this set is affected by the previous knowledge one has over the objects [Murphy et al., 1985]. Inspecting the unknown object p^x itself can bring into light new knowledge.

On what premises DP weights are attributed? They depend on how well a given DP classifies new objects. As shown later, we demonstrate that this ability changes from one dataset to the next. For this reason, DP weights are set every time a new dataset is under analysis. DP weights are individually calculated by testing to how many new unseen records a particular DP applies, and how well it classifies them. These two criteria correspond to *ambit* and *precision* respectively. Weights are computed learning from the training file and testing against an evaluation file. Weight calculation is explained in subsection 6.3.

Once weighted, how DP's are used to select p^1 or p^2?

To each cell is applied a *merit ()* function, which correspond to the joint application of allowable combinations of weighted DP's. Several functions are used to fulfil the task of this function to which we refer next.

As DP criteria are first weighted we use function *apply()* to determine a given criterion's applicability or *ambit* which contributes to its weight. In this function a given DP is applied to both cells p^1 and p^2. We say that a particular DP "applies" to a given object when it produces a better result applied to one of these cells. Function *apply()* returns a Boolean value and is shown in Fig 6.1.

One weighted, the primary usage of each individual criterion is to help selecting a cell and consequently its class for a new query cell p^x. In this context we develop a basic function *criterion()* that applies a given criterion to cell patterns p1 and p2 and returns a real value, which correspond to a measure of "goodness" of that criterion. Different criteria return different values as shown later in Table 6.1.

This in turn allows the direct comparison between criteria applied to the same DP which is done by function *apply()* from Definition 28 which allows to determine to which cell the criterion applies best.

As the weight of each criterion is already calculated, a final result corresponds to the sum of al applicable criteria multiplied by its pre-determined weight. This is carried by the *merit()* function applied separately to each cell pattern p^1 and p^2. A pattern with larger merit means larger similarity between a given cell pattern and query cell p^x.

Based on each cell's merit, a final comparison through function *predict()* returns the wining cell and class.

We begin this section by giving the characteristics of each DP criterion, its weight calculation and meaning, along with figures showing its discriminating power on various datasets. Next we explain each of the functions referred above putting it all together in the final *predict()* function.

6.1 Decision parameters

We now explain the meaning and characteristics of each decision parameter. Its weight calculation as well as the class returned when applied as criterion.

6.1.1 Semi-exclusive values

We have already defined the *exclusiveness of a cell* in Equation (3.23) of Section 3.4. This measure of exclusiveness tries to determine if the attribute values of a record belong to *semi-exclusive intervals* or not. The presence of attributes qualifying as *semi-exclusives* within the unknown object p^x can only mean that there is a strong evidence that this cell is likely to be related to the class dominating those same intervals.

The fact that this DP check first within the unknown cell p^x itself looking for one or more semi-exclusive intervals make it different from all others. When this is the case and function *semp*(p^x, φ) applies, function *criterion* verifies if the actual class held by cell p (p^1 or p^2) correspond to the class found in p^x intervals. If so, the function returns the fraction of those intervals.

Notice that this criterion is not applicable directly to cell patterns p^1 and p^2 as the information conveyed by the eventual presence of semi-exclusive intervals on these patterns, gives no reason to prefer one of them as the best representative for p^x.

6.1.2 Distance between selected cells

Distance calculation used for the cell extraction of p^1 and p^2 is different from the one used here. In the first case distance was computed using the search mechanism already explained in Section 3.7.

In the present case we use a standard distance calculation to find out the smallest distance between p^x and cells p^1 and p^2. Its computation is normalized using as divisor

factor the attribute's domain range. This distance basically corresponds to a normalized Manhattan distance:

$$d(p, p' \neq \sum_{i=1}^{n} \frac{|p_i - p'_i|}{Max_i - \min_i} \quad (\mathbf{6.1})$$

Max and min represent observed maximum and minimum values for attribute *i.*

When used within function *criterion(),* it returns the inverse of distance to p^x plus a small constant to avoid zero division:

$$criterion(distance, p, p^x) = 1 \Big/ \left(d(p, p^x) + \varepsilon\right) \quad (\mathbf{6.2})$$

When used by function *apply()* this criterion returns true if find that one of the distances $d_1(p^1, p^x)$ or $d_2(p^2, p^x)$ is smaller. If distances are equal, and in an attempt to deal in part with *noisy* data[17], cell frequencies are used as weight considering the well-known heuristic rule that larger frequencies means closer distance.

6.1.3 The shape of cells

We already have defined a shape vector in Equation (3.26) and a shape similarity function in Equation (3.27) allowing shapes comparisons.

Provided with these tools this criterion returns the inverse distance of the shape similarity function between p and p^x plus some small constant to avoid zero division.

$$criterion(Shapes, p, p^x) = 1 \Big/ \left(sp(p, p^x) + \varepsilon\right) \quad (\mathbf{6.3})$$

6.1.4 Cell strength

A cell can be characterized as *strong* or *weak* depending on the number of its sub-cells associated with a single class label. As it was already shown in Definition 18 in subsection 3.3, the value of function s*trength()* correspond to the value of *i* at the point

[17] Data for which the label is incorrect, some number of attribute values are incorrect or a combination of the two [Brodley 1995]

where a cell's prefix becomes unique in terms of class in the whole training dataset, i.e., when function $nlabels(q_i) = 1$. From this point on, all other sub-cells derived from this one will also hold that same class label.

When $strength(p) = n$, cell strength is minimum. When $strength(p) = 1$, cell strength is maximum. When $strength(p) = 0$, we are probably in the presence of an *outlier,* meaning that two identical cells in the dataset are associated to at least two different classes, thus breaking our basic assumption about *data consistency* described in Section 3.8.1. On the other hand, if $strength(p) = n$, means that only the last attribute value made the difference to associate the cell to a given class. Considering that less relevant attributes are located towards the end of a cell's sequence of values class membership for minimum strength cells is weak. It is less likely that other cells similar to it might have the same class.

This criterion is applicable if one of the competing cells p^1 or p^2 has a larger strength value than the other. In this case function *apply()* will return true. When this is the case, it represents a larger area of the hyperspace where the class distribution is homogeneous. An unknown new instance close to this area increases its chances of sharing the same class, unless we are dealing with an area with greater noise. In these cases this parameter is not very effective.

Applying function *criterion* to this parameter returns the strength value plus one subtracted from *n,* the number of attributes in the cell pattern. So the largest strength value corresponds to n and the weakest value correspond to one.

6.1.5 Frequency of cells and sub-cells

In Equation (3.14) from Section 3.2 we defined function $freq(q_i)$, in order to obtain the number of existing sub-cells of size i within the training set.

As explained later in Section 7.2, the tree structure holds pattern frequencies, interval values (the discretized discrete value of the corresponding attribute) and a flag label. For this reason, we could rewrite Equation (3.11) as:

$$p = <(q_1, freq(q_1), labels(q_1)), (q_2, freq(q_2), labels(q_2),..,(q_n, freq(q_n), labels(q_n))> \quad (\mathbf{6.4})$$

Although sub-cell frequency is used in both distance calculations used in this thesis, we still consider *frequency of cells* as one more decision parameter on its own right. Not

all sub-cell frequencies are of interest. Here we are interested in the frequency of sub-cell q^i where nlabels(q_i) = 1. This frequency is given by Equation (3.18)

Because of the recursive division of the space into hyper planes in Trie-Class, which are orthogonal to the axes, frequency values rapidly decrease as we descend down tree levels, as noticed in [Arya, 1998].

In this context, and if we agreed on the fact that most relevant information occupies a very reduced area in the objects space [Faloutsos, 1995; Berchtold, 1996], then in many situations a larger frequency of cells in well defined areas of the hyperspace are a good indicator for some unknown object close to this area. Several identical sub-cell objects will have more influence on the generated hypotheses that just one, a typical disadvantage of decision trees [Cios et al., 1998]

Therefore, for sub-cells with i component elements where *labels*(q_i) = 1, function *apply()* using this criterion return true if one of competing sub-cells q_i or q_i' has larger frequency than the other. When used within function *criterion()*, it returns the frequency of the sub-cell provided the label constrain is true.

6.1.6 The Majority Class

We have already defined *majority class* in Section (3.3). In most Machine Learning algorithms this is a simple and effective criterion for classification. In general, the majority class or *default class* serves also as the low limit boundary for classification accuracy. An algorithm classifying with accuracy figures below this value would be useless.

In populations with two classes, c_1 and c_2, where class c_1 is strongly predominant, this parameter will serve to the algorithm to predict c_2, only when strong evidence is found that this is the case [Johnson, 1998]. Hence, this criterion applies if one of the selected cells exhibits the same class as the majority class and thus function *apply()* returns true. In this case, function *criterion()* returns 1, zero otherwise.

6.2 Basic functions definitions for the selection of a representative cell's class

We define next all functions used in the class selection process, as well as the way DP weights are calculated and its usage in function *merit()*.

Definition 27. We define function *criterion()* that applies a given criterion to cell pattern $p = cel(r)$. This function returns a real value calculated by a given DP according to Table 6.1.

Function *criterion*() is applied differently according with each DP characteristics. Some of these criteria are just applied to near cells p^1 and p^2, while others also depend on cell p^x for its calculation. Table 6.1 resumes the application of this function to each criterion and its returning value.

Table 6.1 Function criterion return values by DP

Function criterion() calculation by DP	Returned value	p^x dependent?
criterion(Semi-exclusives, p, px) = (semp(px, φ)	(0..1)	yes
criterion(Shapes, p, px) =1 / (sp(p, px) + ε)	a value	yes
criterion(Strength, p) = (n - strength(p)) + 1	(1..n)	no
criterion(Distance, p, px) = 1 / (d(p, px) + ε)	a value	yes
criterion(Frequency, p) = freq(p)	(1..N)	no
criterion(MajorityClass, p) = (label(p) = = lmaj()) ? 1 : 0	(0 1)	no

Parameter *n* corresponds to the number of attributes in the object and *N* is the number of records in the training dataset.

A given criterion can be applicable or not to a record. This constitutes one of the measures Trie-Class uses to determine the adaptability of each DP criterion to different datasets. Function *apply()* defined next helps to do that.

Definition 28. We assume the existence of function *apply()* that returns a Boolean as a result of comparing the results produced by a given criterion applied to both cells p^1 and p^2, using cell p^x as reference.

```
Boolean apply(DP, r)
{p^x = cel (r);
(p^1, p^2) = neighbours(p^x);
 return !(criterion(DP, p^1, p^x) = = criterion(DP, p^2, p^x)); }
```

Fig 6.1 Function *apply()* returns true if a criterion applies to a given cell

When the result of this comparison yields zero we say that the corresponding criterion is not applicable. Else, function *apply()* does indeed apply although does not discriminate which criterion is best. It simply verifies that it is applicable.

6.3 Obtaining the weight of decision parameters

Before using decision parameters to select a class using function *merit()* we must determine its weights, that is, how well they classify records from different datasets.

We have already said that the ability of DP's to classify new records changes with dataset characteristics. These weights are obtained after training decision parameters using roughly 80% of records from the training set, with the remaining 20% being used as evaluation set. These sets are mutually exclusive and distinct from the test set.

Implicitly we are assuming that results obtained with the evaluation set will be later similar when the criterion is applied to the test set.

According with its performance on the evaluation set and some heuristics, a weight is assigned to decision parameters. A DP criterion with more weight means greater influence in deciding which cell bests represent the new object.

Weight is calculated using two parameters: *ambit* and *precision* degrees, an idea similar to the *support* and *confidence* concepts used in decision rules [Agrawal et al., 1993].

Definition 29. If E is some evaluation set formed by N records r, the *ambit* of a decision parameter DP correspond to the fraction of records $r \in E$ where that criterion applies:

$$ambit(DP) = \#\frac{\{r \in E \mid apply(Dp, r) \neq 0\}}{N} \qquad \textbf{(6.5)}$$

Along with this concept of ambit, we define next the classification precision of a given DP.

Definition 30. The *degree of precision* of some decision parameter *DP* corresponds to the fraction of cells *p* where function *apply()* is not zero and the cell is correctly classified by function *predictr()* applying function *merit()* for this criterion alone.

$$precision(DP) = \frac{\#\{r \in E \mid apply(DP, r) \neq 0 \wedge (predictr(r) = label(r))\}}{\#\{r \in E \mid apply(DP, r) \neq 0\}} \quad \textbf{(6.6)}$$

Function *predictr()* assign a class to a given record *r*. It is show next in Fig. 6.2

```
string predictr(r)
{ p^x = cel(r);
  (p^1, p^2) = neighbours( p^x);
  c = predict(p^1,p^2);
  return c;
}
```

Fig 6.2 Function predictr*()* predicts the label of a given record

Function *predict()* is explained later in Section 6.4. The next example illustrates the use of *ambit* and *precision* concepts.

Example 6.1

If an evaluation set contains 100 cells, and criterion *distance* is applicable to 25 of them, the *ambit* for this criterion is 25%. In the remaining 75% of cases these two criteria cancels each other out. The two candidate cells are at the same distance from the unknown object. As an example from Table 6.2, we see that criterion shape has an *ambit* of 74.5%, corresponding to the fraction of evaluation records where the criterion applies.

Table 6.2 presented next shows *ambit* and *precision* values for each DP criterion and some datasets used in this thesis. Look for example the line corresponding to forest

cover dataset and the column for decision parameter *semi-exclusive.* Within the subset of those cells where this criterion applies, it correctly classified 88.1% of them.

This table confirms that DP's are data dependent, a fact shown by the variations observed in parameters *ambit* and *precision*. DP *semi-exclusive* shows on average the best precision with 93.9%. This is not surprise, as exclusiveness present in cell p^x is a strong assumption about the true hypothesis of the class. At the same time, it shows a reduced ambit or sphere of action. The next two parameters that follow very close are parameters *frequency* and *shapes*. It is rather surprising the performance of *shapes,* being such a simple similarity function. On average it applied to 84.7% of records with an average precision of 90.4%.

Table 6.2 Ambit and Precision values for decision parameters in various datasets

Datasets				Degree of ambit and precision for each DP in percentage					
Name	Set type	Nº recs.		Semi-Excl	Shapes	Distance	Frequency	Strength	Majority
forest	Training	28457	Ambit	25.7	99.9	99.9	43.7	29.9	48.7
(7 classes)	Evaluation	5691	Precision	88.1	86.0	82.0	81.0	74.5	72.2
pendigits	Training	7495	Ambit	0.01	94.2	100	80.8	50.2	10.4
(10 classes)	Evaluation	1499	Precision	100.0	98.8	98.4	98.5	98.3	97.7
landsat	Training	3219	Ambit	41.2	68.6	88.0	57.3	49.6	37.8
(7 classes)	Evaluation	644	Precision	95.2	87.4	76.7	89.1	85.0	62.8
adult	Training	22612	Ambit	6.6	76.0	92.0	57.9	60.5	78.8
(2 classes)	Evaluation	4522	Precision	98.6	87.1	83.4	92.5	89.6	86.1
Cancer-W	Training	343	Ambit	34.8	99.6	87.4	89.3	86.1	67.0
(2 classes)	Evaluation	69	Precision	93.7	100	97.7	98.7	97.8	96.0
Hypothyroid	Training	1332	Ambit	5.5	99.9	100	99.7	31.6	92.1
(6 classes)	Evaluation	266	Precision	96.2	99.4	99.3	99.7	99.7	99.3
Heart (Statlog)	Training	135	Ambit	42.7	100	100	19.1	12.0	55.1
(2 classes)	Evaluation	27	Precision	81.5	81.1	77.5	77.7	77.6	84.3
dermatology	Training	180	Ambit	36.5	39.7	100	51.6	58.4	30.6
(6 classes)	Evaluation	36	Precision	97.7	83.7	81.1	87.3	94	89.6
			Average Ambit	24.1	84.7	95.9	62.4	47.3	52.6
			Average Precision	93.9	90.4	87.0	90.6	89.6	86.0

Altogether, this makes it a very important component among decision parameters. On the other hand, *distance* remains the most solid criterion of all when we use both its *ambit* and *precision* for comparison purposes.

The table also shows that *majority class* is at the bottom of the classification, hence indicating the usefulness of developing other decision parameters, as a mean of improving classification accuracy.

Adapting decision parameters to a given task is the confirmation that there is no classification algorithm performing well in all cases. [Mitchell, 1980; Brodley, 1995]. In [Shaffer, 1994] it is proposed for instance to try different induction paradigms, each one in turn, and to use cross-validation to choose the one that appears to perform best. Other approaches combine empirical with analytical evidence as in [Pazzani et al., 1992; Michalski et al., 1993]. Still others use multi-strategy learning by combining multiple methods in one algorithm [Domingos, 1996].

What combinations of *ambit* and *precision* values for a DP represent a better criterion in a given dataset?

We use a heuristic that in general gives more weight to DP's exhibiting large values for both *ambit* and *precision*. The contribution of these two factors is not equal though, as more weight is given to parameter *ambit* over *precision.* The reason for this being simply the fact that if the extent of a criterion is insignificant or very small, the value of factor *precision,* whatever it might be, is immaterial. On the contrary, a significant ambit of a criterion then a precision figure might be interesting if relatively high for classification purposes. Function $\alpha(DP)$ measures the weight of a given decision parameter, which is calculated using the following heuristic:

$$\alpha(DP) = ((((2ap) / (3a)) + 1) / (((3a) / (2p)) + 1)) + 3p + 2a \qquad \textbf{(6.7)}$$

Variables *a* and *p* stand for *ambit* and *precision* calculated according with Equations (6.5) and (6.6) respectively. Function $\alpha(DP)$ ranks over every other percentage combination of *ambit* and *precision* favouring *ambit* as observed by the value assigned to the coefficients. In general, when variables *a* and *p* increases, α increase also. The intuition here is simple. Assign more weight to those DP that extent over a large number of cases and at the same time have better classification skills. And within this general evaluation criterion, favours slightly more the value of ambit. A very high precision only applicable to a bunch of cases is not as good as a somewhat lower classification

value, but covering a larger fraction of records. In any case, as the discovery process seems, as a rule, to require human judgement [Langley, 1998], these figures can lead to modifications in the way weights are calculated.

In Fig. 6.3 below we show the variations in the values of function $\alpha(DP)$ depending on various combinations of *ambit* and *precision*.

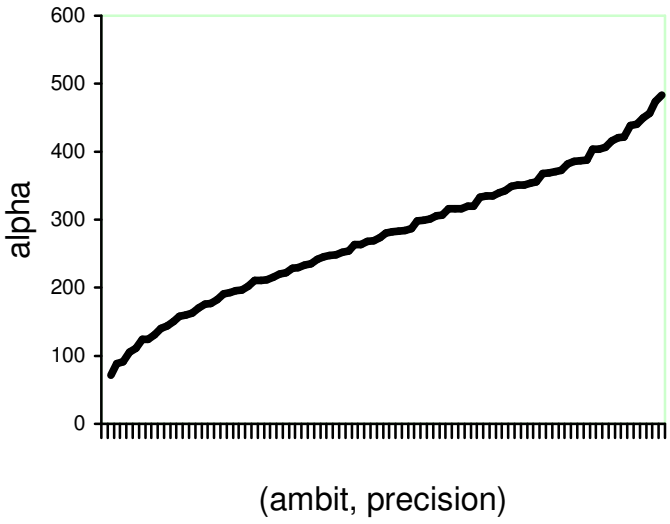


Fig. 6.3 Variation in weight α for various combinations of *ambit* and *precision*

In Appendix 3 you can find the table of values originating the graph of Fig. 6.3.

Ranking decision parameters is done, calculating the value of function $\alpha(DP)$ from Equation (6.7) for each criterion and setting them in decreasing order.

In Table 6.3 we show the result of applying Equation (6.7) to *ambit* and *precision* values from Table 6.2.

Table 6.3 Decision parameters weights for different datasets

dataset Name	Weight values by DP and dataset					
	Exclusive	Shapes	Distance	Frequency	Strength	Majority
Forest cover	256	501	494	301	243	301
Pendigits	200	505	524	459	356	227
Landsat	320	397	443	362	328	247
Adult	217	197	469	370	374	429
Cancer-W	358	354	363	368	359	351

Hypothyroid	209	526	526	525	298	499
Heart (Statlog)	299	493	486	215	192	345
Dermatology	310	293	493	339	375	275
Average weight	271.1	408.3	474.8	367.4	315.6	334.3
Fraction of total avg. values	12.5%	18.8%	21.9%	16.9%	14.5%	15.4%

The last line in Table 6.3 corresponds to the fraction that each weight represents overall in the merit function for the considered datasets. This can be interpreted as the average influence of each decision parameter when applied into the *merit* function. Although parameter *Distance* continues to be the more important (21.9%), the participation of each other parameter is very homogeneous, perhaps with the exception of *Semi-exclusives*. In general, this denotes a combined effort to help choosing the best representative cell pattern when all these aspects are together considered.

6.4 Predicting the final output class

Decision parameters are weighted just once for a dataset. The classification process starts next. Trie-Class is presented with a new test file to classify. Each new record is discretized using the same algorithms used to create the training file stored in a tree, and converted into cell p^x which becomes the first input to the function. Two near candidates cell patterns p^1 and p^2 are extracted from the training dataset using the algorithm described in Section 3.7 using function *neighbours()*. They also are input to the function.

Next, function *criterion()* is applied to both cell patterns p^1 and p^2 using the six available decision parameters. Once each criterion is calculated, we proceed to measure the merit of each considered cell p. This is done using function *merit()*.

Definition 31. We assume the existence of function *merit()* which measures how similar a given cell pattern is with respect to some unknown object p^x.

$$merit(p) = \sum_{i=1}^{6} criterion\left(DP_i, p, p^x\right) \cdot \alpha\left(DP_i\right) \qquad (\mathbf{6.8})$$

This function returns the aggregate value resulting from the application of function *criterion()* to all six decision parameters pondered by its corresponding weight.

Resulting values produced by the *criterion()* function are normalized as their return values should be equally considered. This requires normalizing the *distance, shape* and *strength* criteria. In the case of both distance criteria, its intervals ranges from zero to the maximum distance observed between p^1, p^2 and p^x, so it is: [0 $max(d(p^x,p))$].

Therefore, on each case distance figures will be divided by the maximum value observed. The same is done with criterion *strength,* but this time applied to strength values.

Function *merit()* returns a real value. In the case when all DP criteria values except one are set to zero, function merit can be used to measure the goodness of a single criterion for a particular cell pattern.

Function *merit()* represent a similarity measure among cell patterns within a given data space, allowing their comparison with respect to another cell pattern (p^x in our case). In this sense we can say that it could be used as a new metric with its own similarity measure for classification problems. Therefore, and although not implemented in the present thesis, the use of this function could substitute completely the initial similarity measure used to extract cells p^1 and p^2. Probably this would be done at the expense of a larger algorithmic complexity and a different data structure given the number of parameters used.

Once we know the merit value for each contending cell, the application of a final function *predict()* gets the winner class to be attributed to p^x.

```
label predict(p1,p2)
{if (merit(p1) > merit(p2)
     return label(p1)
else
if (merit(p2) > merit(p1)
    return label(p2)
else return lmaj();
}
```

Fig 6.4 Function that predicts the label class for a new query p^x.

Trie-Class always assign a class to each new object under scrutiny. The *majority class* is attributed in the default case, on the condition that one of the two cell patterns p^1 or p^2 actually exhibit this class (which in the case of datasets with more than two classes might not be true). If it is not, the pattern holding the criterion with the largest weight value will be chosen instead.

7 Implementation

7.1 General overview

The drawing in Fig.7.1 shows the general idea on how Trie-Class algorithm is implemented. There are three main steps in the construction of our classifier: pre-processing data, building the required structures and running the classifier.

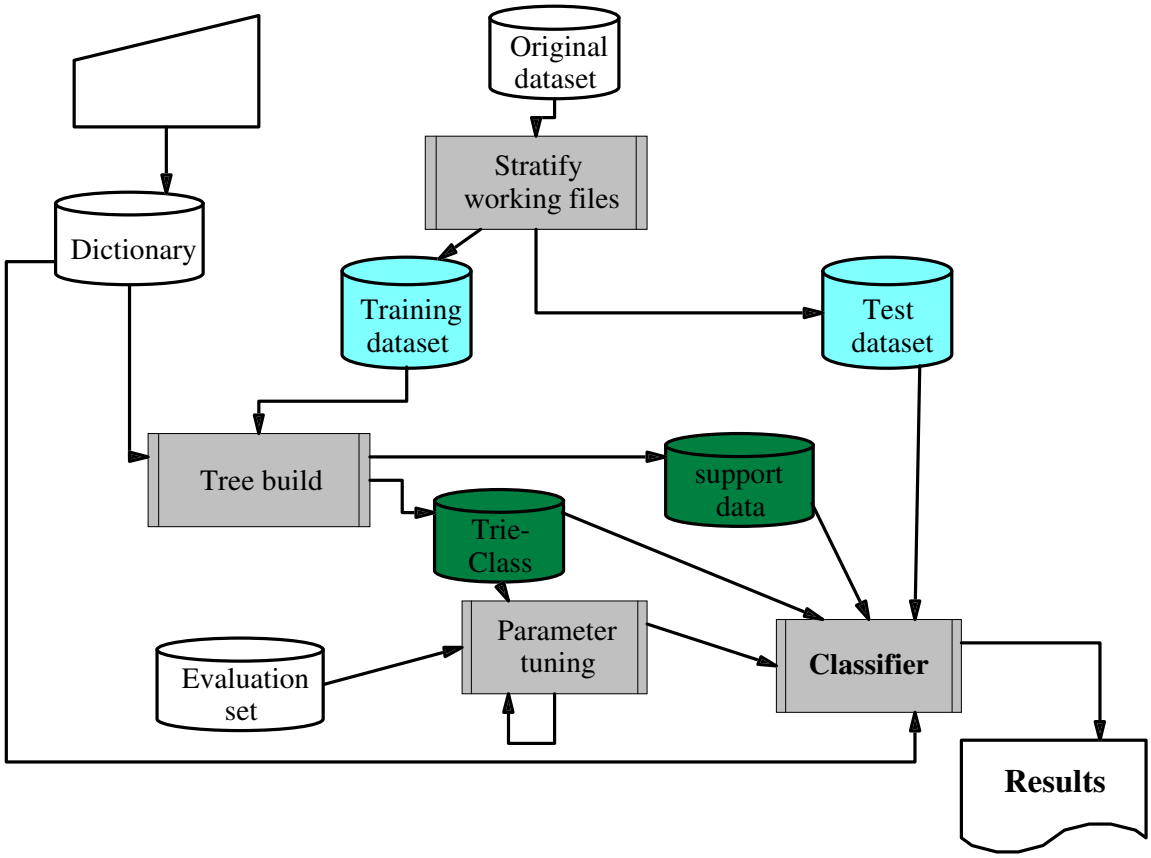


Fig 7.1 Trie-Class main modules

As every other algorithm learning by induction, Trie-Class begins by preparing the training and test datasets. The training file will be used for "learning" and evaluating the functioning of the algorithm. The test set is used once to finally classify unseen records. Sample stratification, explained in Section 4 is used to obtain these subsets.

All attribute records within these files are discretized. This discretization is done using interval values specified on the dictionary file for each attribute. In practice, in many cases of domains with small number of values, the discretization process does not alter the original values of an attribute and hence no domain compression takes place. For instance consider the famous Cancer dataset, which consist of 10 attributes, all with identical numeric domain values ranging from 0 to 10. If decided by the user, indicating an interval of 1 for each domain in the dictionary file would produce this effect.

Trie-Class can handle missing values in categorical attributes if they form part of the allowable values of an attribute.

Watching at the diagram it can be observed that the storage of records is not "*lazy"*, a characteristic of many instance-based methods.

Trie-Class uses a trie as tree structure to hold cell information, which will be used as patterns at classification time. This tree structure does not hold training data on its original format. *C-trie* keeps count on cell frequencies within each attribute interval. These frequencies are used by the *frequency* DP criterion as explained earlier in Section 6. Besides this tree, a second file is created, which contains supporting information needed by the algorithm. Basically it contains information on *semi-exclusive intervals,* as defined in Equation (3.22) by function *semk()*, as well as information on joint probability values for each symbolic attribute, needed for the distance calculations of symbolic attributes as stated in Definition 26 and Equation (4.2). As for the first type of information the file contains orderly lists of attributes. For each of them the file stores those intervals where the semi-exclusive property holds. As it was explained in Definition 19 in Section 3.4, the value of parameter ϕ is user-defined.

These two files appear labelled in Fig. 7.1 as "*Trie*" and "*supporting data"* respectively.

A dictionary permanently loaded into main memory during tree construction and classification completes the information for Trie-Class to work. It includes attribute information: data type, interval size, maximum and minimum values and a class flag. (For a complete layout of the dictionary see Annexe I).

In order to assign weights to decision parameters, Trie-Class divides the training set itself into training and evaluation sets with approximately 80 and 20% of records respectively. Decision parameters are tested against this last subset in order to decide

the weight to assign to each decision parameter. This last sub-process is iterative as depend on prediction error results, as suggested by the arrow pointing to itself in the par*ameter tuning* process of Fig. 7.1. Once decision parameters have their weights the classification algorithm is ready to run against test data.

In the rest of this chapter, we explain tree growing, its characteristics, related work and the search process. Finally, we argue that our search algorithm using best sub-cells to obtain p^1 when compared with regular k-NN methods as the sole decision criterion increases classification accuracy and decrease execution time.

7.2 Building a *trie* as the main tree structure

A fundamental and very well studied technique for storing and retrieving data is to use *m-ary* trees, also known as *digital trees, lexicographic trees* or simply *tries*, which is its most widespread name and the one we use in this thesis.

Tries were first proposed in [de la Briandais, 1959] although the term *trie,* taken from information re*trie*val has been given by [Fredkin, 1960]. Tries are used to store multimedia images, web pages, string matching, remote sensing imagery, genetic sequences, etc using all kind of trie variations: *Patricia trees* [Morrison, 1968], *Two-tries* [Aoe, 1996], *Triangulation tries* [Bergman, 1994], *R-trees* [Guttman, 1984], *Quadtrees* [Samet, 1984], *Burst Tries* [Heinz, *LC-tries* [Nilsson, 1999], among several others.

Along the paths of the tree these structures do not store data at the nodes, which is usually the case in regular trees. In a trie a set of strings from an alphabet containing *m* symbols is stored in a natural way in an *m-ary* tree where each string corresponds to a unique path. Branching at the j^{th} level is determined by the value of the j^{th} element from the key. There are two types of nodes in a trie: *branch* nodes containing only pointers to a number of children and *leaf* or *element* nodes, containing the string or key. Leaves have no children. The *root* of the trie contains disjoint index values representing the first letter or element of the string. At index position *i*, the pointer to the next letter points to the sub-tree of all words starting with that letter. A pointer to the j^{th} character of a key is located at the j^{th} level of the trie. All words containing a common prefix are located in the same path represented by the various node levels. Trie structures represent incomplete trees. Its leaves are not at the same level as shown in Figure 7.2.

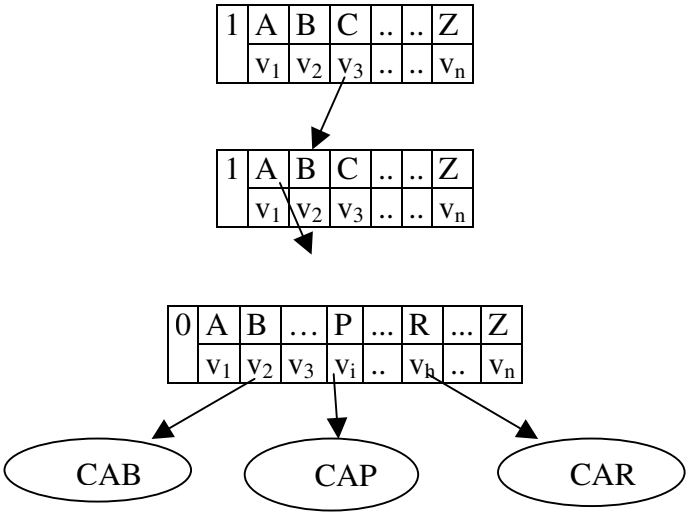


Fig. 7.2 Example of a classical trie after insertion of words

A leftmost binary field is sometimes used as a leaf indicator; a bit 0 indicates a leaf node; otherwise a branch node. Our own tree structure is show next in Fig. 7.3.

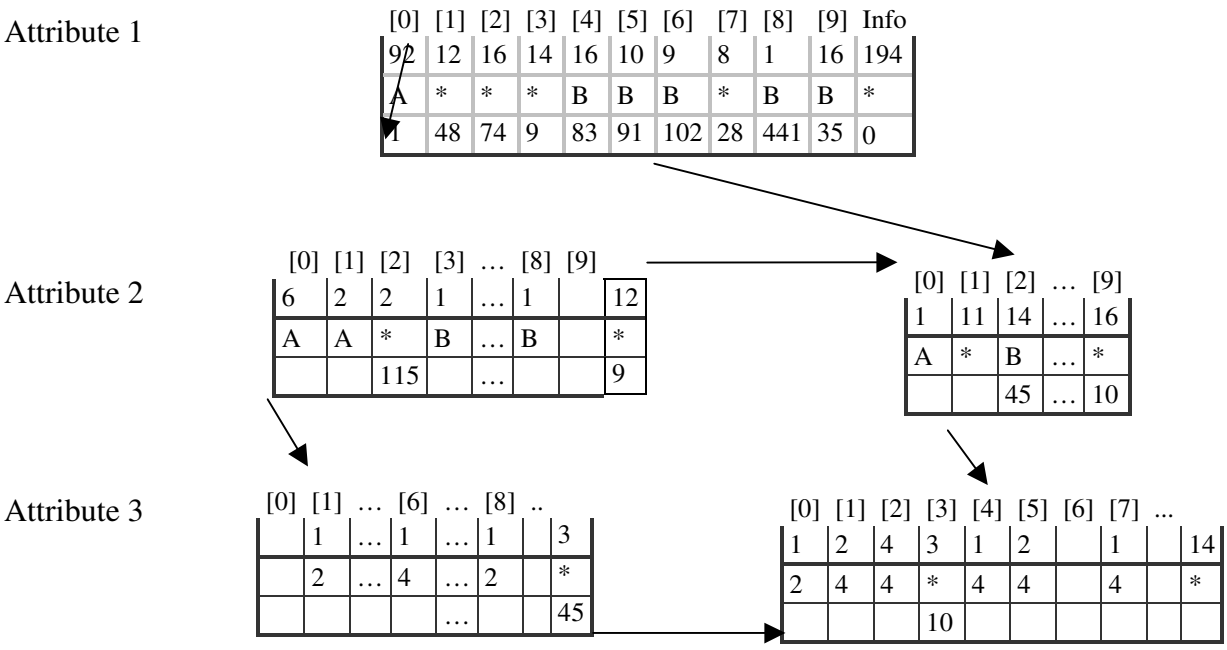


Fig. 7.3 Section of *C-trie* showing 3 equal domain attribute levels

This structure slightly differs from the classical *trie* structure.

From Equation (3.6) we know that each attribute value belonging to a record's sequence is converted into an integer value that we call *cell component* v_i. Its value ranges from 0 to s_i, which corresponds to the attribute's domain.

It is using the v_i component values from a cell vector p that the tree is built. Each cell component value serves as the branching factor. This structure is permanently stored in secondary memory. We call this tree the *C-trie.* As shown in Figure 7.3, every node in the *C-trie* is formed by an array of j attribute interval values corresponding to cell component value v_i. Like regular tries, *C-trie* is also a kind of deterministic finite automaton (DFA) [Cohen, 1990].

All input cells are n dimensional vectors. For this reason and contrary to normal tries *C-trie* contains a fixed number of levels, one for each of the n attributes in the cell vector. It also has no *leaves*, the last level corresponds to level n. The i^{th} tree level corresponds to the i^{th} cell component value v_i. Classes are not stored at leaves as is the case with decision trees. They are indicated at each index positions within a node. In the example of Fig 7.3 there are two classes *A* and *B*.

With the exception of the *root* node, all nodes in a level are linked together by pointers forming n linked-lists, thus making easier to travel along that level. Cells within each node have a record structure containing three pieces of information: a counter field *ctr* holding sub-cell frequency, a class *flag* indicator, and a pointer *ptr* to the next cell element down the tree. The class *flag* keeps track of sub-cell's class membership in a sort of "binary" fashion. As long as one or more identical sub -cells q_i from Equation (3.12) exhibits the same class, that class appears in the *flag* field at the i^{th} level. When a new cell p comes along for insertion, and its class c is different from the existing one at q_i, then the *flag* field becomes undetermined class-wise at sub-cell q_i, a fact marked with a '*' in the *flag* field. For instance, for interval 0 on the root node correspond a frequency of 92, a class "A" and pointer address of 1 pointing to next node. This means a unique class exists for this full cell throughout the dataset. However, for interval 1 with frequency 12, the class is '*', meaning that two or more sub-cells relate to two or more different classes. At some point along the cell path the class flag becomes associated with one class only. This corresponds to a cell *strength* defined in Equation (3.21). Every node contains an extra cell at the end of the array. It holds the sum of cell frequencies in a node, the general class observed in the entire partition and a

pointer to the next node of the same level. For instance in level 3, the leftmost node points to node number 45, the next node at the same level. This number coincides with the value of the pointer used by interval 2 in the rightmost node of level 2.

As is the case with other trees, such as the optimised *kd-tree* [Friedman et al, 1977] *C-trie* recursively subdivides the n^{th}-dimensional space using hyper planes orthogonal to the coordinate axes.

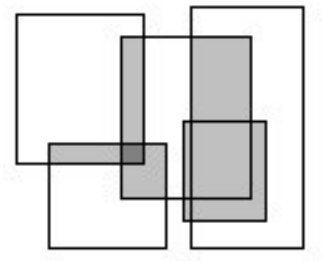


Fig. 7.4 Overlapped class regions in a two-dimensional space.

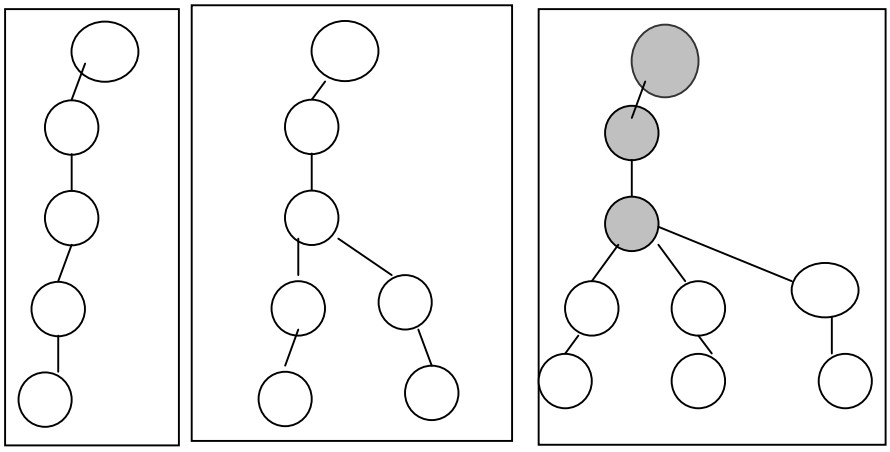
As one descends along any tree path, sub-cell cardinality decreases very rapidly. In the last level, it represents the number of identical cells *p* existing in the whole training file. Keeping track of frequencies can be very useful in determining isolated sub-cells that could result into *outliers*. Also, a map of frequencies like this can be useful to create clusters of similar cell prefixes, a task that comes almost naturally with the structure of tries.

An original contribution of Trie-Class with respect to the spatial class distribution is its ability to keep track of cell class membership at the sub-cell level. Overlapped and non-overlapped class areas are exactly mapped as shown in the example of Fig. 7.4 for two-dimensional data. In simple terms, overlap is the data space region covered by sub-cells where function $nlabels(q_i) > 1$ (see Definition 16 and Equation 3.20b) Example 7.1, illustrate the same with vectors of numeric value.

Example 7.1

Imagine we insert into a trie cell p^1 = <*3,1,1,1,3,"A"*> with class "A" as shown in Fig.7.5 (a). A second cell p^2 = <*3,1,1,3,2,"A"*> is inserted next in 7.5(b) also with the same class. In 7.5(c) a cell p^3 = <*3,1,1,7,4,"B"*> is introduced.

Sub-cell q_3 = <*3,1,1, u*> becomes immediately overlapped. By this we mean that from the point of view of classes, two classes *"share"* the same prefix.



(a) (b) (c)

Fig. 7.5 Overlap class regions in the hyperspace

From sub-cell q_4 onwards, sub-cells are associated with just one class, which correspond to class *"A"* in the case of cells p^1 and p^2 and *"B"* in the case of cell p^3.

The information contained in these overlapped and non-overlapped class distribution regions is used for class assignment of new instances.

7.3 Insertion algorithm

Trie-Class creates its trie incrementally as described next in Table 7.1.

```
Create empty node as root;
for each training record r ∈ R:
    node_number ← 0;   /*all insertions begin at root node */
    c ← label(r);          /* obtain cell class */
    for  each attribute a_i ∈ r , i[1 n], do:
          v ← ord(a_i)   /* discretize the attribute value */
          counter[v] ← counter[v] + 1;
          if  class[v] = nil class[v] ← c;
          else
                If  c not equal to class[v]
                    class[v] ← '*';  /* undefined class */
          If   address[v] = nil  /*create a new node only if necessary; */
               node ← new sequential file record
          address[v] ← node;
          update node;
          node_number ← address[v];
    end;
end.
```

Table. 7.1 Pseudo-code for insertion algorithm

Each new attribute is inserted in a new node unless it exists before. Therefore, cell sub-cells exhibiting identical attribute values share the same nodes including up to the point where the last cell component elements differs from each other. From there on, new nodes will be created for the remaining cell component elements.

Each attribute belonging to a cell is inserted in a node representing consecutive tree levels. Attributes are all linked together by the corresponding address fields.

7.4 Discussion on the actual implementation

Very high in the list of desired performance capabilities for a good near neighbour engine algorithm is the need for a fast, efficient retrieval algorithm. The reason for using tries is that these structures have proven to be very fast on search problems [Bergman, 1994;Merret et al., 1996; Alber et al., 2001]. Tries also have excellent retrieval

properties for spatial data when dealing with a large number of dimensions in datasets [Aoe, 1996; Merret, 1996] as well as for approximate searching of similar objects such as remote sensing images [Alber, 2001] or similar but not identical cells as do it here.

From the insertion algorithm of previous section, we see that only required nodes for new sub-cells are created. In other words all cell prefixes shares the same nodes. This is a characteristic of regular tries. Exploiting this overlap of paths near the root helps in achieving some degree of natural compression, which depends on cells spatial distribution.[Merret, 1996]. Additional compression in front of dataset with a large number of dimensions, could be achieved by using compression schemes such as a DAWG graph [Appel, 1988] or the double array TAIL presented by [Aoe, 1989] which share all transition states, or using a single node to stack common cell prefixes [Aoe, 1996], [Andersson, 1994]. There are still several known mechanisms offered to compress trie size such as *Patricia trees* [Gonnet et al., 1991], *X-tree* [Berchtold et al., 1996] and *Burst tries* [Heinz et al., 2002] among others.

Nevertheless, all these compression schemes in our case would reduce even further information on cells, already limited by discretization. Also, some of these compress mechanisms require going through the input file more than once to achieve its purposes. At this point, we want to remember the fact that our purpose is not perfecting trie compression techniques, but to produce a simple, efficient and accurate classification algorithm.

In any case, very large dimension datasets pose a space problem. If compression is desired for these cases, it could be achieved by one of the following simple methods. The first one would be splitting *C-trie* into sub-trees holding different index ranges, although this might influence I/O access time. The second and more important would be to compress the first levels of the tree up to the point where sub-cells become associated with classes, leaving all remaining suffixes in some linked list. Although this operation would require processing a second time the training file, tree size would be smaller. Suffix elements could also be keep in remaining common nodes.

Perhaps the best alternative would be creating a forest of trees each one holding only cells of the same class. Each structure would represent the spatial distribution of one class in the total data hyperspace. Searching the closest elements in these trees would be carried on each tree using the same method as the one we use in Trie-Class. Several

small subsets of close neighbours each belonging to one class would participate in the final selection process using decision parameters. In these trees, equal binning discretization method would have no importance whatsoever in terms of information loss. It remains to see the time complexity of such forest structure.

Mixing strategies for tries is not new as a mean to balance its fast searching capabilities with a large space usage [Knuth, 1997]. In both cases though, searching for identical or similar cells would increase search time costs by introducing sequential search mechanisms in these "big" nodes or linked lists. Compression techniques seem to be consistent with the fact that the most relevant attributes are indeed first located into the tree and these common prefixes are indeed strong representatives of the correct mapping between cells and classes.

The search process described in Section 3.7 is constant and independent of the size of the training file, a very important factor. This search process could be also considered as searching in an ordered file as a matrix of *i* rows and *j* columns, with the search done on columns represented by the ordered array of nodes, as is the case with some algorithms such as [Micó, 1996]. The search is done starting from the i^{th} column corresponding to a given element value in a circular way increasing the radius each time by one unit, looking each time to the next elements [i+1] and [i –1] discarding all others as soon as an existing cell value is found. For this reason algorithm's complexity is constant and equal to $O(\log n)$ on the average case.

Search time is always constant in Trie-Class, unless used the "*look ahead*" mechanism. Search complexity is logarithmic, if we use total nodes visited as a measure of complexity, as done in other cases [Yanilos, 1993].

Keeping the count of frequencies at sub-cell level allows us to have a graphical distribution of cell density. This not only helps in breaking ties when selecting neighbour elements within a given node, as it could be used to extend the use of this structure for *clustering* as well [Anderberg, 1973].

Search time is fast in *C-trie*. Taking advantage of array indexing, for any given index value *j* we look for existing cell values to the "left" starting at *j, j*-1,..0, and to the right starting at *j*+1 within interval [1..i]. Once cell(s) found within the node, we eliminate from the search the rest of the tree, concentrating in the following sub-tree. This is equivalent to take into account the triangle inequality [Burkhard, 1973] to significantly

reduce the number of direct distance calculations needed for an efficient search algorithm as in [Berman, 1999]. The search phase is done in $O(n_i)$ time complexity.

Trie-Class can learn, due to the fact that is persistent. New training cells can be easily added. Record deletion is more complicated but is not considered as a functional part of the algorithm. Changing the training file is interpreted as growing again a new tree.

It should not be neglected the fact that *C-trie* was designed to hold a sample from the database, whose only requirement is to be representative of the data in the statistical sense. This means that most of the time we are dealing with a manageable number of records.

Although the actual structure for prototyping is done using dynamically sized arrays for every node, linked lists could also be used to save array size in sparse distributions. As it is well known, this structure unless indexed, has a drawback of a sequential search. Alternatively, *hashing* tables containing internal node indexes could also be used, but constructing them requires also extra time.

7.5 Dictionary and other supporting files

Like many other data mining applications, ours also use a user-provided dictionary file. Basically it contains information on all attributes, the type of data, i.e. numeric discrete, continuous or symbolic, the minimum and maximum possible values they can take (their domain), the size of the interval to be used as a domain partition in the tree structure and a flag indicating whether this is the class field or not.

An example of the dictionary can be found in the Appendix I.

It is worth saying at this point that with an extra single read of the training sample most of this information could be automatically detected. The only requirement to be supplied by the user would be the size of the interval for each attribute. This information is crucial for tree construction, and allows the user adjust algorithm efficiency by altering the interval for whichever attribute. This user interface with the software is very important for all classification algorithms in data mining, where to a large degree they play a key role in the success of the end result. There is nothing compared with this knowledge, if such knowledge exists, and cannot be overlooked with the obsession of automation.

Along with *C-trie* and dictionary files Trie-Class uses a couple more of files containing information devoted to two different purposes.

One of them is to keep information on *semi-exclusive intervals* as defined in Equation (3.22), which is basically an ordered table keeping for each attribute and partition interval, values which relate to one class only. These are sometimes called *"pure attributes"* [Breiman, 1984] or *"primary"* [Turney, 1996] in the literature. These attributes are informative of the class when considered by themselves [Kohavi, 1997].

Optionally, the user can decide to have this file information somehow softened: the information contains interval values for those attributes where one of the classes holds a user-defined threshold percentage of the number of training cells. Whichever the degree of exclusiveness is selected, this file is used at generalization time when cell values are checked for the presence of one or more of these values.

A second file, also on disk is used to keep information on symbolic attributes frequencies. For each symbolic attribute the file keeps one record for each class containing the frequency of each value. These are used in the distance calculation for these types of attributes, specifically in the calculation of the joint probability $P(v \cap c)$ already explained in Section 4.2.

These two files appear under the name "support data" in the diagram of Fig. 7.1.

8 Conclusions and Future work

In this dissertation, we explored specific paradigms for data classification, namely, decision trees and instance-based methods in an effort to develop an experimental algorithm able to improve some of its aspects while simplifying algorithmic complexity.

The order of the conclusions presented here is arbitrary with respect to its importance degree. Rather, we have followed the sequential order in which these topics appear on this work.

There are literally dozens of algorithms to solve classification problems in the literature. Our approach was in general to keep it as simple as possible, considering the truthfulness of the well-known paradigm of the Minimum Description Length principle. Within this context we did retain two of the more popular methods, *instance-based* and *decision trees* as inspiration to develop our own. From the first one we took the main idea of not using a central model developed to classify all records – as done for instance in decision trees - but to use training records themselves as patterns to locally represent on each case the best model to assign its class to some unknown query. From the second of these methods, we have taken the idea of using a tree to store actual records as a means of rapidly searching records in the data hyperspace. This is as far as it goes the similarity between our algorithm and decision trees because in this kind of paradigm tree nodes are used as threshold decision values that together represent a general model used to classify in the same manner all test records. In our case, the use of a trie serves only the purpose of an index with very fast access, but not as a generator of a classification model. In fact our algorithm in this respect has a totally opposed behaviour to decision trees and it is similar to the nearest neighbour method.

Trie-Class use a simple algorithm overall, formed by small contributions along the various phases of the Data Mining process.

- The development of the concept of *sub-cells,* as a method for early class identification as well as pattern characterization for model selection (Section 3.3).
- A sub-optimal search method for the extraction of near neighbours, different from the traditional distance calculation, which gives elimination power to more relevant attributes (Section 3.7).

- A simple mechanism to differentiate relevant and non-relevant attributes using a one-dimension projection of attribute values and *semi-exclusive* intervals (Section 4.3).
- The use of *joint probabilities* to solve the distance calculation problem in the presence of symbolic attributes (Section 4.2).
- The use of Decision Parameters in the final pattern selection process uses concepts such as cell *strength*, *semi-exclusivity* and *shapes* (Section 6.1). These parameters enrich the information about objects. By having a weight according with training data characteristics (Section 6.3), they adapt the algorithm to the data under inspection.

8.1 Conclusions

Our experimental results from Section 5 show that on average Trie-CLASS performs at least as good as several of the leading classifiers reported, whether this comparison is done against classifiers running in our test bench or whether we compare with results found in the bibliography[18]. In particular this is true with respect to the landmark classifier C4.5 [Quinlan, 1986] and the instance-based learning *k-NN* algorithm [Aha, 1991]. In eleven out of thirteen files compared against C4.5, ours was better. It also appears clear from these figures that Trie-Class performs equally well with various types of data, numeric or symbolic as well as average dataset sizes and dimensions. Our figures also show that Trie-Class has poorer results when the number of classes is greater than two, perhaps due to the fact that the actual algorithm is only implemented to extract two cell patterns representing two different classes.

A clear improvement over regular *NN* methods is the search mechanism used to extract selected records using a greedy strategy. Trie-Class extracts near objects using the concept of similarity in turn assimilated to a distance calculation. Its searching method restricts the search area within the trie according with previous values found at sub-cell levels, thus avoiding the visit to all unnecessary tree branches. The extraction of additional cells restricts even further the search space, as its class must be different

[18] As new results on classifiers performance appear every day in the literature, some of our figures could be out of date.

from the class of the previous cells extracted. Overall, reduced areas of the data space are searched to obtain close neighbours.

Greedy search strategies are in general sub-optimal, as they can loss better solutions. The counter part to this been that some complex algorithmic problems can find some acceptable solution. Our results, mixing a greedy search with look-ahead for ties situations prove to be encouraging. In fact, Trie-Class obtain better results than *IBk*, a Weka implementation of a *k-NN* algorithm, when the value of $k = 1$.

Feature subset selection is the process of identifying and removing as much irrelevant and redundant information as possible. Searching the feature space within reasonable time is necessary, especially for the case o data with large number of features. For this reason reducing data dimensionality is dealt using a heuristic search strategy as opposed to an exhaustive search of the feature space prohibitive most of the time. They are more feasible and can give good results, although they do not guarantee finding the optimal subset. Regularities on data are found in Trie-Class using every other feature one at a time, independently from others using a previously discretized single-dimension space. Using this criterion attributes can be ordered by degree of relevance, allowing the removal of irrelevant values without diminishing severely classification accuracy. Feature selection is done before tree growth. Most relevant attributes produce the initial data space divisions and thus most similar objects remains close, a problem affecting several classification algorithms. This fact also influences distance calculation, because more elimination power is given to more relevant attributes largely reducing the search space.

We have already said that Trie-Class extracts two near cells as a first approximation to classify new objects. In a next step it uses a "voting" mechanism to make a final decision that is different from all other *k-NN* algorithms we know of. This selection is done through the use of *decision parameters,* which allow the extraction of further information from pre-selected cell patterns. This represents richer knowledge about these competing neighbours, a procedure that goes beyond the standard mechanism of using *distance* as the sole criterion. Moreover, decision parameters are weighted according with its ability to classify new records, dynamically adapting the whole algorithm to the changing characteristics of data. This adaptation of the algorithm constitutes an important step towards fighting the known fact that not all classification

algorithms performs equally well with different datasets. We have no knowledge of these technique been used before.

Distance calculation for symbolic attributes constitutes a problem of its own, dealt in different ways by different authors. Trie-Class uses a heterogeneous mechanism depending on the type of value (discrete, continuous or symbolic). In the specific case of symbolic attributes it uses a simple mechanism of low complexity based on the joint probability distribution of classes within attributes and its corresponding values, resembling somehow the functioning of Bayesian Networks at a given node. This mechanism works better than the simple overlap solution and is cheaper in complexity than more sophisticated methods.

The choice of using a multi-way tree indexed on attribute values works as a very fast index and we believe it is a good solution for the type of search carried on. It has been demonstrated that this structure allows a very fast search and presents a low computational complexity for the required type of proximity search [Bentley, 1997] as well as in the case of large multimedia databases. Contrary to standard tries, useful information represented by records class membership is not found at tree leaves but at each tree level, i.e. associated with sub-cells, allowing the drawing of a very useful class map in the data space. Moreover, difficult choices of threshold values as in the case of decision trees are avoided.

In this structure search time is independent of the file size and exhibit low algorithmic complexity, a problem found in many search methods as our results show with respect to execution time.

The gain we obtain with a fast search has the cost of sometimes using a larger disk space, as our data structure is disk resident. As disk space has sky rocketed in terms of capacity, and at the same time with systematic decreasing prices and increasing access speeds in the last decade, our choice seems to be adequate. In any case, the eventual use of pruning at the level of sub-cells or prefixes belonging to a single class can diminish easily tree size, not to mention the fact that Trie-Class requires only a representative sample not the entire population in order to classify and thus the size of the required structure is always under control. The algorithm implemented by Trie-Class can be alternatively implemented using any database management system. This could simply

handle all required data and carry the search mechanism using some of the existing database techniques.

8.2 Future work

Trie-Class extracts two near neighbours in order to select the class of one of them as the class to assign to a new query object. In this respect, as a proposal for further work, an obvious way of decreasing tree size and perhaps improve classification accuracy in datasets with more than two classes, would be the use of a forest with as many trees as classes exist in a given dataset. Each one of these trees would hold records belonging to one class only. At search time the actual search algorithm would be used to extract one or two cell patterns per tree, each one of them associated with a single class.

Trie-Class tree structure called *C-trie* allows the identification of classes at the sub-cell level. Manipulating this map of classes would allow a graphical representation of clusters of classes and its frequencies.

Clustering techniques could be easily implement with Trie-Class, an aspect in Data Mining that was out of the scope of this work. As clusters represent objects with common characteristics, all six *decision parameters* are a good solution to identify these common objects, especially applied at sub-cell levels. The application of these criteria would extend the use of distance as the sole similarity criterion used in many clustering algorithms, allowing a richer similarity concept and thus allowing the selection of clusters with a strong internal strength. In this sense, Trie-Class can become a bivalent tool, allowing the implementation of classification as well as clustering techniques.

One of the decision parameters used to select the best representative pattern is *shapes*, a vector of values representing inter-attribute relationships, which are used to identify pattern similarity. Considering the encouraging results of this decision parameter in classification, it would be worth investigating further the possibility of creating a whole new metric space using this shape criterion.

Finally, another aspect not implemented in this thesis is the fact that we use decision parameters and the *merit()* function as a mean of selecting the most representative cell pattern. We could well substitute the original search mechanism to extract near neighbours all together and replace it by the value provided by this function. Thus, it would be used to define a new similarity metric. This might represent a richer similarity

concept if compared with the use of distance as the only similarity criterion between objects.

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Appendix I. Example of Dictionary corresponding to the Annealing Dataset

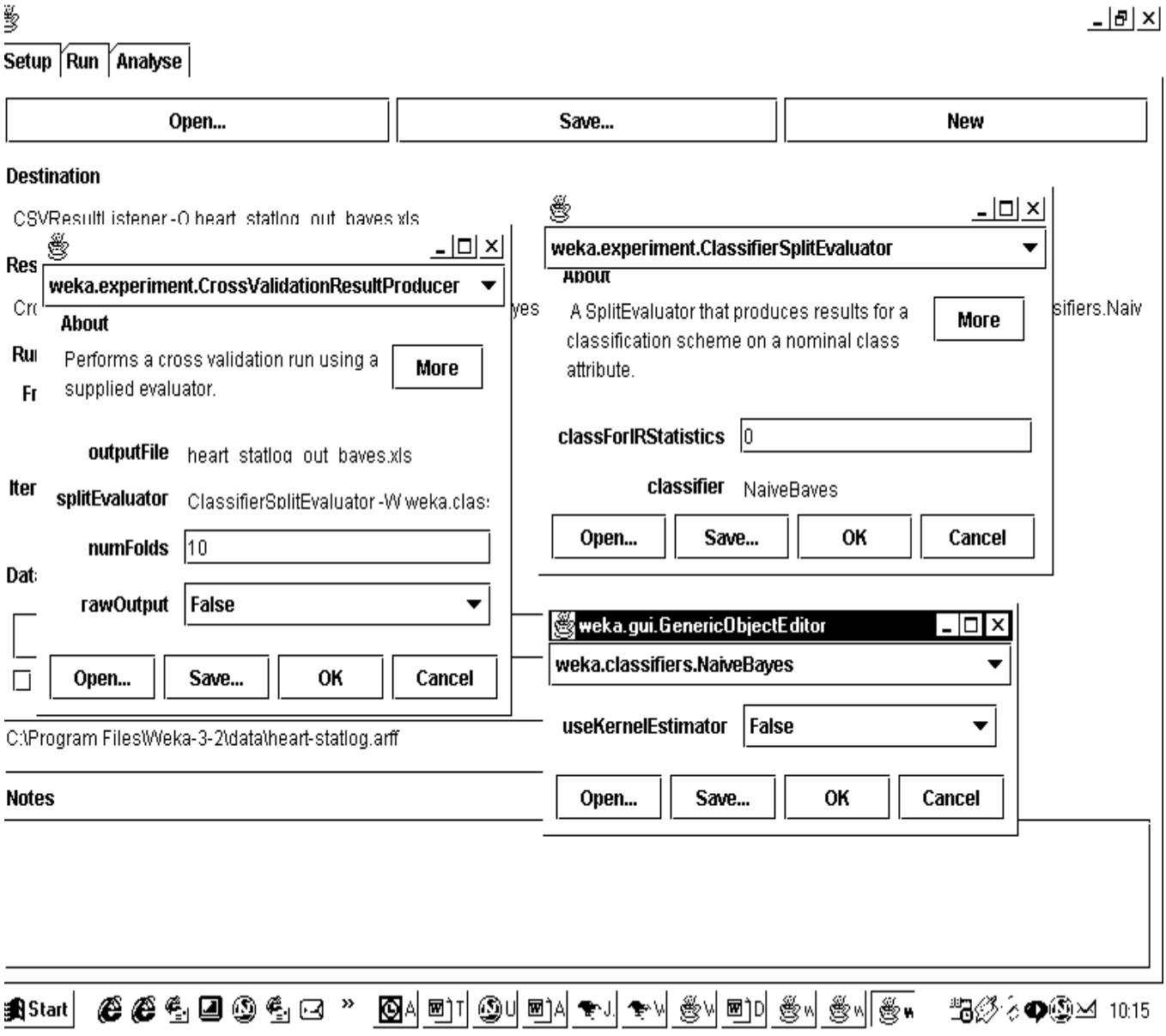
Each line contains the following elements:
Number, description, Type, initial value, end value, interval size, class flag, #,symbolic values.
Allowable types: N=discrete, R=continuous, D=symbolic known values, S= symbolic unknown values, C=Class

---

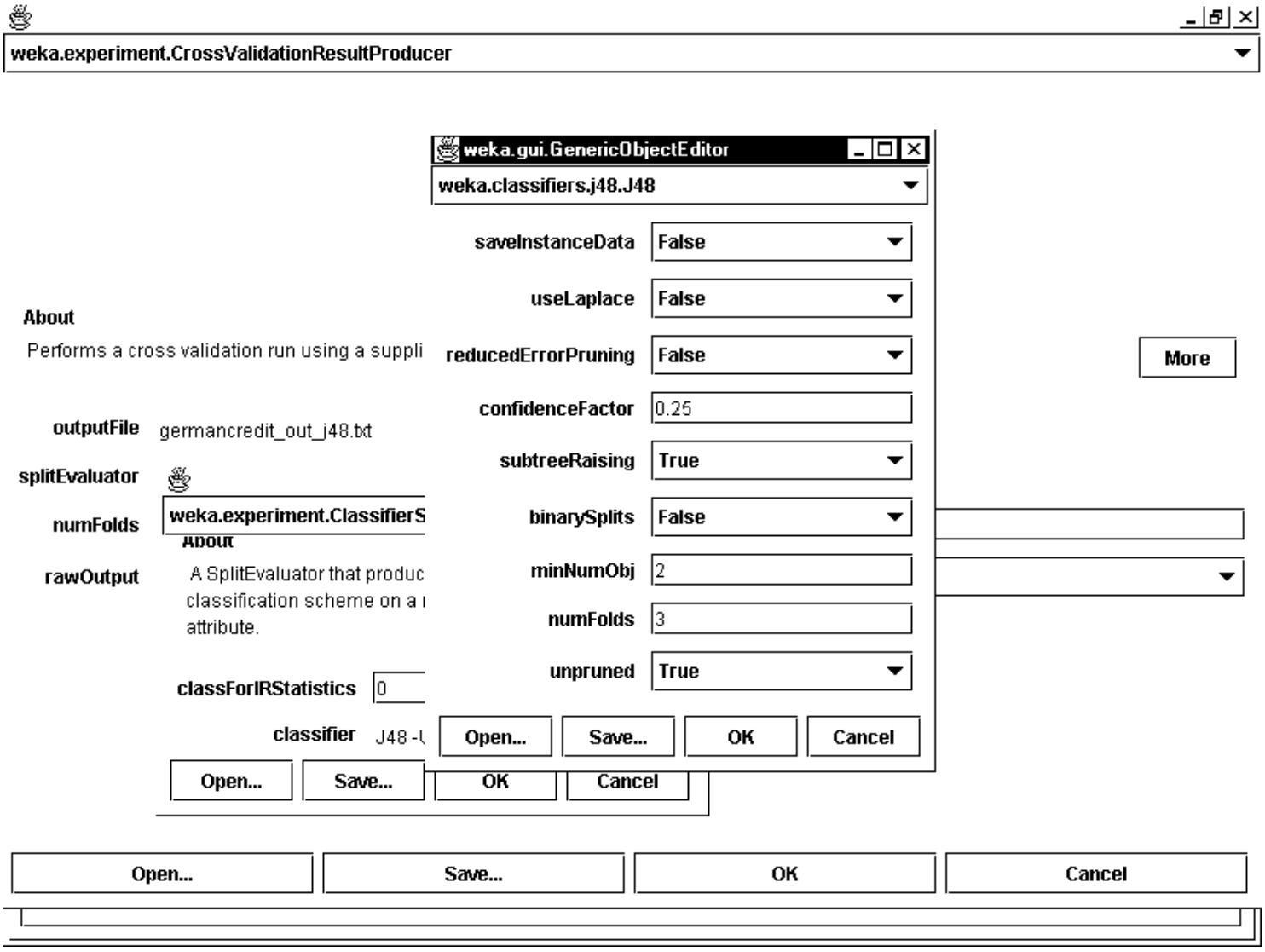
1,	hardness,		N,	0,	85,	1,	N
2,	width,		R,	0,	1525,	20,	N
3,	surface-quality,		D,	0,	6,	1,	N,#,-,D,E,F,G,
4,	carbon,		N,	0,	70,	1,	N
5,	steel,		D,	0,	10,	1,	N,#,-,R,A,U,K,M,S,W,V,
6,	family,		D,	0,	11,	1,	N,#,-,GB,GK,GS,TN,ZA,ZF,ZH,ZM,ZS,
7,	strength,	N,	0,	700,	10,	N	
8,	chrom,		D,	0,	3,	1	,N,#,C,-,
9,	oil,		D,	0,	4,	1,	N,#,-,Y,N,
10,	ferro,		D,	0,	3,	1,	N,#,Y,-,
11,	len,		R,	0,	4880,	40,	N
12,	enamelability,		D,	0,	7,	1,	N,#,-,1,2,3,4,5,
13,	surface-finish,		D,	0,	4,	1,	N,#,P,M,-,
14,	formability,		D,	0,	7,	1,	N,#,-,1,2,3,4,5,
15,	packing,	D,	0,	5,	1,	N,#,-,1,2,3,	
16,	phos,		D,	0,	3,	1,	N,#,P,-,
17,	exptl,		D,	0,	3,	1,	N,#,Y,-,
18,	BlueBrightVarnClean,		D,	0,	6,	1,	N,#,B,R,V,C,-,
19,	product-type,		D,	0,	4,	1,	N,#,C,H,G,
20,	temper_rolling,		D,	0,	3,	1,	N,#,-,T,
21,	condition,		D,	0,	5,	1,	N,#,-,S,A,X,
22,	non-ageing,		D,	0,	3,	1,	N,#,-,N,
23,	bc,		D,	0,	3,	1,	N,#,Y,-,
24,	bf,		D,	0,	3,	1,	N,#,Y,-,
25,	bt,		D,	0,	3,	1,	N,#,Y,-,
26,	bw/me,		D,	0,	4,	1,	N,#,B,M,-,
27,	bl,		D,	0,	3,	1,	N,#,Y,-,
28,	m,		D,	0,	3,	1,	N,#,Y,-,
29,	cbond,		D,	0,	3,	1,	N,#,Y,-,

30,	marvi,	D,	0,	3,	1,	N,#,Y,-,
31,	corr,	D,	0,	3,	1,	N,#,Y,-,
32,	lustre,	D,	0,	3,	1,	N,#,Y,-,
33,	jurofm,	D,	0,	3,	1,	N,#,Y,-,
34,	s,	D,	0,	3,	1,	N,#,Y,-,
35,	p,	D,	0,	3,	1,	N,#,Y,-,
36,	shape,	D,	0,	3,	1,	N,#,COIL,SHEET,
37,	thick,	R,	0,	4000,	40,	N
38,	bore,	D,	0,	5,	1,	N,#,0000,0500,0600,0760,
39,	classes,	C,	0,	5,	0,	S

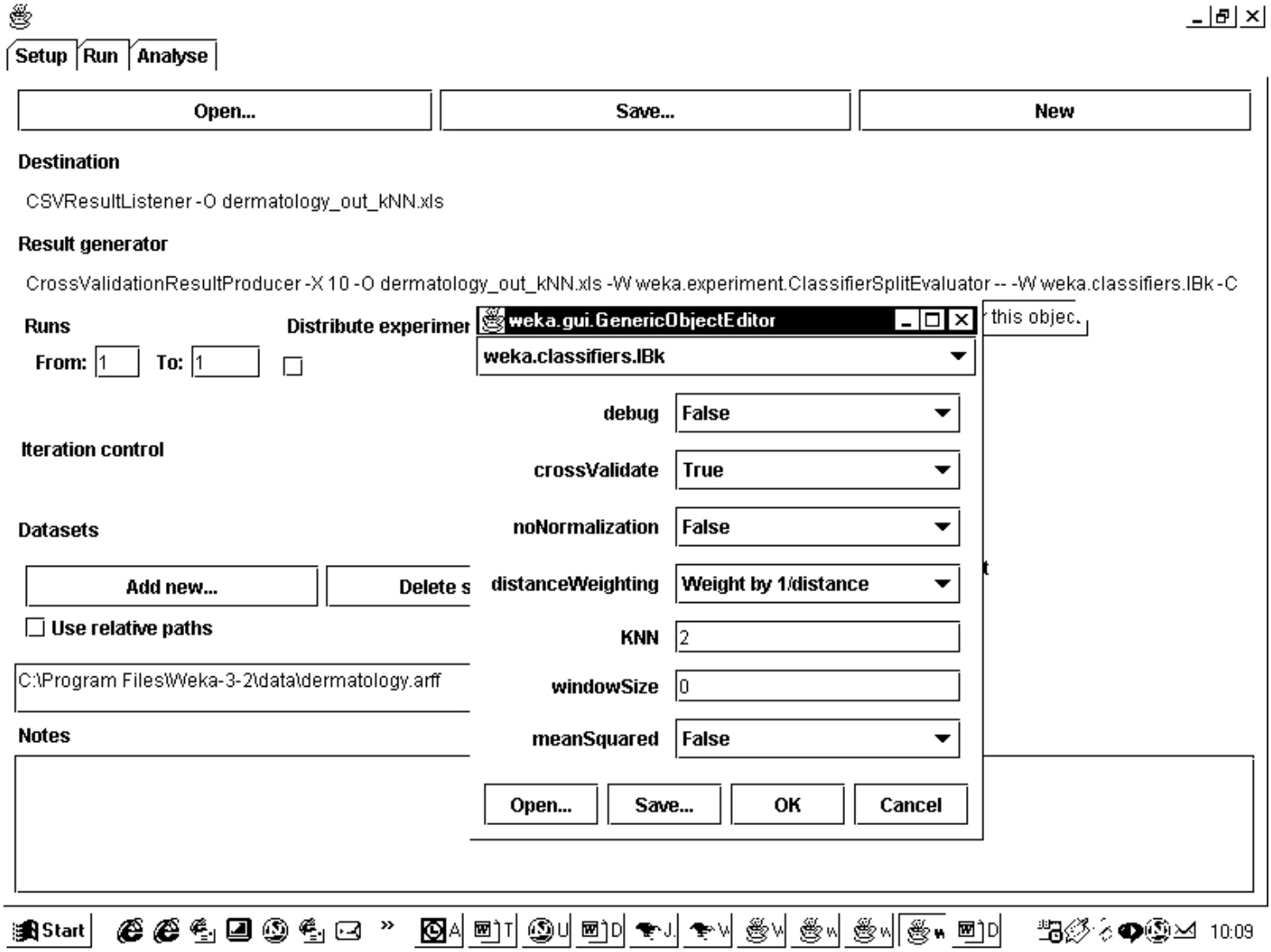
Appendix II. Settings for the execution of the Naive Bayes classifier



Parameter values settings for the execution of the J48 (C4.5) classifier.



Parameter values settings for the execution of the IBk (k-NN) classifier.



Appendix III. Alpha values for Decision Parameters

Table A-1 Weights (alpha) for various ambit and precision values expressed in percentage

ambit	precision	alpha	ambit	precision	alpha
10	10	53	50	60	282
10	20	72	50	70	301
10	30	91	50	80	320
10	40	111	50	90	339
10	50	131	50	100	359
10	60	151	60	10	233
10	70	171	60	20	247
10	80	191	60	30	263
10	90	211	60	40	281
10	100	230	60	50	298
20	10	88	60	60	316
20	20	106	60	70	335
20	30	124	60	80	354
20	40	144	60	90	373
20	50	163	60	100	392
20	60	183	70	10	269
20	70	202	70	20	283
20	80	222	70	30	299
20	90	242	70	40	316
20	100	262	70	50	333
30	10	124	70	60	351
30	20	141	70	70	369
30	30	158	70	80	388
30	40	177	70	90	406
30	50	196	70	100	425
30	60	215	80	10	306
30	70	235	80	20	320
30	80	254	80	30	335
30	90	274	80	40	351
30	100	294	80	50	368
40	10	160	80	60	386
40	20	176	80	70	403
40	30	193	80	80	422
40	40	211	80	90	440
40	50	230	80	100	459
40	60	249	90	10	342
40	70	268	90	20	356

40	80	287	90	30	371
40	90	306	90	40	387
40	100	326	90	50	403
50	10	196	90	60	421
50	20	211	90	70	438
50	30	228	90	80	456
50	40	246	90	90	474
50	50	264	90	100	493