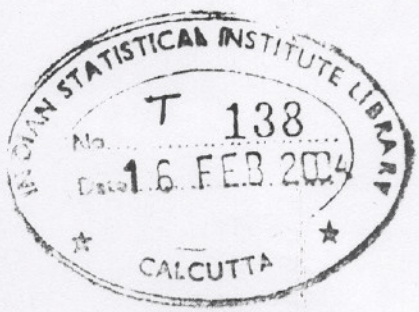
CERTAIN PATTERN RECOGNITION TASKS FOR DATA MINING PROBLEMS

Pabitra Mitra
Machine Intelligence Unit
Indian Statistical Institute
Kolkata - 700108
India.



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In the Lotus Feet of Mother

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pabitra Mitra
(Pabitra Mitra)

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Chapter 1

Introduction and Scope of the Thesis

1.1 Introduction

Pattern recognition (PR) is an activity that we humans normally excel in. We do it almost all the time, and without conscious effort. We receive information via our various sensory organs, which is processed instantaneously by our brain so that, almost immediately, we are able to identify the source of the information, without having made any perceptible effort. What is even more impressive is the accuracy with which we can perform recognition tasks even under non-ideal conditions, for instance, when the information that needs to be processed is vague, imprecise or even incomplete. In fact, most of our day-to-day activities are based on our success in performing various pattern recognition tasks. For example, when we read a book, we recognize the letters, words and, ultimately, concepts and notions, from the visual signals received by our brain, which processes them speedily and probably does a neurobiological implementation of template-matching!

The discipline of Pattern Recognition (or pattern recognition by machine) essentially deals with the problem of developing algorithms and methodologies/devices that can enable the computer-implementation of many of the recognition tasks that humans normally perform. The motivation is to perform these tasks more accurately, or faster, and perhaps, more economically than humans and, in many cases, to release them from drudgery resulting from performing routine recognition tasks repetitively and mechanically. The scope of PR also encompasses tasks humans are not good at, like reading bar codes. The goal of pattern recognition research is to devise ways and means of automating certain decision-making processes that lead to classification and recognition.

Machine recognition of patterns can be viewed as a two-fold task, consisting of learning the invariant and common properties of a set of samples characterizing a class, and of deciding that a new sample is a possible member of the class by noting that it has properties common to those of the set of samples. The task of pattern recognition by a computer can be described as a transformation from the measurement space $\mathcal{M}$ to the feature space $\mathcal{F}$ and finally to the decision space $\mathcal{D}$, i.e.,

$$\mathcal{M} \rightarrow \mathcal{F} \rightarrow \mathcal{D}.$$

Here the mapping $\delta : \mathcal{F} \rightarrow \mathcal{D}$ is the decision function, and the elements $d \in \mathcal{D}$ are

termed as decisions.

PR has been a thriving field of research for the past few decades, as is amply borne out by the numerous books [30, 32, 41, 118, 123, 125] devoted to it. In this regard, mention must be made of the seminal article by Kanal [61], which gives a comprehensive review of the advances made in the field till the early nineteen-seventies. More recently, a review article by Jain *et al.* [60] provides an engrossing survey of the advances made in statistical pattern recognition till the end of the twentieth century. Though the subject has attained a very mature level during the past four decades or so, it remains evergreen to the researchers due to continuous cross-fertilization of ideas from disciplines like computer science, physics, neurobiology, psychology, engineering, statistics, mathematics and cognitive science. Depending on the practical need and demand, various modern methodologies have come into being, which often supplement the classical techniques [111].

In recent years, the rapid advances being made in computer technology have ensured that large sections of the world population have been able to gain easy access to computers on account of falling costs worldwide, and their use is now commonplace in all walks of life. Government agencies, and scientific, business and commercial organizations are routinely using computers not just for computational purposes but also for storage, in massive databases, of the immense volumes of data that they routinely generate, or require from other sources. Large-scale computer networking has ensured that such data has become accessible to more and more people. In other words, we are in the midst of an information explosion, and there is urgent need for methodologies that will help us bring some semblance of order into the phenomenal volumes of data that can readily be accessed by us with a few clicks of the keys of our computer keyboard. Traditional statistical data summarization and database management techniques are just not adequate for handling data on this scale, and for extracting intelligently, information or, rather, knowledge that may be useful for exploring the domain in question or the phenomena responsible for the data, and providing support to decision-making processes. This quest had thrown up some new phrases, for example, *data mining* and *knowledge discovery in databases (KDD)* [24, 37, 38, 51, 52, 55].

The massive databases that we are talking about are generally characterized by the presence of not just numeric, but also textual, symbolic, pictorial and aural data. They

may contain redundancy, errors, imprecision, and so on. KDD is aimed at discovering natural structures within such massive and often heterogeneous data. Therefore PR plays a significant role in KDD process. However, KDD is being visualized as not just being capable of knowledge discovery using generalizations and magnifications of existing and new pattern recognition algorithms, but also the adaptation of these algorithms to enable them to process such data, the storage and accessing of the data, its preprocessing and cleaning, interpretation, visualization and application of the results, and the modeling and support of the overall human-machine interaction.

Data mining is that part of knowledge discovery which deals with the process of identifying valid, novel, potentially useful, and ultimately understandable patterns in data, and excludes the knowledge interpretation part of KDD. Therefore, as it stands now, data mining can be viewed as applying PR and machine learning principles in the context of voluminous, possibly heterogeneous data sets [111].

The objective of the thesis is to provide some results of investigations, both theoretical and experimental, addressing certain pattern recognition tasks essential for data mining. Tasks considered include data condensation, feature selection, case generation, clustering, classification and rule generation/evaluation. Various methodologies have been developed using both classical and soft computing approaches (integrating fuzzy logic, artificial neural networks, rough sets, genetic algorithms). The emphasis of the proposed methodologies is given on (a) handling data sets which are large (both in size and dimension) and involve classes that are overlapping, intractable and/or having nonlinear boundaries, and (b) demonstrating the significance of granular computing in soft computing paradigm for generating linguistic rules and dealing with the knowledge discovery aspect. Before we describe the scope of the thesis, we provide a brief review of pattern recognition, knowledge discovery in data bases, data mining, challenges in application of pattern recognition algorithms to data mining problems, and some of the possible solutions.

Section 1.2 presents a description of the basic concept, features and techniques of pattern recognition briefly. Next, we define the KDD process and describe its various components. In Section 1.4 we elaborate upon the data mining aspects of KDD, discussing its components, tasks involved, approaches and application areas. The pattern recognition perspective of data mining is introduced next and related research challenges are mentioned. The problem of scaling up pattern recognition algorithms

to large data sets is discussed in Section 1.6. Some broad approaches to achieving scalability are listed. Finally, Section 1.7 discusses the scope of the thesis.

1.2 Pattern Recognition in Brief

A typical pattern recognition system consists of three phases namely, *data acquisition, feature selection/extraction* and *classification/clustering.* In the data acquisition phase, depending on the environment within which the objects are to be classified/clustered, data are gathered using a set of sensors. These are then passed on to the feature selection/extraction phase, where the dimensionality of the data is reduced by retaining/measuring only some characteristic features or properties. In a broader perspective, this stage significantly influences the entire recognition process. Finally, in the classification/clustering phase, the selected/extracted features are passed on to the classifying/clustering system that evaluates the incoming information and makes a final decision. This phase basically establishes a transformation between the features and the classes/clusters. Different forms of transformation can be a Bayesian rule of computing *a posterior* class probabilities, nearest neighbor rule, linear discriminant functions, perceptron rule, nearest prototype rule etc [30, 32].

1.2.1 Data acquisition

Pattern recognition techniques are applicable in a wide domain, where the data may be qualitative, quantitative, or both; they may be numerical, linguistic, pictorial, or any combination thereof. The collection of data constitutes data acquisition phase. Generally, the data structures that are used in pattern recognition systems are of two types : *object data vectors* and *relational data.* Object data, set of numerical vectors, are represented in the sequel as $Y = \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n\}$, a set of n feature vectors in the p-dimensional measurement space Ω_Y. An sth object, $s = 1, 2, \ldots, n$, observed in the process has vector $\mathbf{y}_s$ as its numerical representation; y_{si} is the ith $(i = 1, 2, \ldots, p)$ feature value associated with the sth object. Relational data is a set of n^2 numerical relationships, say $\{r_{sq}\}$, between pairs of objects. In other words, r_{sq} represents the extent to which sth and qth objects are related in the sense of some binary relationship ρ. If the objects that are pairwise related by ρ are called $O = \{o_1, o_2, \ldots, o_n\}$, then

$\rho : O \times O \rightarrow I\!R.$

1.2.2 Feature selection/extraction

Feature selection/extraction is a process of selecting a map of the form $X = f(Y)$, by which a sample $\mathbf{y}$ $(=[y_1, y_2, \ldots, y_p])$ in a p-dimensional measurement space Ω_Y is transformed into a point $\mathbf{x}$ $(=[x_1, x_2, \ldots, x_{p'}])$ in a p'-dimensional feature space Ω_X, where $p' < p$. The main objective of this task [30], is to retain/generate the optimum salient characteristics necessary for the recognition process and to reduce the dimensionality of the measurement space Ω_Y so that effective and easily computable algorithms can be devised for efficient classification. The problem of feature selection/extraction has two aspects – formulation of a suitable criterion to evaluate the goodness of a feature set, and searching the optimal set in terms of the criterion. In general, those features are considered to have optimal saliencies for which interclass/intraclass distances are maximized/minimized. The criterion of a good feature is that it should be unchanging with any other possible variation within a class, while emphasizing differences that are important in discriminating between patterns of different types.

The major mathematical measures so far devised for the estimation of feature quality are mostly statistical in nature, and can be broadly classified into two categories – *feature selection in the measurement space* and *feature selection in a transformed space*. The techniques in the first category generally reduce the dimensionality of the measurement space by discarding redundant or least information carrying features. On the other hand, those in the second category utilize all the information contained in the measurement space to obtain a new transformed space; thereby mapping a higher dimensional pattern to a lower dimensional one. This is referred to as feature extraction.

1.2.3 Classification

The problem of classification is basically one of partitioning the feature space into regions, one region for each category of input. Thus it attempts to assign every data point in the entire feature space to one of the possible (say, M) classes. In real life, the complete description of the classes is not known. We have instead, a finite and

usually smaller number of samples which often provides partial information for optimal design of feature selector/extractor or classifying/clustering system. Under such circumstances, it is assumed that these samples are representative of the classes. Such a set of typical patterns is called a *training set.* On the basis of the information gathered from the samples in the training set, the pattern recognition systems are designed, *i.e.*, we decide the values of the parameters of various pattern recognition methods. Design of a classification or clustering scheme can be made with labeled or unlabeled data. When the computer is given a set of objects with known classifications (*i.e.*, labels) and is asked to classify an unknown object based on the information acquired by it during training, we call the design scheme *supervised learning*; otherwise we call it *unsupervised learning.* Supervised learning is used for classifying different objects, while clustering is performed through unsupervised learning.

Pattern classification, by its nature, admits many approaches, sometimes complementary, sometimes competing, to provide solution of a given problem. These include *decision theoretic approach* (both *deterministic* and *probabilistic*), *syntactic approach, connectionist approach, fuzzy and rough set theoretic approach* and *hybrid or soft computing approach.*

In the decision theoretic approach, once a pattern is transformed, through feature evaluation, to a vector in the feature space, its characteristics are expressed only by a set of numerical values. Classification can be done by using deterministic or probabilistic techniques [30, 32]. In deterministic classification approach, it is assumed that there exists only one unambiguous pattern class corresponding to each of the unknown pattern vectors. *Nearest neighbor classifier (NN rule)* [32] is an example of this category.

In most of the practical problems, the features are usually noisy and the classes in the feature space are overlapping. In order to model such systems, the features $x_1, x_2, \ldots, x_i, \ldots, x_p$ are considered as random variables in the probabilistic approach. The most commonly used classifier in such probabilistic systems is the *Bayes maximum likelihood classifier* [32].

When a pattern is rich in structural information (*e.g.*, picture recognition, character recognition, scene analysis) *i.e.*, the structural information plays an important role in describing and recognizing the patterns, it is convenient to use syntactic approaches [41] which deal with the representation of structures via sentences, grammars and au-

tomata. In the syntactic method [41], the ability of selecting and classifying the simple pattern primitives and their relationships represented by the composition operations is the vital criterion of making a system effective. Since the techniques of composition of primitives into patterns are usually governed by the formal language theory, the approach is often referred to as linguistic approach. An introduction to a variety of approaches based on this idea can be found in [41].

A good pattern recognition system should possess several characteristics. These are on-line adaptation (to cope with the changes in the environment), handling nonlinear class separability (to tackle real life problems), handling of overlapping classes/clusters (for discriminating almost similar but different objects), real-time processing (for making a decision in a reasonable time), generation of soft and hard decisions (to make the system flexible), verification and validation mechanisms (for evaluating its performance), and minimizing the number of parameters in the system that have to be tuned (for reducing the cost and complexity). Moreover, the system should be made artificially intelligent in order to emulate some aspects of the human processing system. Connectionist approaches (or artificial neural network based approaches) to pattern recognition are attempts to achieve these goals, and have drawn the attention of researchers because of its major characteristics like adaptivity, robustness/ruggedness, speed and optimality.

All these approaches to pattern recognition can again be fuzzy set theoretic [14, 62, 118, 165] in order to handle uncertainties, arising from vague, incomplete, linguistic, overlapping patterns etc., at various stages of pattern recognition systems. Fuzzy set theoretic classification approach is developed based on the realization that a pattern may belong to more than one class, with varying degree of class membership. Accordingly, fuzzy decision theoretic, fuzzy syntactic, fuzzy neural approaches are developed [14, 19, 118, 123].

More recently, the theory of rough sets [127, 132, 133, 158] has emerged as another major mathematical approach for managing uncertainty that arises from inexact, noisy, or incomplete information. It is turning out to be methodologically significant to the domains of artificial intelligence and cognitive sciences, especially in the representation of and reasoning with vague and/or imprecise knowledge, data classification, data analysis, machine learning, and knowledge discovery [156, 158].

Investigations have also been made in the area of pattern recognition using genetic

algorithms [129]. Like neural networks, genetic algorithms (GAs) [46] are also based on powerful metaphors from the natural world. They mimic some of the processes observed in natural evolution, which include cross-over, selection and mutation, leading to a stepwise optimization of organisms.

There have been several attempts over the last decade to evolve new approaches to pattern recognition and deriving their hybrids by combining the merits of several techniques [123]. Recently, a consolidated effort is being made to integrate mainly fuzzy logic, artificial neural networks, genetic algorithms and rough set theory, for developing an efficient new paradigm called *soft computing*. Soft computing [167] is a consortium of methodologies which works synergistically and provides in one form or another flexible information processing capabilities for handling real life ambiguous situations. Its aim is to exploit the tolerance for imprecision, uncertainty, approximate reasoning and partial truth in order to achieve *tractability, robustness, low cost solutions*, and *close resemblance to human like decision making*. In other words, it provides the foundation for the conception and design of high MIQ (Machine IQ) systems, and therefore forms the basis of future generation computing systems. An integration of neural network and fuzzy set theories, commonly known as the neuro-fuzzy approach, is perhaps the most visible hybrid paradigm [122, 123] in soft computing framework. Rough-fuzzy [127] and neuro-rough [109, 126] hybridizations are also proving to be fruitful frameworks for modeling human perceptions and providing means for computing with words. Significance of the recently proposed computational theory of perceptions (CTP) [169] may also be mentioned in this regard.

1.3 Knowledge Discovery in Databases

Knowledge discovery in databases (KDD) is defined as [37]:

> *The nontrivial process of identifying valid, novel, potentially useful, and ultimately understandable patterns in data.*

In this definition, the term *pattern* goes beyond its traditional sense to include models or structures in data. *Data* is a set of facts F (e.g., cases in a database), and a *pattern* is an expression E in a language L describing the facts in a subset F_E (or a

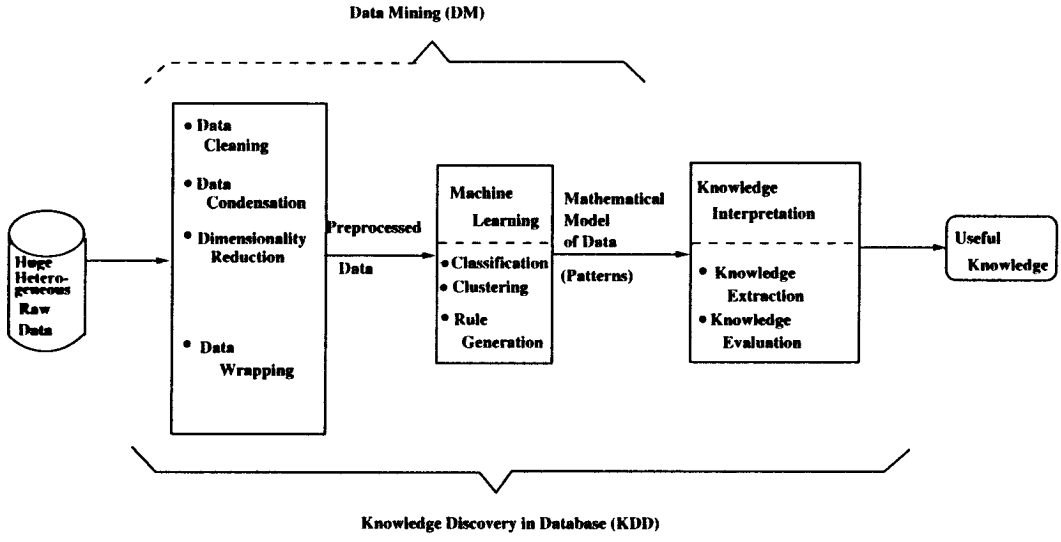


Figure 1.1: The KDD process [111]

model applicable to that subset) of F. E is called a pattern if it is simpler than the enumeration of all facts in F_E.

The discovered patterns should be valid on new data with some degree of certainty. Also, the patterns need to be novel (at least to the system and preferably to the user) and potentially useful, that is, lead to some benefit to the user. Finally, the patterns should be understandable (if not immediately) after some postprocessing.

Data mining is a step in the KDD process that consists of applying data analysis and discovery algorithms which, under acceptable computational limitations, produce a particular enumeration of patterns (or generate a model) over the data. It uses *historical* information to discover regularities and improve future decisions [95].

The overall KDD process is outlined in Figure 1.1. It is interactive and iterative involving, more or less, the following steps [37, 38]:

1. *Data cleaning and preprocessing*: includes basic operations, such as noise removal and handling of missing data. Data from real-world sources are often erroneous, incomplete, and inconsistent, perhaps due to operation error or system implementation flaws. Such low quality data needs to be cleaned prior to data mining.

2. *Data condensation and projection*: includes finding useful features and samples to represent the data (depending on the goal of the task) and using dimensionality

reduction or transformation methods.

3. *Data integration and wrapping*: includes integrating multiple, heterogeneous data sources and providing their descriptions (wrappings) for ease of future use.

4. *Choosing the data mining function(s) and algorithm(s)*: includes deciding the purpose (e.g., classification, regression, summarization, clustering, discovering association rules and functional dependencies, or a combination of these) of the model to be derived by the data mining algorithm and selecting methods (e.g., neural networks, decision trees, statistical models, fuzzy models) to be used for searching patterns in data.

5. *Data mining*: includes searching for patterns of interest in a particular representational form or a set of such representations.

6. *Interpretation and visualization*: includes interpreting the discovered patterns, as well as the possible visualization of the extracted patterns. One can analyze the patterns automatically or semi-automatically to identify the truly interesting/useful patterns for the user.

7. *Using discovered knowledge*: includes incorporating this knowledge into the performance system, taking actions based on knowledge.

Thus, KDD refers to the overall process of turning low-level data into high-level knowledge. Perhaps the most important step in the KDD process is data mining. However, the other steps are also important for the successful application of KDD in practice. For example, steps 1, 2 and 3, mentioned above, have been the subject of widespread research in the area of *data warehousing*. We now focus on the data mining component of KDD.

1.4 Data Mining

Data mining involves fitting models to or determining patterns from observed data. The fitted models play the role of inferred knowledge. Deciding whether the model reflects useful knowledge or not is a part of the overall KDD process for which subjective

human judgment is usually required. Typically, a data mining algorithm constitutes some combination of the following three components [37].

- **The model**: The function of the model (*e.g.*, classification, clustering) and its representational form (*e.g.*, linear discriminants, neural networks). A model contains parameters that are to be determined from the data.
- **The preference criterion**: A basis for preference of one model or set of parameters over another, depending on the given data. The criterion is usually some form of goodness-of-fit function of the model to the data, perhaps tempered by a smoothing term to avoid overfitting, or generating a model with too many degrees of freedom to be constrained by the given data.
- **The search algorithm**: The specification of an algorithm for finding particular models and parameters, given the data, model(s), and a preference criterion.

A particular data mining algorithm is usually an instantiation of the model/preference/search components.

1.4.1 Data mining tasks

The more common model tasks/functions in current data mining practice include:

1. *Association rule discovery*: describes association relationship among different attributes. The origin of association rules is in market basket analysis. A *market basket* is a collection of items purchased by a customer in an individual *customer transaction*. One common analysis task in a transaction database is to find sets of items, or *itemsets*, that *frequently* appear together. Each pattern extracted through the analysis consists of an itemset and its *support* i.e., the number of transactions that contain it. Businesses can use knowledge of these patterns to improve placement of items in a store or for mail-order marketing. The huge size of transaction databases and the exponential increase in the number of potential frequent itemsets with increase in the number of attributes (items) make the above problem a challenging one. The Apriori algorithm [1] provided one early solution which was improved by subsequent algorithms using partitioning, hashing, sampling and dynamic itemset counting.

2. *Clustering*: maps a data item into one of several clusters, where clusters are natural groupings of data items based on similarity metrics or probability density models. Clustering is used in several exploratory data analysis tasks, customer retention and management, and web mining. The clustering problem has been studied in many fields, including statistics, machine learning and pattern recognition. However, large data considerations were absent in these approaches. Recently, several new algorithms with greater emphasis on scalability have been developed, including those based on summarized cluster representation called *cluster feature* (Birch [171], ScaleKM [16]), sampling (CURE [49]) and density joins (DBSCAN [35]).

3. *Classification*: classifies a data item into one of several predefined categorical classes. It is used for the purpose of predictive data mining in several fields e.g., in scientific discovery, fraud detection, atmospheric data mining and financial engineering. Several classification methodologies have already been discussed earlier in Section 1.2.3. Some typical algorithms suitable for large databases are based on Bayesian techniques and decision trees.

4. *Sequence analysis*: models sequential patterns, like time-series data [79]. The goal is to model the process of generating the sequence or to extract and report deviation and trends over time. The framework is increasingly gaining importance because of its application in bioinformatics and streaming data analysis.

5. *Regression*: maps a data item to a real-valued prediction variable. It is used in different prediction and modeling applications.

6. *Summarization*: provides a compact description for a subset of data. A simple example would be mean and standard deviation for all fields. More sophisticated functions involve summary rules, multivariate visualization techniques and functional relationship between variables. Summarization functions are often used in interactive data analysis, automated report generation and text mining.

7. *Dependency modeling*: describes significant dependencies among variables.

Some other tasks required in some data mining applications are, outlier/anomaly detection, link analysis, optimization and planning.

1.4.2 Data mining tools

A wide variety and number of data mining algorithms are described in the literature - from the fields of statistics, pattern recognition, machine learning and databases. They represent a long list of seemingly unrelated and often highly specific algorithms. Some representative groups are mentioned below:

1. Statistical models (e.g., linear discriminants [32, 55])
2. Probabilistic graphical dependency models
3. Decision trees and rules [145]
4. Inductive logic programming based models
5. Example based methods (e.g., nearest neighbor [5], lazy learning [3] and case based reasoning [74] methods)
6. Neural network based models [24, 88, 108]
7. Fuzzy models [24, 89, 134]
8. Rough set theory based models [75, 82, 105]
9. Genetic algorithm based models [64]
10. Hybrid and soft computing models [63, 104]

The data mining algorithms determine both the flexibility of the model in representing the data and the interpretability of the model in human terms. Typically, the more complex models may fit the data better but may also be more difficult to understand and to fit reliably. Also, each representation suits some problems better than the other. For example, decision tree classifiers can be very useful for finding structure in high dimensional spaces and are also useful in problems with mixed continuous and categorical data. However, they may not be suitable for problems where the true decision boundaries are nonlinear multivariate functions.

1.4.3 Applications of data mining

A wide range of organizations including business companies, scientific laboratories and governmental departments have deployed successful applications of data mining. While early adopters of this technology have tended to be in information-intensive industries such as financial services and direct mail marketing, the technology is applicable to any company looking to leverage a large data warehouse to better manage their operations. Two critical factors for success with data mining are: a large, well-integrated data warehouse and a well-defined understanding of the process within which data mining is to be applied. Several domains where large volumes of data are stored in centralized or distributed databases include the following.

- *Financial Investment*: Stock indices and prices, interest rates, credit card data, fraud detection.
- *Health Care*: Several diagnostic information stored by hospital management systems.
- *Manufacturing and Production*: Process optimization and trouble shooting.
- *Telecommunication network*: Calling patterns and fault management systems.
- *Scientific Domain*: Astronomical observations, genomic data, biological data.
- *The World Wide Web.*

The results of a recent survey conducted at the *www.kdnuggets.com* web site regarding the usage of data mining algorithms in different domains are presented in Figure 1.2.

1.5 Pattern Recognition in Data Mining

In the previous section we have discussed the generic components of a data mining system, common data mining tasks/tools and related principles and issues that appear in designing a data mining system. At present, the goal of KDD community is to develop a unified framework of data mining which should be able to model typical data mining tasks, be able to discuss the probabilistic nature of the discovered patterns

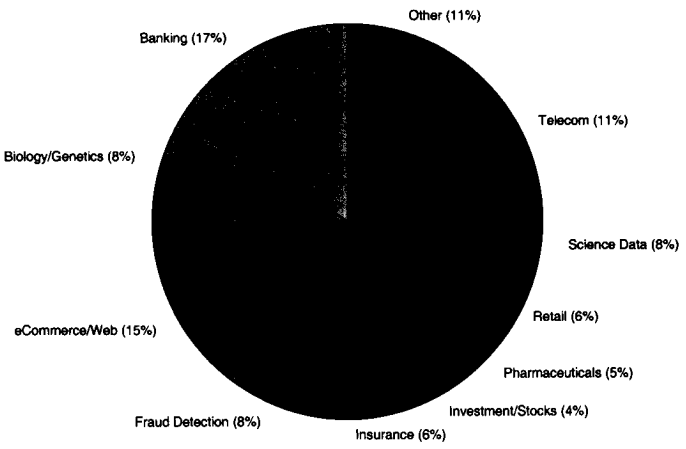


Figure 1.2: Application areas of data mining

and models, be able to talk about data and inductive generalizations of the data, and accept the presence of different forms of data (relational data, sequences, text, web). Also, the framework should recognize that data mining is an interactive and iterative process, where comprehensibility of the discovered knowledge is important and where the user has to be in the loop [92, 146].

Pattern recognition and machine learning algorithms seem to be the most suitable candidates for addressing the above tasks. It may be mentioned in this context that historically the subject of knowledge discovery in databases has evolved, and continues to evolve, from the intersection of research from such fields as machine learning, pattern recognition, statistics, databases, artificial intelligence, reasoning with uncertainties, expert systems, data visualization, and high-performance computing. KDD systems incorporate theories, algorithms, and methods from all these fields. Therefore, before elaborating the pattern recognition perspective of data mining, we describe briefly two other prominent frameworks, namely, the database perspective and the statistical perspective of data mining.

Database perspective of data mining

Since most business data resides in industrial databases and warehouses, commercial companies view mining as a sophisticated form of database querying [51, 59]. Research based on this perspective seeks to enhance the expressiveness of query languages (rule

query languages, meta queries, query optimizations), enhance the underlying model of data and DBMSs (the logical model of data, deductive databases, inductive databases, rules, active databases, semistructured data etc.) and improve integration with data warehousing systems (online analytical processing (OLAP), historical data, meta-data, interactive exploring). The approach also has close links with search based perspective of data mining, exemplified by the popular work on association rules [1] at IBM Almaden.

The database perspective has several advantages including scalability to large databases present in secondary and tertiary storage, generic nature of the algorithms (applicability to a wide range of tasks and domains), capability of handling heterogeneous data, and easy user interaction and visualization of mined patterns. However, it is still ill-equipped to address the full range of knowledge discovery tasks. The reasons being: inability to mine complex patterns and model non-linear relationships (the database models being of limited richness), unsuitability for exploratory analysis, lack of induction capability, and restricted scope for evaluating the significance of mined patterns [146].

Statistical perspective of data mining

Statistical perspective views data mining as computer automated exploratory data analysis of (usually) large complex data sets [45, 55]. The term 'data mining' existed in statistical data analysis literature long before its current definition in computer science community. However, the abundance and massiveness of data has provided impetus to development of algorithms which, though rooted in statistics, lays more emphasis on computational efficiency. Presently, statistical tools are used in all the KDD tasks like preprocessing (sampling, outlier detection, experimental design), data modeling (clustering, expectation maximization, decision trees, regression, canonical correlation etc), model selection, evaluation and averaging (robust statistics, hypothesis testing) and visualization (principal component analysis, Sammon's mapping).

The advantages of statistical approach are its solid theoretical background, and easiness of posing formal questions. Tasks such as classification and clustering fit easily into this approach. What seems to be lacking are ways for taking into account the iterative and interactive nature of the data mining process. Also scalability of the methods to

very large, specially tertiary memory data, is still not fully achieved.

1.5.1 Pattern recognition/machine learning perspective of data mining

At present pattern recognition and machine learning provide the most fruitful framework for data mining [67, 95]. Not only does it provide a wide range of models (linear/non-linear, comprehensible/complex, predictive/descriptive, instance/rule based) for data mining tasks (clustering, classification, rule discovery), methods for modeling uncertainties (probabilistic, fuzzy) in the discovered patterns also form part of PR research. Another aspect which makes pattern recognition algorithms attractive for data mining are their capability of learning or induction. As opposed to many statistical techniques that require the user to have a hypothesis in mind first, PR algorithms automatically analyze data and identify relationships among attributes and entities in the data to build models that allow domain experts to understand the relationship between the attributes and the class. Data preprocessing tasks like instance selection, data cleaning, dimensionality reduction, handling missing data are also extensively studied in pattern recognition framework. Besides these, other data mining issues addressed by PR methodologies include, handling of relational, sequential and symbolic data (syntactic PR, PR in arbitrary metric spaces), human interaction (knowledge encoding and extraction), knowledge evaluation (description length principle) and visualization.

Pattern recognition is at the core of data mining systems. However, pattern recognition and data mining are not equivalent considering their original definitions. There exists a gap between the requirements of a data mining system and the goals achieved by present day pattern recognition algorithms. Development of new generation PR algorithms is expected to encompass more massive data sets involving diverse sources and types of data that will support mixed-initiative data mining, where human experts collaborate with the computer to form hypotheses and test them. The main challenges to PR as a unified framework for data mining are mentioned below.

1.5.2 Research issues and challenges

1. *Massive data sets and high dimensionality.* Huge data sets create combinatorially explosive search spaces for model induction which may make the process of extracting patterns infeasible owing to space and time constraints. They also increase the chances that a data mining algorithm will find spurious patterns that are not generally valid.

2. *User interaction and prior knowledge.* Data mining is inherently an interactive and iterative process. Users may interact at various stages, and domain knowledge may be used either in the form of a high level specification of the model, or at a more detailed level. Visualization of the extracted model is also desirable.

3. *Overfitting and assessing the statistical significance.* Data sets used for mining are usually huge and available from distributed sources. As a result, often the presence of spurious data points leads to overfitting of the models. Regularization and resampling methodologies need to be emphasized for model design.

4. *Understandability of patterns.* It is necessary to make the discoveries more understandable to humans. Possible solutions include rule structuring, natural language representation, and the visualization of data and knowledge.

5. *Nonstandard and incomplete data.* The data can be missing and/or noisy.

6. *Mixed media data.* Learning from data that is represented by a combination of various media, like (say) numeric, symbolic, images and text.

7. *Management of changing data and knowledge.* Rapidly changing data, in a database that is modified/deleted/augmented, may make the previously discovered patterns invalid. Possible solutions include incremental methods for updating the patterns.

8. *Integration.* Data mining tools are often only a part of the entire decision making system. It is desirable that they integrate smoothly, both with the database and the final decision making procedure.

In the next section we discuss the issues related to the large size of the data sets in more detail.

1.6 Scaling Pattern Recognition Algorithms to Large Data Sets

Organizations are amassing very large repositories of customer, operations, scientific and other sorts of data of gigabytes or even terabytes size. KDD practitioners would like to be able to apply pattern recognition and machine learning algorithms to these large data sets in order to discover useful knowledge. The question of *scalability* asks whether the algorithm can process large data sets efficiently, while building from them the best possible models.

From the point of view of complexity analysis, for most scaling problems the limiting factor of the data set has been the number of examples and their dimension. A large number of examples introduces potential problems with both time and space complexity. For time complexity, the appropriate algorithmic question is: what is the growth rate of the algorithm's run time as the number of examples and their dimensions increases? As may be expected, time-complexity analysis does not tell the whole story. As the number of instances grows, space constraints become critical, since, almost all existing implementations of learning algorithm operate with training set entirely in main memory. Finally, the goal of learning algorithm must be considered. Evaluating the effectiveness of a scaling technique becomes complicated if degradation in the quality of the learning is permitted. Effectiveness of a technique for scaling pattern recognition/learning algorithms is measured in terms of the above three factors, namely, time complexity, space complexity and quality of learning.

Many diverse techniques, both general and task specific, have been proposed and implemented for scaling up learning algorithms. An excellent survey of these methods is provided in [143]. We discuss here some of the broad categories relevant to the thesis. Besides these, other hardware driven (parallel processing, distributed computing) and database driven (relational representation) methodologies are equally effective.

Data reduction

The simplest approach for coping with the infeasibility of learning from a very large data set is to learn from a reduced/condensed representation of the original massive

data set [11]. The reduced representation should be as faithful to the original data as possible, for its effective use in different mining tasks. At present the following categories of reduced representations are mainly used:

- *Sampling/Instance selection*: Various random, deterministic and density biased sampling strategies exist in statistics literature. Their use in machine learning and data mining tasks has also been widely studied [22, 71, 84]. Note that merely generating a random sample from a large database stored on disk may itself be a non-trivial task from a computational viewpoint. Several aspects of instance selection, e.g., instance representation, selection of interior/boundary points, instance pruning strategies, have also been investigated in instance based and nearest neighbor classification frameworks [164]. Challenges in designing an instance selection algorithm include accurate representation of the original data distribution, making fine distinctions at different scales and noticing rare events and anomalies.

- *Data squashing*: It is a form of lossy compression where a large data set is replaced by a small data set and some accompanying quantities, while attempting to preserve its statistical information [33].

- *Indexing data structures*: Systems such as kd-trees [13], R-trees, hash tables, AD-trees, multiresolution kd-trees [29] and cluster feature (CF)-trees [16] partition the data (or feature space) into buckets recursively, and store enough information regarding the data in the bucket so that many mining queries and learning tasks can be achieved in constant or linear time.

- *Frequent itemsets*: They are often applied in supermarket data analysis and require that the attributes are sparsely valued [1].

- *DataCubes*: Use a relational aggregation database operator to represent chunks of data [47].

The last four techniques fall into the general class of representation called 'cached sufficient statistics' [106]. These are summary data structures that lie between the statistical algorithms and the database, intercepting the kinds of operations that have the potential to consume large time if they were answered by direct reading of the data

set. Case-based reasoning [74] also involves a related approach where salient instances (or descriptions) are either selected or constructed and stored in the case base for later use.

Dimensionality reduction

An important problem related to mining large data sets, both in dimension and size, is of selecting a subset of the original features [83]. Preprocessing the data to obtain a smaller set of representative features, retaining the optimal/salient characteristics of the data, not only decreases the processing time but also leads to more compactness of the models learned and better generalization.

Active learning

Traditional machine learning algorithms deal with input data consisting of independent and identically distributed (iid) samples. In this framework, the number of samples required (*sample complexity*) by a class of learning algorithms to achieve a specified accuracy can be theoretically determined [12, 163]. In practice, as the amount of data grows, the increase in accuracy slows, forming the learning curve. One can hope to avoid this slow down in learning by employing selection methods for sifting through the additional examples and filtering out a small non-iid set of relevant examples that contain essential information. Formally, active learning studies the closed-loop phenomenon of a learner selecting actions or making queries that influence what data are added to its training set. When actions/queries are selected properly, the sample complexity for some problems decreases drastically, and some NP-hard learning problems become polynomial in computation time [6, 25].

Data partitioning

Another approach to scaling up is to partition the data, avoiding the need to run algorithms on very large data sets. The models learned from individual partitions are then combined to obtain the final *ensemble* model. Data partitioning techniques can be categorized based on whether they process subsets sequentially or concurrently. Several model combination strategies also exist in literature [44] including, boosting,

bagging, ARCing classifiers, committee machines, voting classifiers, mixture of experts, stacked generalization, Bayesian sampling, statistical techniques and soft computing methods. The problems of feature partitioning and modular task decomposition for achieving computational efficiency have also been studied.

Granular computing

Granular computing (GrC) may be regarded as a unified framework for theories, methodologies and techniques that make use of granules (i.e., groups, classes or clusters of objects in a universe) in the process of problem solving. In many situations, when a problem involves incomplete, uncertain and vague information, it may be difficult to differentiate distinct elements and one is forced to consider granules. On the other hand, in some situations though detailed information is available, it may be sufficient to use granules in order to have an efficient and practical solution. Granulation is an important step in the human cognition process. From a more practical point of view, the simplicity derived from granular computing is useful for designing scalable data mining algorithms [82, 127, 136]. There are two aspects of granular computing, one deals with formation, representation and interpretation of granules (algorithmic aspect) while the other deals with utilization of granules for problem solving (semantic aspect). Several approaches for granular computing have been suggested in literature including fuzzy set theory [168], rough set theory [132], power algebras and interval analysis. The rough set theoretic approach is based on the principles of set approximation and provides an attractive framework for data mining and knowledge discovery.

Efficient search algorithms

The most straightforward approach to scaling up machine learning is to produce more efficient algorithms or to increase the efficiency of existing algorithms. As mentioned earlier the data mining problem may be framed as a search through a space of models based on some fitness criteria. This view allows for three possible ways of achieving scalability.

- *Restricted model space*: Simple learning algorithms (e.g., two-level trees, decision stump) and constrained search involve a 'smaller' model space and decrease the

complexity of the search process.

- *Knowledge encoding*: Domain knowledge encoding, providing an initial solution close to the optimal one, results in fast convergence and avoidance of local minima. Domain knowledge may also be used to guide the search process for faster convergence.
- *Powerful algorithms and heuristics*: Strategies like greedy search, divide and conquer, modular computation are often found to provide considerable speed-ups. Programming optimization (efficient data structures, dynamic search space restructuring) and the use of genetic algorithms, randomized algorithms and parallel algorithms may also obtain approximate solutions much faster compared to conventional algorithms.

1.7 Scope of the Thesis

The objective of the thesis is to provide some results of investigations, both theoretical and experimental, addressing certain pattern recognition tasks essential for data mining. Tasks considered include data condensation, feature selection, case generation, clustering, classification and rule generation/evaluation. Various methodologies have been developed using both classical and soft computing approaches (integrating fuzzy logic, artificial neural networks, rough sets, genetic algorithms). The emphasis of the proposed methodologies is given on handling data sets which are large (both in size and dimension) and involve classes that are overlapping, intractable and/or having nonlinear boundaries. Several strategies based on data reduction, dimensionality reduction, active learning, granular computing and efficient search heuristics are employed for dealing with the issue of 'scaling up' in learning problem. The problems of handling linguistic input and ambiguous output decision, learning of overlapping/intractable class structures, selection of optimal parameters, and discovering human comprehensible knowledge (in the form of linguistic rules) are addressed in soft computing framework.

Methodologies developed for data condensation and feature selection are based on classical approach and are useful in the preprocessing stage of data mining. An active support vector learning algorithm and a modular rough-fuzzy multilayer perceptron (MLP) trained with genetic algorithm (GA) are developed for performing classification

and generating comprehensive linguistic rules. New measures for evaluating rules are also presented. Granular computing based on rough-fuzzy approach is used for efficient generation of cases (class prototypes). The case knowledge is further utilized in conjunction with graph theoretic approach and expectation maximization (EM) clustering algorithm for obtaining non-convex clusters.

The effectiveness of the algorithms is demonstrated on different real life data sets, mainly large in dimension and/or size, taken from varied domains e.g, geographical information systems, remote sensing imagery, population census, speech recognition and cancer management. Superiority of the models over several related ones is found to be statistically significant. The results of the investigations are summarized below under different chapter headings.

1.7.1 Density based multiscale data condensation [100]

In Chapter 2, a generic multiscale data reduction methodology is described [100]. It preserves the salient characteristics of the original data set by representing the probability density underlying it. The representative points are selected in a multiresolution fashion, which is novel with respect to the existing density based approaches. A scale parameter (k) is used in non-parametric density estimation so that the data can be viewed at varying degrees of detail depending on the value of k. This type of multiscale representation is desirable in various data mining applications. At each scale the representation gives adequate importance to different regions of the feature space based on the underlying probability density.

It is observed experimentally that the multiresolution approach helps to achieve lower error with similar condensation ratio compared to several related schemes. The reduced set obtained is found to be effective for a number of mining tasks like classification, clustering and rule generation. The algorithm is also found to be efficient in terms of sample complexity, in the sense that the error level decreases rapidly with the increase in size of the condensed set.

1.7.2 Unsupervised feature selection using feature similarity [101]

Chapter 3 describes an unsupervised feature selection algorithm [101] suitable for data sets, large in both dimension and size. Conventional methods of feature selection involve evaluating different feature subsets using some index and selecting the best among them. The index usually measures the capability of the respective subsets in classification or clustering depending on whether the selection process is supervised or unsupervised. A problem of these methods, when applied to large data sets, is the high computational complexity involved in searching.

We digress from the aforesaid conventional view and propose a method which is based on measuring similarity between features and then removing the redundancy therein. This does not need any search and, therefore, is fast. Since the method achieves dimensionality reduction through removal of redundant features, it is more related to feature selection for compression rather than for classification.

The method involves partitioning of the original feature set into some distinct subsets or clusters so that the features within a cluster are highly similar while those in different clusters are dissimilar. A single feature from each such cluster is then selected to constitute the resulting reduced subset. The algorithm is generic in nature and has the capability of multiscale representation of data sets. A new feature similarity measure, called maximum information compression index, is introduced. It is also demonstrated how 'representation entropy' can be used for quantifying the redundancy in a set.

Superiority of the algorithm, over related methods, is demonstrated extensively on different real life data with dimension ranging from 4 to 649. Comparison is made on the basis of both clustering/classification performance and redundancy reduction. Effectiveness of the maximal information compression index and the effect of scale parameter are also studied.

1.7.3 Active support vector learning [99, 102]

While Chapters 2 and 3 deal with some preprocessing tasks of data mining, Chapter 4 is concerned with its classification/learning aspect. Here we present two active learn-

ing strategies [99, 102] for handling the large quadratic programming (QP) problem of support vector machine (SVM) classifier design. The first one is an error driven incremental method for active support vector learning. The method involves selecting a chunk of q new points, having equal number of correctly classified and misclassified points, at each iteration by resampling the data set, and using it to update the current SV set. The resampling strategy is computationally superior to random chunk selection, while achieving higher classification accuracy. Since it allows for querying multiple instances at each iteration, it is computationally more efficient than those that are querying for a single example at a time.

The second algorithm deals with active support vector learning in statistical query framework. Like the previous algorithm, it also involves queries for multiple instances at each iteration. The intermediate statistical query oracle, involved in the learning process, returns the value of the probability that a new example belongs to the actual support vector set. A set of q new points is selected according to the above probability, and is used along with the current SVs to obtain the new SVs. The probability is estimated using a combination of two factors: the margin of the particular example with respect to the current hyperplane, and the degree of confidence that the current set of SVs provides the actual SVs. The degree of confidence is quantified by a measure which is based on the local properties of each of the current support vectors and is computed using the nearest neighbor estimates.

The methodology in the second part has some more advantages. It not only queries for the error points (or points having low margin) but also a number of other points far from the separating hyperplane (interior points). Thus, even if a current hypothesis is erroneous there is a scope for it being corrected owing to the interior points. If only error points were selected the hypothesis might have actually been worse. The ratio of selected points having low margin and those far from the hyperplane is decided by the confidence factor, which varies adaptively with iteration. If the current SV set is close to the optimal one, the algorithm focuses only on the low margin points and ignores the redundant points that lie far from the hyperplane. On the other hand, if the confidence factor is low (say, in the initial learning phase) it explores a higher number of interior points. Thus, the trade-off between efficiency and robustness of performance is adequately handled in this framework. Also, the efficiency of most of the existing active SV learning algorithms depends on the sparsity ratio (*i.e.*, the ratio

of the number of support vectors to the total number of data points) of the data set. Due to the adaptive nature of the query in the proposed algorithm, it is likely to be efficient for a wide range of sparsity ratio.

Experiments have been performed on five real life classification problems. The number of patterns ranges from 351 to 495141, dimension from 9 to 34, and the sparsity ratio from 0.01 to 0.51. Our algorithms, particularly the second one, are found to provide superior performance in terms of classification accuracy, closeness to the optimal SV set, training time and margin distribution, as compared to several related algorithms for incremental and active SV learning. Effectiveness of the confidence factor, used in statistical queries, is also studied.

In the previous three chapters we have used classical approach for developing methodologies for data condensation, feature selection and active learning. The next two chapters (Chapters 5 and 6) emphasize on demonstrating the effectiveness of integrating different soft computing tools, e.g., fuzzy logic, artificial neural networks, rough sets and genetic algorithms for performing certain tasks in data mining.

1.7.4 Rough-fuzzy case generation and clustering [119, 120, 121]

In Chapter 5 the principle of granular computing in rough fuzzy framework is exploited for efficient case (representative class prototypes) generation [119, 120], and clustering [121] of large data sets. It has two parts. First we propose a rough-fuzzy hybridization scheme for case generation. Fuzzy set theory is used for linguistic representation of patterns, thereby producing a fuzzy granulation of the feature space. Rough set theory is used to obtain the dependency rules which model different informative regions in the granulated feature space. The fuzzy membership functions corresponding to the informative regions are stored as cases along with the strength values. Case retrieval is made using a similarity measure based on these membership functions. Unlike the existing case selection methods, the cases here are cluster granules, and not the sample points. Also, each case involves a reduced number of relevant (variable) features. Because of this twofold information compression the algorithm has low time requirement in generation as well as retrieval of cases. Superiority of the algorithm in

terms of classification accuracy, and case generation and retrieval time is demonstrated experimentally on data sets having large dimension and size.

Next, an integration of a minimal spanning tree (MST) based graph-theoretic technique and expectation maximization (EM) algorithm with rough set initialization is described for non-convex clustering [121]. Rough set initialization is performed using dependency rules generated on a fuzzy granulated feature space. EM provides the statistical model of the data and handles the associated uncertainties. Rough set theory helps in faster convergence and avoidance of the local minima problem, thereby enhancing the performance of EM. MST helps in determining non-convex clusters. Since it is applied on Gaussians rather than the original data points, time requirement is very low. Comparison with related methods is made in terms of a cluster quality measure and computation time. Its effectiveness is also demonstrated for segmentation of multispectral satellite images into different landcover types [121].

1.7.5 Modular Rough-fuzzy MLP: Evolution, rule generation and evaluation [97, 98, 124]

So far, we have demonstrated in Chapter 5 a judicious integration of fuzzy sets and rough sets for providing an efficient granular computing paradigm. Chapter 6 provides a synergistic integration of four soft computing components, namely, fuzzy sets, rough sets, neural networks and genetic algorithms along with modular decomposition strategy, for generating a rough-fuzzy multilayer perceptron (MLP) [124]. The resulting connectionist system achieves gain in terms of performance, learning time and network compactness for classification and linguistic rule generation.

Here, the role of the individual components is as follows. Fuzzy sets handle uncertainties in the input data and output decision of the neural network, and provide linguistic representation (fuzzy granulation) of the feature space. Multilayer perceptron is well known for providing a connectionist paradigm for learning and adaptation. Rough set theory is used to extract domain knowledge in the form of linguistic rules, which are then encoded into a number of fuzzy MLP modules or subnetworks. Genetic algorithms (GAs) are used to integrate and evolve the population of subnetworks as well as the fuzzification parameters through efficient searching. A concept of variable mu-

tation operator is introduced for preserving the localized structure of the constituting knowledge based subnetworks, while they are integrated and evolved. The nature of the mutation operator is determined by the domain knowledge extracted by rough sets.

The modular concept, based on 'divide and conquer' strategy, provides accelerated training, preserves the identity of individual clusters, reduces the catastrophic interference due to overlapping regions, and generates a compact network suitable for extracting a minimum number of rules with high certainty values. Knowledge discovery aspect is quantitatively studied through some rule evaluation indices. Two new indices viz., 'certainty' and 'confusion' in a decision are defined in this regard. The effectiveness of the network and the rule extraction algorithm is extensively demonstrated through experiments along with comparisons. In some cases the rules generated are also validated by domain experts. The investigation, besides having significance in soft computing research, has potential for application to large scale problems involving knowledge discovery tasks [104], particularly related to mining of linguistic classification rules.

1.7.6 Conclusions and scope for further research

The concluding remarks along with the scope for further research are made in Chapter 7. ♦

Twenty one different data sets, used in the experiments, are described in brief in the Appendix.

Chapter 2

Density Based Multiscale Data Condensation

2.1 Introduction

The current popularity of data mining and data warehousing, as well as the decline in the cost of disk storage, has led to a proliferation of terabyte data warehouses [38]. Mining a database of even a few gigabytes is an arduous task for machine learning techniques, and requires advanced parallel hardware and algorithms. An approach for dealing with the intractable problem of learning from huge databases is to select a small subset of data for learning [143]. Databases often contain redundant data. It would be convenient if large databases could be replaced by a small subset of representative patterns so that the accuracy of estimates (e.g., of probability density, dependencies, class boundaries) obtained from such a reduced set should be comparable to that obtained using the entire data set.

The simplest approach for data reduction is to draw the desired number of random samples from the entire data set. Various statistical sampling methods such as random sampling, stratified sampling, and peepholing [22] have been in existence. However, naive sampling methods are not suitable for real world problems with noisy data, since the performance of the algorithms may change unpredictably and significantly [22]. Better performance is obtained using *uncertainty sampling* [81] and active learning [152], where a simple classifier queries for informative examples. The random sampling approach effectively ignores all the information present in the samples not chosen for membership in the reduced subset. An advanced condensation algorithm should include information from all samples in the reduction process.

Some widely studied schemes for data condensation are built upon classification based approaches, in general, and the k-NN rule, in particular [27]. The effectiveness of the condensed set is measured in terms of the classification accuracy. These methods attempt to derive a minimal consistent set, *i.e.*, a minimal set which correctly classifies all the original samples. The very first development of this kind is the condensed nearest neighbor rule (CNN) of Hart [54]. Other algorithms in this category including the popular IB3, IB4 [2], reduced nearest neighbor and iterative condensation algorithms are summarized in [164]. Recently a local asymmetrically weighted similarity metric (LASM) approach for data compression [150] is shown to have superior performance compared to conventional k-NN classification based methods. Similar concepts of data reduction and locally varying models based on neural networks and Bayes classifier are

discussed in [141] and [86] respectively.

The classification based condensation methods are however specific to (*i.e.*, dependent on) the classification tasks and the models (e.g., k-NN, perceptron) used. Data condensation of more generic nature is performed by classical vector quantization methods [48] using a set of codebook vectors which minimize the quantization error. An effective and popular method of learning the vectors is by using the self-organizing map [72]. However, if the self-organizing map is to be used as a pattern classifier, the codebook vectors may be further refined using the learning vector quantization algorithms [72]. These methods are seen to approximate the density underlying the data [72]. Since learning is inherent in the methodologies, the final solution is dependent on initialization, choice of learning parameters, and the nature of local minima.

Another group of generic data condensation methods are based on the density based approaches, which consider the density function of the data for the purpose of condensation rather than minimizing the quantization error. These methods do not involve any learning process and therefore are deterministic (*i.e.*, for a given input data set the output condensed set is fixed). Here one estimates the density at a point and selects the points having 'higher' densities, while ensuring a minimum separation between the selected points. These methods bear resemblance to density based clustering techniques like the DBSCAN algorithm [35], popular for spatial data mining. DBSCAN is based on the principle that a cluster point contains in its neighborhood a minimum number of samples, *i.e.*, the cluster point has density above a certain threshold. The neighborhood radius and the density threshold are user specified. Astrahan [9] proposed a classical data reduction algorithm of this type in 1971, in which he used a hypersphere (disc) of radius d_1 about a point to obtain an estimate of density at that point. The points are sorted based on these estimated densities, and the densest point is selected, while rejecting all points that lie within another disc of radius d_2 about the selected point. The process is repeated till all the samples are covered. However, selecting the values of d_1 and d_2 is a non-trivial problem. A partial solution using a minimal spanning tree based method is described in [23]. Though the above approaches select the points based on the density criterion, they do not directly attempt to represent the original distribution. The selected points are distributed evenly over the entire feature space irrespective of the distribution. A constant separation is used for instance pruning. Interestingly, Fukunaga [43] suggested a non-parametric algorithm for selecting a

condensed set based on the criterion that density estimates obtained with the original set and the reduced set are *close*. The algorithm is however search based and requires large computation time.

Efficiency of condensation algorithms may be improved by adopting a multiresolution representation approach. A multiresolution framework for instance based learning and regression has been studied in [29] and [107] respectively. It uses a k-d tree [13] to impose a hierarchy of data partitions which implicitly condense the data into homogeneous blocks having variable resolutions. Each level of the tree represents a partition of the feature space at a particular scale of detail. Prediction for a query point is performed using blocks from different scales; finer scale blocks are used for points close to the query and cruder scale blocks for those far from the query. However, the blocks are constructed by simple median splitting algorithms which do not directly consider the density function underlying the data.

We describe in this chapter a density based multiresolution data reduction algorithm [100] that uses discs of adaptive radii for both density estimation and sample pruning. The method attempts to accurately represent the entire distribution rather than the data set itself. The accuracy of this representation is measured using nearest neighbor density estimates at each point belonging to the entire data set. The method does away with the difficult choice of radii d_1 and d_2 as in Astrahan's method discussed above. In the proposed method, k-NN density estimates are obtained for each point and the points having higher density are selected subject to the condition that the point does not lie in a region 'covered' by any other selected point. A selected point 'covers' a disc around it with volume inversely proportional (by a factor σ, say) to the (estimated) density at that point, as illustrated in Figure 2.1. Hence the regions having higher density are represented more accurately in the reduced data sets compared to sparse regions. The proportionality factor (σ) and k used for k-NN density estimation controls the condensation ratio and the accuracy of representation.

The condensation algorithm can obtain reduced sets which represent the data at different scales. The parameter k acts as the scale parameter, and the data is viewed at varying degrees of detail depending on the value of k. This type of multiscale representation of data is desirable for various applications like data mining. At each scale the representation gives adequate importance to different regions of the feature space based upon the probability density as mentioned before. The above scheme induces

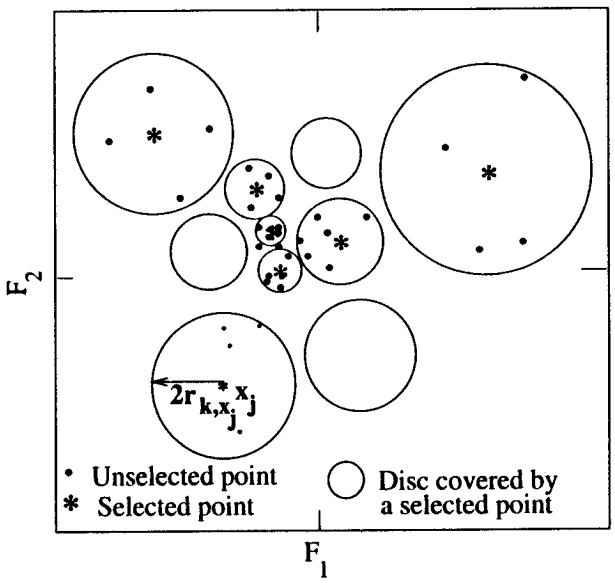


Figure 2.1: Multiresolution data reduction

a scale which is both efficient in terms of density estimation error and natural to the data distribution.

It is observed from experiments that the multiresolution approach helps to achieve lower error with similar condensation ratio compared to several related data condensation schemes. The reduced set obtained was found to be effective for a number of data mining applications like classification, clustering and rule generation. The suggested algorithm is also found to be scalable and efficient in terms of sample complexity, in the sense that the error level decreases quickly with the increase in size of the condensed set. In the next section we describe aspects of multiscale representation.

2.2 Multiscale Representation of Data

Multiscale representation of data refers to visualization of the data at different 'scales', where the term scale may signify either unit, frequency, radius, window size or kernel parameters. The importance of scale has been increasingly acknowledged in the past decade in the areas of image and signal analysis and computer vision with the development of several scale inspired models like pyramids, wavelets and multiresolution techniques. Recently scale-based methods have also become popular in clustering [80]

and density estimation. In these methodologies, the concept of scale has been implemented using variable width radial basis function Network, annealing based clustering and variable window density estimates.

The question of scale is natural to data condensation. At a very coarse scale the entire data may be represented by only a few number of points, and at a very fine scale all the sample points may constitute the condensed set, the scales in between representing varying degrees of detail. In many data mining applications (e.g., structure discovery in remotely sensed data, identifying population groups from census data) it is necessary that the data be represented in varying levels of detail. Data condensation is only a preliminary step in the overall data mining process and several higher level learning operations may be performed on the condensed set later. Hence the condensation algorithm should be able to obtain representative subsets at different scales, as demanded, in an *efficient* manner.

The proposed method for data condensation, discussed in Section 2.1, obtains condensed sets of different degrees of detail by varying a scale parameter k. It may be noted that such variable detail representation may be achieved by other approaches also, including random sampling. However, unlike random sampling the scales induced by the proposed method are not prespecified by the sizes of the condensed sets but follow the natural characteristics of the data. As far as efficiency of the scaling procedure is concerned, it may be noted that in most of the multiscale schemes for representing data or signal, including wavelets, efficiency is achieved by a lenient representation of the 'unimportant' regions and a detailed representation of the 'important' regions, where the notion of importance may vary from problem to problem. We have followed a similar principle in the proposed condensation algorithm where at each scale the different regions of the feature space are represented in the condensed set based on the densities of those regions estimated at that particular scale. Figure 2.2 illustrates the concept of variable scale representation. The data consists of 2000 points selected randomly from two nonoverlapping circles of radius 1 unit and centers at (2,0) and (5,0) respectively (Figure 2.2(a)). Figures 2.2(b)-(e) shows representation of the data by condensed sets at different levels of detail. It can be seen that in Figure 2.2(b) only two points cover the entire data set. In Figure 2.2(c) four points are used to represent the entire data set. Figure 2.2(d) and (e) are more detailed representations of the data.

For a particular scale the basic principle of the proposed data condensation algorithm

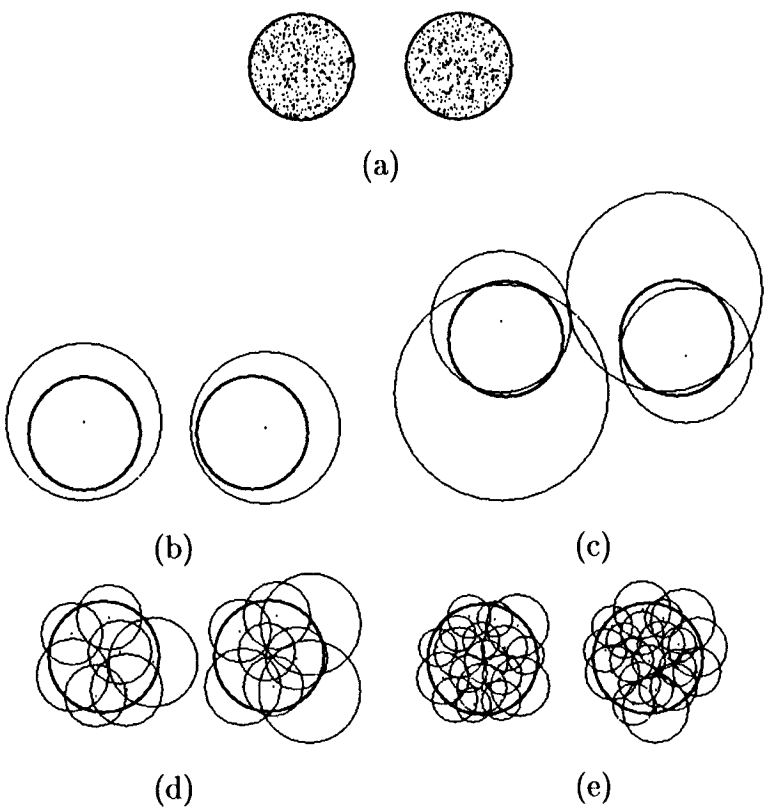


Figure 2.2: Representation of data set at different levels of detail by the condensed sets. '.' is a point belonging the condensed set, the circles about the points denote the discs covered that point. The two bold circles denote the boundaries of the data set.

involves sorting the points based on *estimated densities*, selecting the denser points and removing other points that lie within certain distances of the selected points in a multiresolution manner. A non-parametric method of estimating a probability density function is the k-nearest neighbor method. In k-NN based estimation technique the density of a point is computed based upon the volume of disc about that point which includes a fixed number, say k, other points [87]. Hence, the radius of the disc is smaller in a densely populated region than in a sparse region. The volume of the disc is inversely proportional to the probability density function at the center point of the disc. This behavior is advantageous for the present problem from the point of view of multiresolution representation over different regions of feature space. This is the reason that the k-NN density estimate is considered in the proposed condensation algorithm.

Before we present the data condensation algorithm, we describe in brief the k-NN based density estimation technique in the next section.

2.3 Nearest Neighbor Density Estimate

Let $\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_N}$ be independent observations on a p-dimensional random variable $\mathbf{X}$, with a continuous probability density function f. The problem is to estimate f at a point $\mathbf{z}$.

Let $d(\mathbf{x}, \mathbf{z})$ represent the Euclidean distance between $\mathbf{x}$ and $\mathbf{z}$. A p-dimensional hypersphere of radius r about $\mathbf{z}$ is designated by $S_{r,\mathbf{z}}$, *i.e.*, $S_{r,\mathbf{z}} = \{\mathbf{x} | d(\mathbf{x}, \mathbf{z}) \leq r\}$. The volume or Lebesgue measure of the hypersphere $S_{r,\mathbf{z}}$ will be called A_r. Let us describe a non-parametric method for estimating f suggested by Loftsgaarden [87].

Let $k(N)$ be a sequence of positive integers such that $\lim_{N\to\infty} k(N) = \infty$, and $\lim_{N\to\infty} k(N)/N = 0$. Once $k(N)$ is chosen and a sample set $\{\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N\}$ is available, $r_{k(N),\mathbf{z}}$ is determined as the distance from $\mathbf{z}$ to the $(k(N)+1)$th nearest neighbor of $\mathbf{z}$ among $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N$. Hence, an estimate of f is given by

$$\hat{f}_N(\mathbf{z}) = \frac{k(N)}{N} \times \frac{1}{A_{r_{k(N),\mathbf{z}}}} \tag{2.1}$$

It can be proved [87] that the density estimate given by Equation 2.1 is asymptotically unbiased and consistent. It may however be noted that k-NN estimates suffer from the 'curse of dimensionality' problem in high dimensional spaces.

A condensation algorithm should obtain a subset which is representative of the original data distribution. We discuss some measures of accuracy of such representations in terms of the error in k-NN density estimate discussed above.

Measures of error in density estimate

Let $\mathbf{x}_1, \ldots, \mathbf{x}_N$ be N independent samples drawn from a distribution f. The closeness between two estimates g_1 and g_2 of f is measured by a criterion of the form

$$\hat{J} = \frac{1}{N} \sum_{i=1}^{N} D(g_1(\mathbf{x}_i), g_2(\mathbf{x}_i)) \ ,$$

where $\mathbf{x}_i$ is the ith sample, and $D(.,.)$ is a measure of the distance between $g_1(\mathbf{x}_i)$ and $g_2(\mathbf{x}_i)$. It may be noted that $\hat{J}$ is a random variable, and an estimate of the quantity J, where

$$J = E(\hat{J}) = \int D(g_1(\mathbf{z}), g_2(\mathbf{z})) f(\mathbf{z}) d\mathbf{z}$$

In our case we have a density estimate $\hat{f}_N$ for f, from $\{\mathbf{x}_1, \ldots \mathbf{x}_N\}$ using the k-NN density estimation method already described. Now we like to choose n points, $n << N$, from $\mathbf{x}_1, \ldots, \mathbf{x}_N$ such that the density estimate $\hat{\alpha}_n$ obtained from this n points is close to $\hat{f}_N$ where n is not predetermined. In the next section, we present a method that automatically provides the value for n and the set of n points for a given $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$. It may be noted that $\hat{J}$ measures the difference between estimates $\hat{f}_N$ and $\hat{\alpha}_n$ and not the error of each of these estimates with respect to the actual distribution. However, if N is large it is known that $\hat{f}_N$ is a consistent estimate of f [87] (for suitable values of k as mentioned in Equation 2.1). Hence, a small value of $\hat{J}$ indicate closeness of $\hat{\alpha}_n$ to the actual distribution f.

For D we use the form, similar to log-likelihood ratio used in classification [43],

$$D(\hat{f}_N(\mathbf{x}_i), \hat{\alpha}_n(\mathbf{x}_i)) = \left| \ln \frac{\hat{f}_N(\mathbf{x}_i)}{\hat{\alpha}_n(\mathbf{x}_i)} \right| \ , \tag{2.2}$$

A second possibility is a modified version of the kernel of the Kullback-Liebler information number [43], which attaches more weight to the high density region of the distribution

$$D(\hat{f}_N(\mathbf{x}_i), \hat{\alpha}_n(\mathbf{x}_i)) = \left| \hat{\alpha}_N(\mathbf{x}_i) . \ln \frac{\hat{f}_N(\mathbf{x}_i)}{\hat{\alpha}_n(\mathbf{x}_i)} \right| \ . \tag{2.3}$$

We have used both of these quantities to measure the efficacy of the reduction algorithms in subsequent sections. If the estimates are close enough, each of the quantities is close to zero.

2.4 Proposed Data Reduction Algorithm [100]

The proposed data reduction algorithm involves estimating the density at a point using the methods described in the previous section, sorting the points based on the density criterion, selecting a point according to the sorted list, and pruning all points lying within a disc about a selected point with radius inversely proportional to the density at that point.

Algorithm:

Let $B_N = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ be the original data set. Choose a positive integer k.

1. For each point $\mathbf{x}_i \in B_N$ calculate the distance of the kth nearest neighbor of $\mathbf{x}_i$ in B_N. Denote it by $r_{k,\mathbf{x}_i}$.

2. Select the point $\mathbf{x}_j \in B_N$, having the lowest value of $r_{k,\mathbf{x}_j}$ and place it in the reduced set E. Ties in lowest value of $r_{k,\mathbf{x}_j}$ may be resolved by a convention, say according to the index of the samples. From Equation 2.1 it is evident that $\mathbf{x}_j$ corresponds to the point having the highest density $\hat{f}_N(\mathbf{x}_j)$.

3. Remove all points from B_N that lie within a disc of radius $2r_{k,\mathbf{x}_j}$ centered at $\mathbf{x}_j$, and the set consisting of the remaining points be renamed as B_N. Note that since $r^p_{k,\mathbf{x}_j}$ (where p is the dimension of the feature space) is inversely proportional to the estimate of the probability density at $\mathbf{x}_j$, regions of higher probability density are covered by smaller discs and sparser regions are covered by larger discs. Consequently, more points are selected from the regions having higher density.

4. Repeat Step 2 on B_N till B_N becomes a null set.

The $\mathbf{x}_j$'s thus selected and the corresponding $r_{k,\mathbf{x}_j}$ constitute the condensed (reduced) set. □

The procedure is illustrated in Figure 2.1 in $F_1 - F_2$ space. As shown in the figure, each selected point (marked '*') is at the center of a disc that covers some region in the feature space. All other points (marked as '.') lying within the disc except the center is discarded. It can be seen that selected points lying in high density regions have discs of smaller radii, while points in sparser regions correspond to larger discs, *i.e.*, the data is represented in a multiscale manner over the feature space.

Remarks:

1. The algorithm not only selects the denser data points, but does so in a manner such that the separation between two points is inversely proportional to the probability density of the points. Hence, regions in the feature space having higher density are represented by more points than sparser regions. This provides a better representation of the data distribution than random sampling, because different regions of the feature space are given variable importance on the basis of the probability density of that region, *i.e.*, the representation is of multiresolution nature. A technique for performance enhancement and computational time reduction, using such multiresolution representation is discussed in [29].

2. The condensed set obtained may be used to obtain an estimate of the probability density function of the data. This may be done using the k-NN density estimation method discussed in Section 2.3.

3. The parameter k acts as a scale-parameter for the condensation algorithm. The size of the neighborhood, used for density estimate, as well as the pruning radii are dependent on k, and therefore vary with scale. Smaller the value of k more refined is the scale and vice versa. However, independent of the chosen scale, the representation gives adequate importance to the different regions of the feature space depending on their estimated densities at that scale. This type of multiresolution representation helps preserve salient features which are natural to the data over a wide range of scales. In many situations the scale to be used for condensation is dictated by the application. However, if no such application specific requirements exist, the condensed set may be selected from the region where the error versus scale curve (which is exponentially decaying in nature) begins to flatten.

4. It may be noted that the choice of k is a classical problem for k-NN based methods for finite sample sets. Theoretically, the value of k should increase with the size of the data set (N), but at a slower rate than N itself. For data condensation using the proposed method it has also been observed that the value of k should be increased as the data set size N increases to achieve a constant condensation ratio (CR), though the exact nature of the k versus CR curve is distribution dependent. In the experimental results presented in Section 2.5.5 we observe that at high values of k (*i.e.*, low values of CR) the k versus CR curve is sufficiently robust over different data sets.

5. The accuracy of k-NN density depends on the value of k used. Admissible values of k may be obtained from considerations discussed above. However, for very small data sets the choice of lower admissible limit of k is dictated by the size of the data set.

2.5 Experimental Results and Comparisons [100]

In this section we present the results of experiments conducted on some well known data sets of varying dimension and size. Among them the Forest cover type data represents forest cover of 30m × 30m cells obtained from US Forest Service (USFS) Region 2 Resource Information System (RIS). It contains 581012 instances having 54 attributes representing cartographic variables. Each observation is labeled as belonging to one of the 7 different classes (forest cover types). Among the other data sets, the Satellite Image data consists of four 512 × 512 gray scale images of different spectral bands obtained by the Indian Remote Sensing satellite of the city of Calcutta in India. Each pixel represents a 36.25m × 36.25m region. The third large data set used is the PUMS census data for the Los Angeles and Long Beach area. The data contains 133 attributes, mostly categorical and 320000 samples were used. The other data sets for e.g., Wisconsin breast cancer (medical domain data), Pima Indian (also medical domain data), Vowel (speech data), Iris (flower classification data), ringnorm and twonorm (artificial data) are benchmark data sets widely used in literature. The *Norm* data was artificially generated by drawing 500 i.i.d samples from a normal distribution with mean $= \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ and covariance matrix $= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. The data sets are described in detail

in Appendix A.

The organization of the results is as follows. First we present and compare the results concerning error in density estimate and condensation ratio for all ten data sets. Next, we demonstrate the efficacy of our condensation method for three diverse tasks namely classification, clustering and rule generation on the three large data sets. The Forest cover type data is considered to evaluate the *classification* performance, the Satellite image data is considered for *clustering* and the PUMS Los Angeles census data is considered for *rule generation.* Our choice of tasks for the three large data sets described above has been guided by studies performed on them in existing literature as well as the nature of the data sets. Finally we empirically study the scalability property of the algorithm in terms of sample complexity, *i.e.*, the number of samples in the condensed set required to achieve a particular accuracy level.

2.5.1 Density estimation

Here we compare the error between density estimates obtained using the original data set and the reduced set. The proposed algorithm is compared with three representative data reduction schemes (random sampling, vector quantization based and clustering based) described below. Classification based data reduction methods like Condensed Nearest Neighbor are not compared, as error in density estimates is not the optimality criterion for such methods. The methods compared are: Random sampling with replacement, the Self-organizing map (SOM) [72] and Astrahan's clustering based uniform scale method [9]. In Astrahan's method (explained in Section 2.1), for the purpose of density estimation we use radius $d_1 = \sqrt{sup_{i=1,..,n}(inf_{j=1,..,n} d(\mathbf{x}_i, \mathbf{x}_j))}$, and radius $d_2 = \gamma d_1$ for pruning, where γ is a tunable parameter controlling the condensation ratio. The above expression for d_1 produces a radius close to that obtained using the minimal spanning tree based method described in [23]. The following quantities are compared for each algorithm:

1. The condensation ratio (CR), measured as the ratio of the cardinality of the condensed set and the original set, expressed as percentage.

2. The log-likelihood (LLR) ratio for measuring the error in density estimate with the original set and the reduced set as described in Equation 2.2.

3. The Kullback-Liebler information number (KLI), also for measuring the error in density estimate (Equation 2.3).

Test of statistical significance

In our experiments for each data 90% of the samples are selected as training set and the remaining samples are used as test set. Ten such independent random training-test set splits are obtained, and the mean and standard deviation (SD) of the errors are computed over ten runs. Tests of significance were performed for the inequality of means (of the errors) obtained using the proposed algorithm and the other condensation schemes compared. Since both mean pairs and the variance pairs are unknown and different, a generalized version of t-test is appropriate in this context. The above problem is the classical Behrens-Fisher problem in hypothesis testing, a suitable test statistic is described and tabled in [8]. The test statistic is of the form

$$v = \frac{\bar{x}_1 - \bar{x}_2}{\sqrt{\lambda_1 s_1^2 + \lambda_2 s_2^2}}, \tag{2.4}$$

where $\bar{x}_1, \bar{x}_2$ are the means, s_1, s_2 the standard deviations and $\lambda_1 = 1/n_1, \lambda_2 = 1/n_2$, n_1, n_2 are the number of observations. □

In Tables 2.1-2.4 we report along with the individual means and SD's the value of test statistic computed and the corresponding tabled values at an error probability level of 0.05. If the computed value is greater than the tabled value the means are significantly different.

The experiments have been performed for different values of condensation ratios for each algorithm. However, in Tables 2.1 and 2.2, comparison is presented on the basis of error in density estimate for similar values of CR. Alternatively one could have also compared CR for similar values of error in density estimate. In Tables 2.1 and 2.2, results are presented for two different sets of values of CR, e.g., 0.1-3% and 5-20% (of the original data set and not the training set) respectively. The error values were computed using Equations 2.2 and 2.3 with the same value of k as used for condensation. It may be noted that the optimal choice of k is a function of the data size.

It is seen from the results (Tables 2.1 and 2.2) that our multiscale method achieves consistently better performance than Astrahan's method, random sampling and SOM

Table 2.1: Comparison of k-NN density estimation error of condensation algorithms (lower CR)

Data set	Multiscale Algorithm			Uniform Scale method [9]			SOM			Random sampling		
	CR	LLR	KLI	CR	LLR	KLI	CR	LLR	KLI	CR	LLR	KLI
	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD		Mean SD	Mean SD		Mean SD	Mean SD
Norm	3.0 0.001	1.16 0.09	0.16 0.04	3.0 0.001	1.33 0.12	0.20 0.04	3.0	**1.21 0.08**	**0.17 0.004**	3.0	1.38 0.27	0.25 0.10
					(3.76, 1.72)	(2.34, 1.71)		**(1.69, 1.73)**	**(0.02, 1.81)**		(2.56, 1.78)	(2.77, 1.77)
Iris	2.5 0.000	1.83 0.08	0.40 0.04	2.5 0.000	2.02 0.17	0.68 0.08	2.5	2.00 0.01	0.44 0.005	2.5	2.85 0.98	1.01 0.23
					(3.35, 1.76)	(10.38, 1.76)		(7.0, 1.81)	(3.29, 1.81)		(3.44, 1.81)	(8.66, 1.81)
Vowel	3.4 0.00	1.40 0.16	0.10 0.01	3.4 0.001	1.67 0.28	0.165 0.01	3.4	**1.43 0.005**	0.11 0.00	3.4	1.95 0.55	0.41 0.11
					(2.77, 1.74)	(15.24, 1.71)		**(0.88, 1.81)**	(3.32, 1.81)		(3.18, 1.78)	(9.30, 1.81)
Pima	3.2 0.002	1.15 0.11	18.1 1.03	3.2 0.001	1.31 0.17	21.1 4.0	3.2	1.24 0.04	20.4 1.01	3.2	1.99 0.91	25.1 9.1
					(2.62, 1.73)	(2.41, 1.81)		(2.55, 1.78)	(5.22, 1.71)		(3.04, 1.81)	(2.53, 1.81)
Cancer	4.3 0.002	1.37 0.17	17.1 1.4	4.3 0.003	1.61 0.28	19.0 1.04	4.3	1.54 0.11	19.4 0.50	4.3	1.805 0.57	24.0 9.01
					(2.43, 1.76)	(3.80, 1.72)		(2.23, 1.81)	(5.35, 1.78)		(2.43, 1.81)	(2.54, 1.81)
Monk	4.1 0.00	0.64 0.01	0.65 0.04	4.1 0.001	0.70 0.04	0.72 0.05	4.1	0.67 0.01	0.68 0.01	4.1	0.83 0.16	0.88 0.16
					(4.82, 1.81)	(3.62, 1.72)		(7.03, 1.71)	(2.41, 1.81)		(1.86, 1.81)	(2.61, 1.81)
Tnorm	1.0 0.00	0.43 0.01	1.70 0.10	1.0 0.00	0.57 0.07	1.97 0.17	1.0	0.46 0.00	1.81 0.01	1.0	0.59 0.19	2.01 0.56
					(6.56, 1.81)	(4.54, 1.73)		(9.95, 1.81)	(3.30, 1.81)		(5.86, 1.81)	(1.81, 1.78)
Rnorm	2.0 0.00	0.40 0.05	2.11 0.22	2.0 0.001	0.54 0.07	2.95 0.22	2.0	**0.41 0.001**	2.24 0.001	2.0	0.70 0.15	3.01 0.91
					(5.40, 1.73)	(8.95, 1.71)		**(0.63, 1.81)**	(1.96, 1.81)		(6.23, 1.78)	(3.19, 1.81)
Forest	0.1 0.001	0.82 0.01	2.71 0.02	0.1 0.004	2.0 0.02	4.7 0.55	0.1	1.40 0.00	3.20 0.01	0.1	3.8 1.7	7.0 2.50
					(175, 1.76)	(11.99, 1.81)		(192.36, 1.81)	(72.68, 1.76)		(5.81, 1.81)	(5.69, 1.81)
Sat.Img.	0.2 0.001	0.78 0.01	1.18 0.09	0.2 0.002	0.92 0.02	1.40 0.25	0.2	0.88 0.01	1.28 0.00	0.2	1.09 0.15	1.79 0.27
					(20.76, 1.76)	(8.21, 1.81)		(23.45, 1.71)	(3.68, 1.81)		(6.84, 1.81)	(7.10, 1.78)
Census	0.1 0.002	0.27 0.00	1.55 0.10	0.1 0.004	0.31 0.02	1.70 0.15	0.1	0.30 0.01	1.61 0.01	0.1	0.40 0.17	1.90 0.45
					(6.63, 1.81)	(2.76, 1.72)		(14.07, 1.81)	(1.98, 1.81)		(2.53, 1.81)	(2.52, 1.81)

'CR' denotes condensation ratio in %, 'LLR' denotes the log-likelihood error and 'KLI' denotes the Kullback-Liebler information number, the numbers in the parenthesis indicate the computed and tabled values of the test statistic respectively. A higher computed value compared to tabled value indicates statistical significance. The values marked bold denote lack of statistical significance.

Table 2.2: Comparison of k-NN density estimation error of condensation algorithms (higher CR)

Data set	Multiscale Algorithm			Uniform Scale method [9]			SOM			Random sampling		
	CR	LLR	KLI	CR	LLR	KLI	CR	LLR	KLI	CR	LLR	KLI
	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD		Mean SD	Mean SD		Mean SD	Mean SD
Norm	20 0.001	0.38 0.001	0.08 0.00	20 0.002	0.43 0.002 (74.16, 1.76)	0.10 0.001 (61.59, 1.78)	20	0.40 0.001 (46.9, 1.72)	0.09 0.00 (74.16, 1.76)	20	0.49 0.09 (4.05, 1.81)	0.11 0.01 (9.94, 1.81)
Iris	20 0.00	0.82 0.001	0.19 0.001	20 0.001	0.91 0.001 (211, 1.72)	0.25 0.001 (140, 1.72)	20	0.87 0.001 (117, 1.72)	0.22 0.001 (9.90, 1.81)	20	1.04 0.40 (1.82, 1.81)	0.40 0.16 (4.35, 1.81)
Vowel	20 0.001	0.88 0.07	0.05 0.001	20 0.002	0.97 0.10 (2.61, 1.74)	0.09 0.001 (93.8, 1.72)	20	**0.90 0.001 (0.93, 1.81)**	0.07 0.001 (46.90, 1.72)	20	1.25 0.25 (4.73, 1.81)	0.21 0.04 (13.2, 1.81)
Pima	20 0.001	0.50 0.05	8.8 0.32	20 0.002	0.62 0.09 (3.86, 1.78)	10.0 0.81 (4.56, 1.76)	20	0.59 0.002 (5.96, 1.81)	9.1 0.10 (2.96, 1.81)	20	0.81 0.25 (4.16, 1.81)	14.03 4.1 (4.21, 1.81)
Cancer	20 0.001	0.68 0.05	9.1 0.4	20 0.002	0.81 0.07 (5.01, 1.76)	10.4 0.70 (5.34, 1.74)	20	0.77 0.01 (5.85, 1.81)	9.8 0.01 (5.63, 1.81)	20	0.92 0.22 (3.52, 1.81)	11.9 2.09 (4.36, 1.81)
Monk	20 0.002	0.31 0.001	0.32 0.005	20 0.002	0.34 0.002 (44.5, 1.78)	0.35 0.002 (18.47, 1.78)	20	0.32 0.001 (33.01, 1.81)	0.33 0.001 (6.40, 1.81)	20	0.42 0.04 (9.11, 1.81)	0.44 0.04 (9.87, 1.81)
Tnorm	20 0.000	0.22 0.001	0.80 0.005	10 0.001	0.29 0.005 (45.53, 1.81)	1.04 0.02 (38.61, 1.81)	10	0.25 0.00 (70.35, 1.71)	0.88 0.01 (26.40, 1.81)	10	0.35 0.08 (5.40, 1.81)	1.21 0.17 (7.99, 1.81)
Rnorm	20 0.000	0.25 0.005	0.91 0.002	10 0.001	0.29 0.01 (11.86, 1.78)	1.07 0.07 (7.57, 1.81)	10	0.26 0.00 (6.63, 1.81)	1.01 0.00 (32.52, 1.81)	10	0.32 0.09 (2.57, 1.81)	1.21 0.35 (2.84, 1.81)
Forest	5 0.001	0.54 0.005	0.91 0.002	5 0.002	0.62 0.005 (37.5, 1.72)	1.71 0.007 (364, 1.81)	5	0.57 0.002 (18.4, 1.78)	1.04 0.005 (80.0, 1.76)	5	1.72 0.25 (15.6, 1.81)	4.91 1.17 (11.4, 1.81)
Sat.Img.	5 0.001	0.41 0.005	0.71 0.01	5 0.001	0.50 0.007 (34.70, 1.76)	0.81 0.02 (14.83, 1.76)	5	0..47 0.002 (36.95, 1.78)	0.80 0.01 (21.10, 1.71)	5	0.62 0.10 (6.95, 1.81)	0.92 0.14 (4.96, 1.81)
Census	5 0.002	0.17 0.001	0.80 0.01	5 0.002	0.22 0.002 (74.16, 1.76)	0.91 0.007 (27.98, 1.78)	5	0.19 0.00 (46.90, 1.81)	0.88 0.005 (21.95, 1.78)	5	0.28 0.01 (36.3, 1.81)	1.00 0.17 (3.89, 1.81)

for both sets of condensation ratios. For each condensation ratio (two condensation ratios are considered), for each index of comparison (two indices are considered) of density estimation error and for each data set (eleven data sets including three large data sets), the proposed method is found to provide better performance than each of the other three data condensation methodologies compared. Regarding statistical significance tests it can be seen from Tables 2.1 and 2.2 that, out of 132 comparisons, the proposed method is found to provide *significantly* better results in 127 comparisons. Only while comparing with SOM for the *Norm*, Vowel and Ringnorm data sets, the performance of the proposed method is found to be better, but not significantly. (The corresponding entries are marked bold in Tables 2.1 and 2.2.) Experiments were also carried out for other values of the condensation ratio (e.g., 40% and 60%) and similar performance has been observed.

For the purpose of comparison, the condensed sets obtained using different algorithms are also used for kernel density estimates. The kernel estimate is given by

$$\hat{\beta}_n(\mathbf{x}) = \frac{1}{n}\sum_{j=1}^{n} K(\mathbf{x}, \mathbf{u}_j),$$

where $\mathbf{u}_j$'s are points belonging to the reduced set and $K(\cdot,\cdot)$ is the kernel function. We used a Gaussian kernel of the form

$$K(\mathbf{x}, \mathbf{u}_j) = \left[(h^2 2\pi)^{-p/2}\right] \exp\left\{-\frac{1}{2h^2}\delta(\mathbf{x}, \mathbf{u}_j)\right\},$$

where p is the dimension, h bandwidth and $\delta(\mathbf{x}, \mathbf{u}_j)$ the Euclidean distance between $\mathbf{x}$ and $\mathbf{u}_j$. The bandwidth h is chosen as

$$h = \sqrt{\sup_{i=1,..,n} (\inf_{j=1,..,n} d(\mathbf{u}_i, \mathbf{u}_j))},$$

where $\mathbf{u}_i$ and $\mathbf{u}_j$ are points in the condensed set. The reason for selecting the above bandwidth can be explained in terms of minimal spanning trees [23]. The bandwidth satisfies both the conditions for consistent kernel density estimation. The error measures are presented in Tables 2.3 and 2.4 for the same two groups of condensed sets as considered in Tables 2.1 and 2.2 respectively. It is seen from Tables 2.3 and 2.4 that when using kernel estimates, the proposed algorithms produce less error than all the related schemes for all data sets. Statistical significance tests are also presented for all the comparisons, and in 129, of 132 comparisons, the proposed method performs

Table 2.3: Comparison of kernel (Gaussian) density estimation error of condensation algorithms (lower CR, same condensed set as Table 2.1)

Data set	Multiscale Algorithm		Uniform Scale method [9]		SOM		Random sampling	
	LLR	KLI	LLR	KLI	LLR	KLI	LLR	KLI
	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD
Norm	1.04 0.07	0.14 0.03	1.15 0.09	0.17 0.03	1.10 0.07	**0.15 0.004**	1.29 0.25	0.23 0.09
			(3.05, 1.74)	(2.24, 1.74)	(1.92, 1.72)	**(1.04, 1.81)**	(3.05, 1.81)	(3.67, 1.78)
Iris	1.72 0.05	0.37 0.02	1.91 0.14	0.59 0.04	1.88 0.01	0.41 0.002	2.78 0.95	0.98 0.17
			(4.04, 1.78)	(15.56, 1.76)	(9.92, 1.81)	(6.29, 1.81)	(3.52, 1.81)	(11.27, 1.81)
Vowel	1.35 0.09	0.09 0.005	1.61 0.17	0.16 0.01	**1.38 0.002**	0.10 0.00	1.88 0.47	0.37 0.08
			(4.27, 1.76)	(19.8, 1.76)	**(1.05, 1.81)**	(6.32, 1.81)	(3.50, 1.81)	(11.05, 1.81)
Pima	1.07 0.08	17.2 0.81	1.27 0.11	19.9 2.2	1.18 0.01	19.1 0.88	1.91 0.90	23.2 8.9
			(4.65, 1.74)	(3.64, 1.78)	(4.31, 1.81)	(5.02, 1.72)	(2.94, 1.81)	(2.12, 1.81)
Cancer	1.34 0.16	16.8 1.4	1.57 0.20	18.8 0.91	1.51 0.09	19.1 0.47	1.78 0.55	23.3 8.80
			(2.84, 1.74)	(3.78, 1.78)	(2.92, 1.78)	(4.93, 1.79)	(2.43, 1.81)	(2.31, 1.81)
Monk	0.62 0.01	0.63 0.04	0.68 0.03	0.71 0.04	0.66 0.01	0.67 0.01	0.82 0.11	0.87 0.14
			(6.00, 1.78)	(4.47, 1.74)	(8.94, 1.74)	(3.08, 1.81)	(6.00, 1.81)	(5.21, 1.81)
Tnorm	0.42 0.01	1.64 0.05	0.56 0.05	1.92 0.11	0.45 0.00	1.78 0.001	0.57 0.10	1.97 0.44
			(8.68, 1.81)	(6.51, 1.74)	(9.49, 1.81)	(5.53, 1.81)	(4.72, 1.81)	(2.33, 1.81)
Rnorm	0.38 0.03	2.02 0.17	0.53 0.05	2.80 0.19	0.40 0.001	2.19 0.01	0.69 0.09	2.89 0.82
			(8.13, 1.76)	(6.51, 1.74)	(9.49, 1.81)	(5.53, 1.81)	(4.72, 1.81)	(2.33, 1.81)
Forest	0.80 0.007	2.69 0.01	1.95 0.01	4.4 0.53	1.38 0.00	3.10 0.01	3.70 1.43	7.0 2.50
			(325, 1.74)	(10.2, 1.81)	(366, 1.81)	(91, 1.72)	(6.55, 1.81)	(5.45, 1.81)
Sat.Img	0.75 0.005	1.09 0.02	0.88 0.01	1.28 0.09	0.82 0.005	1.22 0.00	0.98 0.10	1.72 0.22
			(36.77, 1.76)	(6.52, 1.81)	(31.3, 1.72)	(20.55, 1.81)	(7.26, 1.81)	(9.02, 1.81)
Census	0.25 0.00	1.46 0.04	0.29 0.01	1.59 0.09	0.27 0.005	1.52 0.005	0.37 0.10	1.82 0.40
			(12.6, 1.81)	(4.17, 1.78)	(12.6, 1.81)	(4.71, 1.81)	(3.79, 1.81)	(2.83, 1.81)

significantly better than the other three algorithms. The cases for which statistical significance could not be established are denoted by bold entries in Tables 2.3 and 2.4.

We have also compared our algorithm with Fukunaga's non-parametric data condensation algorithm [43] only for the *Norm* data set. For a log-likelihood error of 0.5 the condensation ratio achieved by this method is 50%, while the corresponding figure is 23.4% for our method. On the *Norm* data set while the CPU time required by the proposed algorithm is 8.10 secs, the above mentioned algorithm is found to require 2123.05 secs.

In Figure 2.3, we have plotted the points in the condensed set along with the discs covered by them at different condensation ratios for the proposed algorithm and for Astrahan's method. The objective is to demonstrate the multiresolution characteristics of the algorithm in contrast to a fixed resolution method. It is observed that our algorithm represents the original data in a multiresolution manner; the denser regions are more accurately represented compared to the sparser regions. The regions covered by the representative points are uniform for Astrahan's method [9]. It may be observed

Table 2.4: Comparison of kernel (Gaussian) density estimation error of condensation algorithms (higher CR, same condensed set as Table 2.2)

Data set	Multiscale Algorithm		Uniform Scale method [9]		SOM		Random sampling	
	LLR	KLI	LLR	KLI	LLR	KLI	LLR	KLI
	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD	Mean SD
Norm	0.35 0.001	0.07 0.00	1.40 0.001	0.09 0.001	0.37 0.001	0.08 0.001	0.47 0.05	0.10 0.01
			(117, 1.72)	(66, 1.81)	(47, 1.72)	(33.1, 1.81)	(7.95, 1.81)	(9.94, 1.81)
Iris	0.79 0.001	0.17 0.001	0.88 0.001	0.23 0.001	0.86 0.001	0.21 0.001	1.00 0.28	0.37 0.10
			(211, 1.72)	(140, 1.72)	(140, 1.72)	(93.8, 1.72)	(2.48, 1.81)	(6.63, 1.81)
Vowel	0.86 0.05	0.04 0.001	0.95 0.09	0.08 0.001	**0.88 0.001**	0.05 0.001	1.17 0.22	0.20 0.04
			(2.90, 1.74)	(93.8, 1.72)	**(1.32, 1.81)**	(23.45, 1.72)	(4.55, 1.81)	(13.26, 1.81)
Pima	0.47 0.04	8.20 0.28	0.60 0.07	9.10 0.54	0.56 0.001	8.8 0.04	0.80 0.17	14.00 4.10
			(5.34, 1.74)	(4.90, 1.74)	(7.46, 1.81)	(7.03, 1.81)	(6.27, 1.81)	(4.68, 1.81)
Cancer	0.67 0.04	8.70 0.35	0.79 0.05	9.80 0.76	0.74 0.005	9.50 0.01	0.90 0.19	11.5 2.01
			(6.21, 1.76)	(4.66, 1.74)	(5.75, 1.81)	(7.57, 1.81)	(3.92, 1.78)	(4.55, 1.81)
Monk	0.30 0.001	0.31 0.004	0.34 0.001	0.34 0.001	0.31 0.001	0.32 0.001	0.41 0.03	0.44 0.02
			(93.8, 1.72)	(24.1, 1.81)	(23.4, 1.72)	(8.04, 1.78)	(12.15, 1.81)	(21.14, 1.81)
Tnorm	0.21 0.001	0.78 0.004	0.28 0.004	0.99 0.01	0.23 0.00	0.86 0.005	0.34 0.05	1.19 0.10
			(56.3, 1.81)	(64.6, 1.78)	(66.3, 1.81)	(41.4, 1.76)	(8.62, 1.81)	(13.5, 1.81)
Rnorm	0.23 0.002	0.88 0.001	0.28 0.005	1.02 0.05	0.24 0.001	0.97 0.001	0.31 0.05	1.17 0.28
			(30.8, 1.78)	(9.28, 1.81)	(14.8, 1.78)	(211, 1.72)	(4.64, 1.81)	(3.43, 1.81)
Forest	0.53 0.004	0.90 0.002	0.61 0.004	1.70 0.005	0.55 0.001	0.98 0.004	1.70 0.17	4.90 1.00
			(46.9, 1.72)	(492, 1.78)	(16.08, 1.79)	(59.3, 1.74)	(22.8, 1.81)	(13.2, 1.81)
Sat.Img	0.40 0.004	0.70 0.005	0.47 0.007	0.80 0.01	0.45 0.001	0.77 0.005	0.59 0.05	0.90 0.10
			(28.8, 1.74)	(29.6, 1.74)	(40, 1.78)	(32, 1.72)	(12.5, 1.81)	(6.62, 1.81)
Census	0.16 0.001	0.78 0.01	0.22 0.001	0.91 0.005	0.17 0.00	0.87 0.004	0.27 0.01	0.98 0.11
			(140, 1.72)	(35, 1.76)	(33.1, 1.81)	(27.7, 1.78)	(36.3, 1.81)	(6.00, 1.81)

from the figure that multiscale representation is most effective in terms of error when the condensed set is sparse, *i.e.*, the condensation ratio is low (Figure 2.3(a)).

2.5.2 Classification: Forest cover data

As mentioned in Appendix A, the said data represents forest cover types of 30m × 30m cells obtained from US Forest Service (USFS) Region 2 Resource Information System (RIS). There are 581,012 instances, with 54 attributes representing cartographic variables (hillshade, distance to hydrology, elevation, soil type etc), of which 10 are quantitative and 44 binary. The quantitative variables were scaled to the range $[0, 1]$. The task is to classify the observations into seven categories representing the forest cover types, namely – Spruce/Fir, Lodgepole Pine, Ponderosa Pine, Cottonwood/Willow, Aspen, Douglas-fir, Krummholz. About 80% of the observations belong to classes Spruce/Fir and Lodgepole Pine.

We have condensed the training set using different condensation algorithms including

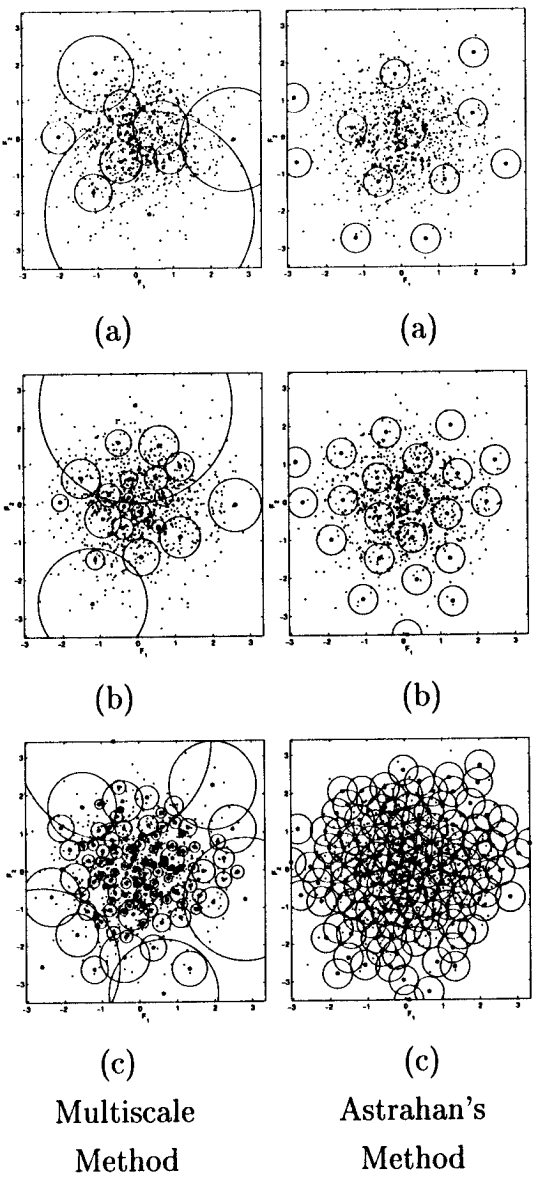


Figure 2.3: Plot of the condensed points (of the *Norm* data) for the proposed algorithm and Astrahan's method, for different sizes of the condensed set. Bold dots represent a selected point and the discs represent the area of $F_1 - F_2$ plane covered by a selected point at their center.

the proposed one. The different condensed sets obtained are then used to design a k-NN classifier (1-NN for LASM) and a multi layer perceptron (MLP) for classifying the test set. The goal is to provide an evidence that the performance of our multiresolution condensation algorithm does not depend on the final use of the condensed set. The following data reduction methods are compared:

1. Random sampling: Sampling with replacement is used to obtain a specific condensation ratio. The condensed set is a representative of the underlying distribution.

2. Stratified sampling: Instead of sampling uniformly over the entire population, subclasses of interest (*strata*) are identified and treated differently. For the given data we considered *class stratification*, *i.e.*, the number of samples selected from each class is proportional to the size of the class in the original set.

3. Condensed nearest neighbor (CNN) [54]: The condensation ratio is varied by changing the parameter k used for k-NN classification. The condensed set obtains a high concentration of points near the class boundaries. It may be mentioned that arbitrarily low condensation ratios cannot be achieved using CNN.

4. Local asymmetrically weighted similarity metric (LASM) [150]: The condensed set is obtained by random sampling, but the metric used for nearest neighbor classification varies locally and is learned from the training set. The value of reinforcement rate used is $\alpha = 0.2$ and the punishment rate used is $\beta = 1.0$.

5. Method of Astrahan [9]: As explained in the last section this is an uniform scale density based method.

6. Learning vector quantization [72]: We have considered the LVQ3 version of the algorithm for comparison. Initial codebook vectors obtained using a self-organizing map are refined here using the LVQ3.

As in the case of density estimate experiments (Section 2.5.1), we have selected 90% of the data randomly as training set and the remaining data is used as test set. Such data splits are performed 10 times independently and the mean and standard deviation (SD) of the classification accuracy on test set, and condensation ratios (CR) obtained

Table 2.5: Classification performance for Forest cover type data

Condensation Algorithm	Condensation Ratio (%)		Classification Accuracy (%) using k-NN		Classification Accuracy (%) using MLP		CPU time (hrs)
	Mean	SD	Mean	SD (test stat.)	Mean	SD (test stat.)	
Proposed method	0.1	0.004	83.10	1.90	70.01	0.90	4.29
LVQ3	0.1	-	75.01	1.01 (12.50, 1.76)	68.08	0.80 (3.33, 1.72)	2.02
LASM	0.1	-	74.50	2.52 (9.08, 1.72) (1-NN)	-	-	5.90
Astrahan	0.1	0.004	66.90	2.10 (18.97, 1.72)	59.80	0.53 (32.81, 1.73)	4.10
Stratified sampling	0.1	-	44.20	5.9 (20.81, 1.81)	36.10	5.95 (18.75, 1.81)	-
Random sampling	0.1	-	37.70	10.04 (14.73, 1.81)	29.80	8.2 (16.16, 1.81)	-
Proposed method	5.0	0.01	97.00	1.81	80.02	1.40	4.52
LVQ3	5.0	-	88.01	1.04 (14.34, 1.76)	74.00	0.92 (11.99, 1.73)	4.05
LASM	5.0	-	87.55	2.50 (10.17, 1.73) (1-NN)	-	-	7.11
Astrahan	5.0	0.01	82.09	2.53 (16.05, 1.73)	66.00	1.4 (23.48, 1.71)	4.40
CNN	5.05	1.01	81.17	3.80 (2.64, 1.73)	75.02	4.1 (1.52, 1.78)	5.51
Stratified sampling	5.0	-	55.20	7.1 (18.92, 1.81)	40.10	7.01 (18.52, 1.81)	-
Random sampling	5.0	-	44.70	8.02 (21.09, 1.81)	35.80	8.8 (16.40, 1.81)	-

for each such splits are presented. Statistical significance tests are also performed to test the inequality of means of the classification accuracy. As before we present the computed value of the test statistic and the tabled value, if the computed value is greater than the tabled value the means are significantly different. We also present the CPU times required by the condensation algorithms on a Digital Alpha 800MHz workstation. The figures shown here are the average values taken over 10 runs.

In Table 2.5, we compare the effect of each method on classification accuracy for condensation ratios of 0.1% and 5%. Note that the lowest condensation ratio that could be achieved for the Forest data using CNN is 3.1%, hence, comparison with CNN is presented only for the 5% case.

It can be seen from Table 2.5 that the proposed methodology achieves higher classification accuracy than the other methods and that this difference is statistically significant. For classification, the same value of k as that used for condensation is considered, except for LASM where 1-NN is used. For classification using MLP, the proposed method and LVQ performs similarly. Results for LASM are not presented for MLP, since if no specialized metric is used LASM represents just a random subset. The performances of both random sampling and stratified sampling are found to be catastrophically poor. The uniform scale method of Astrahan performs poorer than the proposed method, LVQ and LASM.

2.5.3 Clustering: Satellite image data

The satellite image data (Appendix A) contains observations of the Indian Remote Sensing (IRS) satellite for the city of Calcutta, India. The data contains images of four spectral bands. We present in Figure 2.4(a), for convenience, the image for band 4. Here the task is to segment the image into different land cover regions, using four features (spectral bands). The image mainly consists of six classes e.g., clear water (ponds, fisheries), turbid water (the river Ganges flowing through the city), concrete (buildings, roads, airport tarmacs), habitation (concrete structures but less in density), vegetation (crop, forest areas) and open spaces (barren land, playgrounds). Fuzzy segmentation of the image is reported in detail in [116].

Using our methodology we have extracted six prototype points from the entire data set. The remaining points are placed in the cluster of the prototype point to whose sphere (disc) of influence the particular point belongs. Thus the condensation process implicitly generates a clustering (partition/segmentation) of the image data.

We have compared the performance of our algorithm with two other related clustering methods, namely, k-means algorithm [32] and Astrahans density based uniform scale method [9]. For the k-means algorithm we have considered $k = 6$, since there are six classes, and the best result (as evaluated by a cluster quality index) obtained out of ten random initializations is presented. In Astrahan's method six prototype points are obtained, the remaining pixels are then classified by minimum distance classification with these six points.

The results are presented in Figures 2.4(b)-(d). Figure 2.4(d) is seen to have more structural details compared to Figures 2.4(b) and 2.4(c). From the segmented image obtained using the proposed method more number of landmarks known from ground truths can be detected by visual inspection. The segmentation results of the remote sensing images obtained above are also evaluated quantitatively using an index β.

Let n_i be the number of pixels in the ith ($i = 1, \ldots, c$) region obtained by the segmentation method. Let X_{ij} be the vector (of size 4×1) of the gray values of the jth pixel ($j = 1, \ldots, n_i$) for all the images in region i, and $\bar{X}_i$ the mean of n_i gray values of the ith region. Then β is defined as [116]:

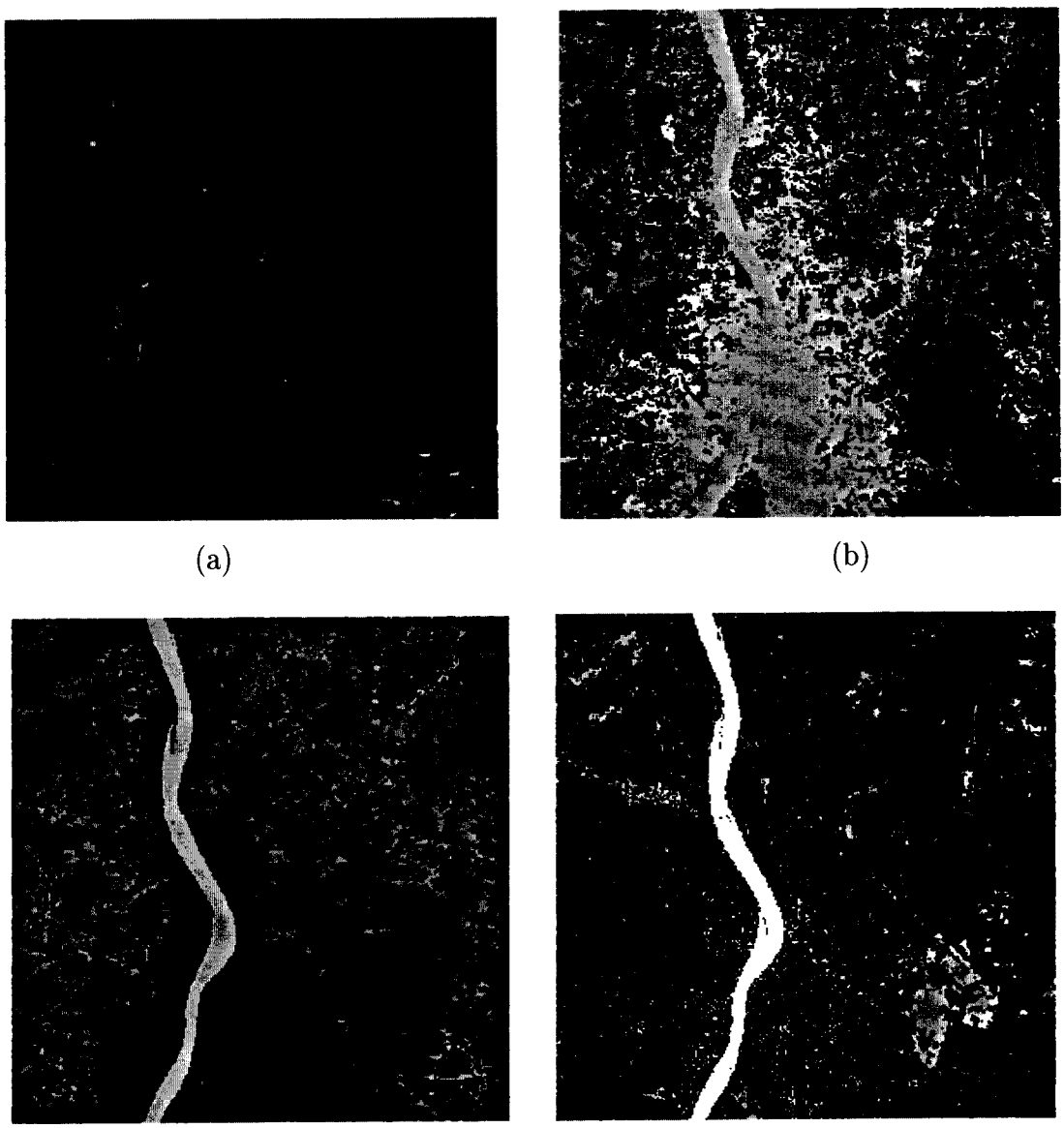


Figure 2.4: IRS images of Calcutta: (a) original Band 4 image, and segmented images using (b) k-means algorithm, (c) Astrahan's method, (d) proposed multiscale algorithm

Table 2.6: β value and CPU time of different clustering methods

Method	k-means	Astrahan's	Proposed
β	5.30	7.02	9.88
CPU time (hrs)	0.11	0.71	0.75

$$\beta = \frac{\sum_{i=1}^{c}\sum_{j=1}^{n_i}(X_{ij}-\bar{X})^T(X_{ij}-\bar{X})}{\sum_{i=1}^{c}\sum_{j=1}^{n_i}(X_{ij}-\bar{X}_i)^T(X_{ij}-\bar{X}_i)} \tag{2.5}$$

where, n is the size of the image and $\bar{X}$ is the mean gray value of the image. It may be noted that X_{ij}, $\bar{X}$ and $\bar{X}_i$ are all 4×1 vectors.

Note that the above measure is nothing but the ratio of the total variation and within-class variation and is widely used for feature selection and cluster analysis [116]. For a given image and c (number of clusters) value, the higher the homogeneity within the segmented regions higher would be the β value. The proposed method has the highest β value as can be seen in Table 2.6.

2.5.4 Rule generation: Census data

The original source for this data set is the IPUMS project. The data (Appendix A) contains 320000 samples and 133 attributes, mostly categorical (integer valued). A study commonly performed on census data is to identify contrasting groups of populations and study their relations. For this data we have investigated two groups of population namely those who have undergone/not undergone 'higher education', measured in terms of number of years in college. It is interesting and useful to generate logical rules depending on the other available attributes which classify these groups. We have considered the attribute educational record, *'edrec'*, and investigated two sets of population, one having more than $4\frac{1}{2}$ years of college education, and the other below that. The task is to extract logical inference rules for the sets.

As a similarity measure between two samples we have used the *Value Difference Metric* (VDM) [164]. Using the VDM, the distance between two values x and v of a single attribute a is defined as

$$vdm_a(x,v) = \sum_{a=1}^{M} \left(\frac{N_{a,x,c}}{N_{a,x}} - \frac{N_{a,v,c}}{N_{a,v}} \right)^2 \tag{2.6}$$

where $N_{a,x}$ is the number of times attribute a had value x; $N_{a,x,c}$ is the number of times attribute a had value x and the output class was c; and M is the number of output classes (2 in our case). Using this distance measure, two values of an attribute are considered to be closer if they have more similar classification, regardless of the magnitude of the values. Using the value difference metric, the distance between two points having p independent attributes is defined as

$$\mathrm{VDM}(\mathbf{x},\mathbf{v}) = \sqrt{\sum_{a=1}^{p} vdm_a^2(\mathbf{x}_a,\mathbf{v}_a)}. \tag{2.7}$$

We have used the popular C4.5 [145] program to generate logical rules from the condensed data sets. We have restricted the size of the rules to conjunction of 3 variables only. As before, 90% of the data is selected as training set and the rules are evaluated on the remaining data. Eleven such splits are obtained and the means and standard deviations (SD) are presented.

For the purpose of comparison with our method, the C4.5 program is also run on condensed sets obtained using: Random sampling, Stratified sampling, Density based Uniform Scale method of Astrahan [9] and Condensed nearest neighbor. Following quantities are computed in Table 2.7:

1. Condensation ratio (CR)
2. Number of rules generated
3. Accuracy of classification on test set (we also present statistical tests of significance for comparing the other methods with the proposed method)
4. Percentage of uncovered samples
5. CPU time

The comparison is performed for a constant condensation ratio of 0.1%. However, for CNN a CR of only 2.2% could be achieved by varying k. The classification accuracy of the proposed method is higher than random sampling, stratified sampling and CNN,

Table 2.7: Rule generation performance for the Census data

Condensation method	CR(%)		# of Rules (rounded to integer)		Classification accuracy (%)			Uncovered samples (%) (%)		CPU time (hrs)
	Mean	SD	Mean	SD	Mean	SD	(Test Stat.)	Mean	SD	
Random sampling	0.1	-	448	88	32.1	8.8	(8.43, 1.81)	40.01	5.5	-
Stratified sampling	0.1	-	305	45	38.8	5.5	(9.71, 1.78)	37.0	5.5	-
CNN	2.2	0.050	270	53	32.0	4.1	(17.55, 1.78)	55.0	4.1	2.80
Astrahan [9]	0.1	0.004	245	50	48.8	4.0	(4.89, 1.78)	25.0	3.1	4.22
Proposed	0.1	0.004	178	30	55.1	1.5		20.2	1.80	4.10

Figures in parentheses indicate the computed value of test statistic and tabled value respectively

it is also significantly higher than Astrahan's method. It is also observed that the uncovered region is minimum for the rules generated from the subset obtained by the proposed algorithm. The rule base size is far smaller than random, statistical sampling and Astrahan's method. Therefore the rules generated from the condensed set is compact yet having high accuracy and cover as compared to other sets.

2.5.5 Experiments on scalability

The scaling property of the condensation algorithm is also studied in a part of the experiment. For this we have examined the *sample complexity* of the algorithm, *i.e.*, the size of condensed set required to achieve an accuracy level (measured as error in density estimate). In Figure 2.5 the log-likelihood error is plotted against the cardinality of the condensed set (as a fraction of the original set), for three typical data sets namely, *Norm* (of known distribution), Vowel (highly overlapping), Wisconsin (large dimension). The solid curve is for the proposed methodology while the dotted one is for random sampling. It can be seen that the proposed methodology is superior to random sampling.

2.5.6 Experiments on choice of k

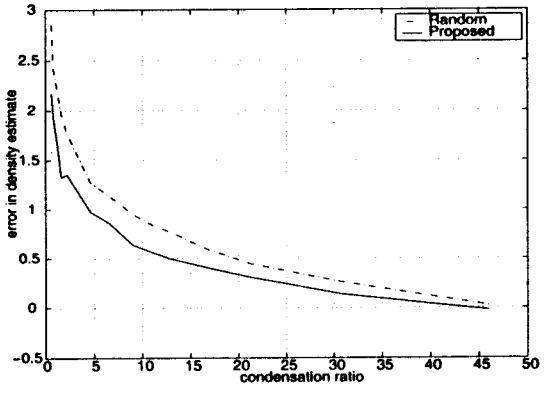
In Section 2.4 we have described the role of k in the proposed algorithm. As k increases, the size of condensed set reduces and vice versa. Here we provide some experimental results in support of the discussion. The effect of varying parameter k on the condensa-

tion ratio (CR) is shown in Figure 2.6, for the three aforesaid data sets (Section 2.5.6). It can be observed that for values of k in the range $\approx$ 7–20 the curves attain low CR values and are close to each other for all the three data sets. For the Vowel data a CR value of 3.4% was obtained at $k = 31$. It may be noted that the curve for the *Norm* (smallest) data set is shifted to the left compared to the other two curves.

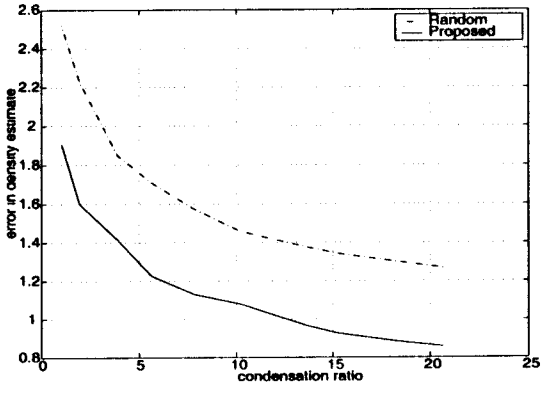
2.6 Conclusions and Discussion

In this chapter, we have presented an algorithm for non-parametric data condensation. The method follows the basic principles of non-parametric data reduction present in literature, but the sample pruning step is done in a multiresolution manner rather than with uniform resolution. It is based on the density underlying the data. The proposed approach is found to have superior performance as compared to some existing data reduction schemes in terms of error in density estimate both for small and large data sets having dimension ranging from 2 to 133. The performance of classification, clustering and rule generation using the condensation algorithm is studied for three large data sets. The algorithm does not require the difficult choice of radii d_1 and d_2, which are critical for Astrahan's method, only the choice of parameter k is necessary. Choice of k is guided by the size of the original data set and the accuracy/condensation ratio desired. The parameter k also provides a parametrization of the concept of scale in data condensation, and the scales induced follow the natural characteristics of the data and, hence, are efficient.

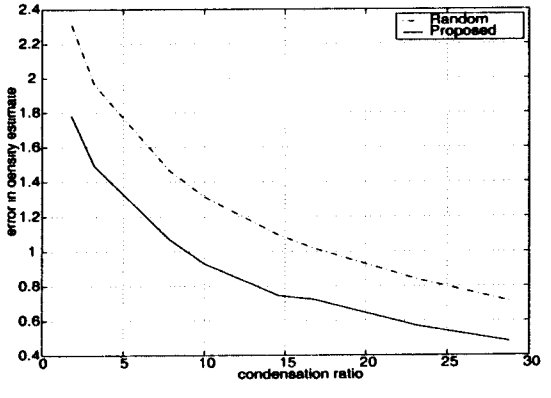
As far as the computational complexity is concerned, the algorithm can be considered to have three computational steps. In the first step, for each point in the original set the distance of the kth nearest neighbor is computed. In the second step, the point having the minimum value of the distance is selected and in the third step, all points lying within a radius of $2r_{k,\mathbf{x}_j}$ of a selected point are removed. It is observed that the computation time required for second and third steps decreases with iteration, since the size of the original set decreases progressively (the rate is dependent on k and the data distribution). The first step is the most time consuming one and it requires $(\mathcal{O}(kN^2))$, where N is the number of data points. A way of reducing the time complexity of nearest neighbor calculation is to use approximate nearest neighbor



(a)



(b)



(c)

Figure 2.5: Variation in error in density estimate (log-likelihood measure) with the size of the Condensed Set (expressed as percentage of the original set) with the corresponding, for (a) the *Norm* data, (b) Vowel data, (c) Wisconsin Cancer data.

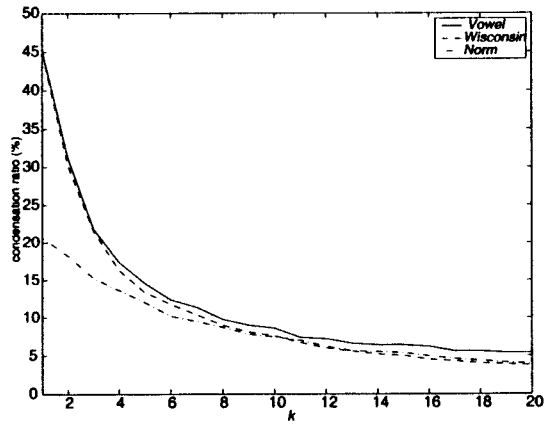


Figure 2.6: Variation of condensation ratio CR (%) with k.

(ANN) computations using specialized data structures like k-d trees [7]. Probabilistic nearest neighbor search methods have also been suggested [36], having expected $\mathcal{O}(1)$ time complexity and $\mathcal{O}(N)$ storage complexity.

The guiding principle of our algorithm is to minimize the error in terms of density estimate rather than the classification score. The justification is to obtain a generic representative condensed set independent of the task performed with it later. In many data mining applications the final task is not always known beforehand or there may be multiple tasks to be performed. In the above circumstances such a condensed representation is more useful. We have performed experiments to show that a condensed set obtained by our method performs well for diverse data mining tasks such as classification, clustering and rule generation.

Chapter 3

Unsupervised Feature Selection using Feature Similarity

3.1 Introduction

An important problem related to mining large data sets, both in dimension and size, is of selecting a subset of the original features [38]. Preprocessing the data to obtain a smaller set of representative features and retaining the optimal salient characteristics of the data not only decreases the processing time but also leads to more compactness of the models learned and better generalization. We use supervised feature selection when class labels of the data are available, otherwise unsupervised feature selection is appropriate. In many data mining applications class labels are unknown; thereby indicating the significance of unsupervised feature selection there.

Conventional methods of feature selection involve evaluating different feature subsets using some index and selecting the best among them. The index usually measures the capability of the respective subsets in classification or clustering depending on whether the selection process is supervised or unsupervised. A problem of these methods, when applied to large data sets, is the high computational complexity involved in searching. The complexity is exponential in terms of the data dimension for an exhaustive search. Several heuristic techniques have been developed to circumvent this problem. Among them the branch and bound algorithm, suggested by Fukunaga and Narendra [30], obtains the optimal subset in expectedly less than exponential computations when the feature evaluation criterion used is monotonic in nature. Greedy algorithms like sequential forward and backward search [30] are also popular. These algorithms have quadratic complexity, but they perform poorly for non-monotonic indices. In such cases, sequential floating searches [144] provide better results, though at the cost of a higher computational complexity. Beam search variants of the sequential algorithms [4] are also used to reduce computational complexity. Recently robust methods for finding out the optimal subset for arbitrary evaluation indices are being developed using genetic algorithms (GAs) [129]. GA based feature selection methods [77] are usually found to perform better than other heuristic search methods for large and medium sized data sets, however they also require considerable computation time for large data sets. Other attempts to decrease the computational time of feature selection include probabilistic search methods like random hill climbing [155], and Las Vegas Filter (LVF) approach [83]. Comparison and discussion of some of the above methods for many real life data sets may be found in [77].

Since the interest of the present study lies with unsupervised feature selection, we discuss here some of the existing methods which can be broadly classified into two categories. Methods in one such category involve maximization of clustering performance, as quantified by some index. These include sequential unsupervised feature selection algorithm [83], wrapper approach based on expectation maximization (EM) [34], maximum entropy based method and the recently developed neuro-fuzzy approach [113]. The other category considers selection of features based on feature dependency and relevance. The principle is that any feature carrying little or no additional information beyond that subsumed by the remaining features, is redundant, and should be eliminated. Various dependence measures like correlation coefficients [50], measures of statistical redundancy [58], or linear dependence [26] have been used. Recently the Relief algorithm [70] and its extensions [76] which identify statistically relevant features have been reported. A fast feature selection algorithm based on information fuzzy network is described in [78]. Another algorithm based on conditional independence uses the concept of Markov blanket [73]. All these methods involve search and require significantly high computation time for large data sets. In [69] an algorithm which does not involve search and selects features by hierarchically merging similar feature pairs is described. However, the algorithm is crude in nature and performs poorly on real life data sets. It may be noted that, principal component analysis (PCA) [30] also performs unsupervised dimensionality reduction based on information content of features. However, PCA involves feature transformation and obtains a set of transformed features rather than a subset of the original features.

In this chapter we propose an unsupervised algorithm [101] which uses feature dependency/similarity for redundancy reduction, but requiring no search. The method involves partitioning of the original feature set into some distinct subsets or clusters so that the features within a cluster are highly similar while those in different clusters are dissimilar. A single feature from each such cluster is then selected to constitute the resulting reduced subset. A new similarity measure, called maximal information compression index, is used in clustering. Its comparison with two other measures namely, correlation coefficient and least square regression error is made. It is also demonstrated how 'representation entropy' can be used for quantifying redundancy in a set.

The nature of both the proposed clustering algorithm and the newly introduced feature similarity measure is geared towards two goals - minimizing the information loss (in

terms of second order statistics) incurred in the process of feature reduction, and minimizing the redundancy present in the reduced feature subset. The feature selection algorithm owes its low computational complexity to two factors - (a) unlike most conventional algorithms, search for the best subset (requiring multiple evaluation of indices) is not involved, (b) the new feature similarity measure can be computed in much less time compared to many indices used in other supervised and unsupervised feature selection methods. Since the method achieves dimensionality reduction through removal of redundant features, it is more related to feature selection for compression rather than for classification.

Superiority of the algorithm, over four related methods *viz*, branch and bound algorithm, sequential floating forward search, sequential forward search and stepwise clustering, is demonstrated extensively on nine real life data of both large and small sample sizes and dimension ranging from 4 to 649. Comparison is made on the basis of both clustering/classification performance and redundancy reduction. Effectiveness of the maximal information compression index and the effect of scale parameter are also studied.

The organization of the chapter is as follows: in the next section we describe measures of similarity between a pair of features. In Section 3.3 we present the proposed feature selection algorithm using the similarity measure and discuss some of its characteristics. In Section 3.5 we provide experimental results along with comparisons.

3.2 Feature Similarity Measure

In this section we discuss some criteria for measuring similarity between two random variables, based on linear dependency between them. In this context we propose a new measure called *maximal information compression index* to be used for feature selection.

There are broadly two possible approaches to measure similarity between two random variables. One is to non-parametrically test the closeness of probability distributions of the variables. Walds-Wolfowitz test and the other run tests [148] may be used for this purpose. However, these tests are sensitive to both location and dispersion of the distributions, hence not suited for the purpose of feature selection. Another approach is to measure the amount of functional (linear or higher) dependency between the vari-

ables. There are several benefits of choosing linear dependency as a feature similarity measure. It is known that if some of the features are linearly dependent on the others, and if the data is linearly separable in the original representation, the data is still linearly separable if all but one of the linearly dependent features are removed [26]. As far as the information content of the variables is concerned, second order statistics of the data is often the most important criterion after mean values [148]. All the linear dependency measures that we will discuss are related to the amount of error in terms of second order statistics, in predicting one of the variables using the other. We discuss below two existing [148] linear dependency measures before explaining the proposed *maximal information compression index.*

Correlation Coefficient (ρ): The most well known measure of similarity between two random variables is the correlation coefficient. Correlation coefficient ρ between two random variables x_1 and x_2 is defined as $\rho(x_1, x_2) = \frac{\text{cov}(x_1,x_2)}{\sqrt{\text{var}(x_1)\text{var}(x_2)}}$, where var( ) denotes the variance of a variable and cov( ) the covariance between two variables. If x_1 and x_2 are completely correlated i.e., exact linear dependency exists, $\rho(x_1, x_2)$ is 1 or -1. If x_1 and x_2 are totally uncorrelated $\rho(x_1, x_2)$ is 0. Hence, $1 - |\rho(x_1, x_2)|$ can be used as a measure of similarity between two variables x_1 and x_2. Following can be stated about the measure:

1. $0 \leq 1 - |\rho(x_1, x_2)| \leq 1$
2. $1 - |\rho(x_1, x_2)| = 0$ if and only if x_1 and x_2 are linearly related.
3. $1 - |\rho(x_1, x_2)| = 1 - |\rho(x_2, x_1)|$ (symmetric)
4. If $u = \frac{x_1 - a}{c}$ and $v = \frac{x_2 - b}{d}$ for some constants a, b, c, d, then $1 - |\rho(x_1, x_2)| = 1 - |\rho(u, v)|$ i.e., the measure is *invariant to scaling and translation* of the variables.
5. The measure is *sensitive to rotation* of the scatter diagram in (x_1, x_2) plane.

Though correlation coefficient contains many desirable properties as a feature similarity measure, properties 4 and 5, mentioned above, make it somewhat unsuitable for feature selection. Since the measure is invariant to scaling, two pairs of variables having different variances may have the same value of the similarity measure, which is

not desirable as variance has high information content. Sensitivity to rotation is also not desirable in many applications.

Least Square Regression Error (e): Another measure of the degree of linear dependency between two variables x_1 and x_2 is the error in predicting x_2 from the linear model $x_2 = a + bx_1$. a and b are the regression coefficients obtained by minimizing the mean square error $e(x_1, x_2)^2 = \frac{1}{n}\sum(e_i(x_1, x_2))^2$, $e_i(x_1, x_2) = x_{2i} - a - bx_{1i}$. The coefficients are given by $a = \bar{x_2}$ and $b = \frac{\text{cov}(x_1, x_2)}{\text{var}(x_1)}$ and the mean square error $e(x_1, x_2)$ is given by $e(x_1, x_2) = \text{var}(x_2)(1 - \rho(x_1, x_2)^2)$. If x_2 and x_1 are linearly related $e(x_1, x_2) = 0$, and if x_1 and x_2 are completely uncorrelated $e(x_1, x_2) = \text{var}(x_2)$. The measure e^2 is also known as the *residual variance*. It is the amount of variance of x_2 unexplained by the linear model. Some properties of e are:

1. $0 \leq e(x_1, x_2) \leq \text{var}(x_2)$
2. $e(x_1, x_2) = 0$ if and only if x_1 and x_2 are linearly related.
3. $e(x_1, x_2) \neq e(x_2, x_1)$ (unsymmetric)
4. If $u = x_1/c$ and $v = x_2/d$ for some constant a, b, c, d, then $e(x_1, x_2) = d^2 e(u, v)$, i.e., the measure e is *sensitive to scaling* of the variables. It is also clear that e is *invariant to translation* of the variables.
5. The measure e is *sensitive to rotation* of the scatter diagram in $x_1 - x_2$ plane.

Note that the measure e is not symmetric (property 3). Moreover, it is sensitive to rotation (property 5).

Now we suggest a measure of linear dependency which has many desirable properties for feature selection not present in the above two measures.

Maximal Information Compression Index (λ_2): Let Σ be the covariance matrix of random variables x_1 and x_2. Define, *maximal information compression index* as $\lambda_2(x_1, x_2) =$ smallest eigenvalue of Σ, i.e.,

$$2\lambda_2(x_1, x_2) = (\text{var}(x_1) + \text{var}(x_2) - \sqrt{(\text{var}(x_1) + \text{var}(x_2))^2 - 4\text{var}(x_1)\text{var}(x_2)(1 - \rho(x_1, x_2)^2)}.$$

The value of λ_2 is zero when the features are linearly dependent and increases as the amount of dependency decreases. It may be noted that the measure λ_2 is nothing but the eigenvalue for the direction normal to the principle component direction of feature pair (x_1, x_2). It is shown in [30] that maximum information compression is achieved if a multivariate (in this case bivariate) data is projected along its principal component direction. The corresponding loss of information in reconstruction of the pattern (in terms of second order statistics) is equal to the eigenvalue along the direction normal to the principal component. Hence, λ_2 is the amount of reconstruction error committed if the data is projected to a reduced (in this case reduced from two to one) dimension in the best possible way. Therefore it is a measure of the *minimum amount of information loss* or the *maximum amount of information compression*, possible.

The significance of λ_2 can also be explained geometrically in terms of linear regression. It can be easily shown [148] that the value of λ_2 is equal to the sum of the squares of the perpendicular distances of the points (x_1, x_2) to the best fit line $x_2 = \hat{a} + \hat{b}x_1$, obtained by minimizing the sum of the squared perpendicular distances. The coefficients of such a best fit line are given by $\hat{a} = \bar{x_1}cot\theta + \bar{x_2}$ and $\hat{b} = -cot\theta$, where $\theta = 2\ \tan^{-1}\left(\frac{2\text{COV}(x_1,x_2)}{\text{var}(x_1)^2-\text{var}(x_2)^2}\right)$. The nature of errors and the best fit lines for least square regression and principal component analysis are illustrated in Figure 3.1. λ_2 has the following properties:

1. $0 \leq \lambda_2(x_1, x_2) \leq 0.5(\text{var}(x_1) + \text{var}(x_2))$
2. $\lambda_2(x_1, x_2) = 0$ if and only if x_1 and x_2 are linearly related.
3. $\lambda_2(x_1, x_2) = \lambda_2(x_2, x_1)$ (symmetric)
4. If $u = \frac{x_1}{c}$ and $v = \frac{x_2}{d}$ for some constant a, b, c, d, then $\lambda_2(x_1, x_2) \neq \lambda_2(u, v)$, i.e., the measure is *sensitive to scaling* of the variables. Since the expression of λ_2 does not contain mean, but only the variance and covariance terms it is *invariant to translation* of the data set.
5. λ_2 is *invariant to rotation* of the variables about the origin (this can be easily verified from the geometric interpretation of λ_2 considering the property that the perpendicular distance of a point to a line does not change with rotation of the axes).

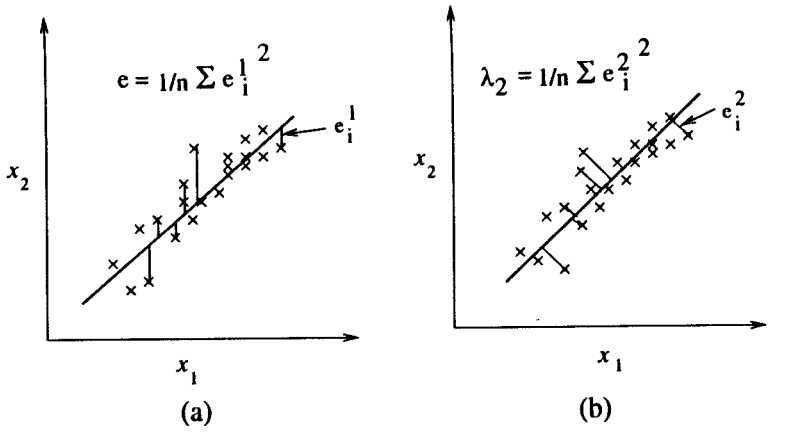


Figure 3.1: Nature of errors in linear regression, (a) Least square fit (e), (b) Least square projection fit (λ_2).

The measure λ_2 possesses several desirable properties like symmetry (property 3), sensitivity to scaling (property 4), and invariance to rotation (property 5). It is a property of the variable pair (x_1, x_2) reflecting the amount of error committed if maximal information compression is performed by reducing the variable pair to a single variable. Hence, it may be suitably used in redundancy reduction.

3.3 Feature Selection Method [101]

The task of feature selection involves two steps, namely, partitioning the original feature set into a number of homogeneous subsets (clusters) and selecting a representative feature from each such cluster. Partitioning of the features is done based on the k-NN principle using one of the feature similarity measures described in Section 3.2. In doing so, we first compute the k nearest features of each feature. Among them the feature having the most compact subset (as determined by its distance to the farthest neighbor) is selected, and its k neighboring features are discarded. The process is repeated for the remaining features until all of them are either selected or discarded.

While determining the k nearest neighbors of features we assign a constant error threshold (ϵ) which is set equal to the distance of the kth nearest neighbor of the feature selected in the first iteration. In subsequent iterations, we check the λ_2 value, corresponding to the subset of a feature, whether it is greater than ϵ or not. If yes, then we

decrease the value of k. Therefore k may be varying over iterations. The concept of clustering features into homogeneous groups of varying sizes is illustrated in Figure 3.2. The algorithm may be stated as follows:

Algorithm:

Let the original number of features be P, and the original feature set be $A = \{F_i, i = 1, \ldots, P\}$. Represent the dissimilarity between features F_i and F_j by $S(F_i, F_j)$. Higher the value of S is, the more dissimilar are the features. The measures of linear dependency (e.g., ρ, e, λ_2) described in Section 3.2 may be used in computing S. Let r_i^k represent the dissimilarity between feature F_i and its kth nearest neighbor feature in R. Then

Step 1: Choose an initial value of $k \leq P - 1$. Initialize the reduced feature subset R to the original feature set A, i.e., $R \leftarrow A$.

Step 2: For each feature $F_i \in R$, compute r_i^k.

Step 3: Find feature $F_{i'}$ for which $r_{i'}^k$ is minimum. *Retain* this feature in R and *discard* k nearest features of $F_{i'}$. (Note: $F_{i'}$ denotes the feature for which removing k nearest neighbors will cause minimum error among all the features in R). **Let** $\epsilon = r_{i'}^k$.

Step 4: **If** $k >$ cardinality$(R) - 1$: $k =$ cardinality$(R) - 1$.

Step 5: **If** $k = 1$: **Go to Step 8.**

Step 6: **While** $r_{i'}^k > \epsilon$ **do**:

(a) $k = k - 1$.

$r_{i'}^k = \inf_{F_i \in R} r_i^k$.

('k' is decremented by 1, until the 'kth nearest neighbor' of at least one of the features in R is less than ϵ-dissimilar with the feature)

(b) **If** $k = 1$: **Go to Step 8.**

(if no feature in R has less than ϵ-dissimilar 'nearest neighbor' select all the remaining features in R)

End While

Step 7: **Go to Step 2.**

Step 8: Return feature set R as the reduced feature set. □

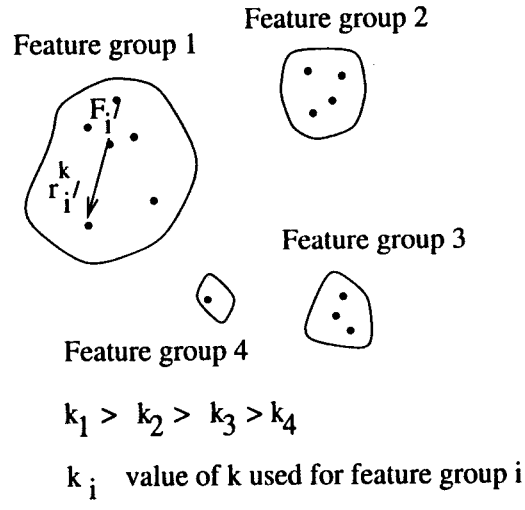


Figure 3.2: Feature clusters

Remarks:

Computational complexity: The algorithm has low computational complexity with respect to both number of features and number of samples of the original data. With respect to the dimension (P) the method has complexity $\mathcal{O}(P^2)$. Among the existing search based schemes only sequential forward and backward search have complexity $\mathcal{O}(P^2)$, though each evaluation is more time consuming. Other algorithms like plus-l-take-r, sequential floating search and branch and bound algorithm [30] have complexity higher than quadratic. Most probabilistic search algorithms also require more than quadratic number of evaluations.

The second factor which contributes to the speedup achieved by the proposed algorithm, is the low computational complexity of evaluating the linear dependency measures of feature similarity. If the data set contains n samples, evaluation of the similarity measure for a feature pair is of complexity $\mathcal{O}(n)$. Thus the feature selection scheme has overall complexity $\mathcal{O}(P^2n)$. Almost all other supervised and unsupervised feature evaluation indices (e.g., entropy, class separability, K-NN classification accuracy) have at least $\mathcal{O}(n^2)$ complexity of computation. Moreover, evaluation of the linear dependency measures involves computation using one dimensional variables only, while the other measures often involve distance computations at higher dimensions. All these factors contribute to the large speedup achieved by the proposed algorithm compared to other feature selection schemes.

Notion of scale in feature selection and choice of k: In our algorithm k controls the size of the reduced set. Since k determines the error threshold (ϵ), the representation of the data at different degrees of details is controlled by its choice. This characteristic is useful in data mining where *multiscale* representation of the data is often necessary. Note that the said property may not always be possessed by other algorithms where the input is usually the desired size of the reduced feature set. The reason is that changing the size of the reduced set may not necessarily result in any change in the levels of details. In contrast, for the proposed algorithm, k acts as a scale parameter which controls the degree of details in a more direct manner.

Non-metric nature of similarity measure: The similarity measures used in the proposed algorithm need not be a metric. Unlike conventional agglomerative clustering algorithms it does not utilize metric property of the similarity measures. Also unlike the step wise clustering method [69] used previously for feature selection, our clustering algorithm is partitional and non-hierarchical in nature.

3.4 Feature Evaluation Indices

Let us now describe some indices that have been considered for evaluating the effectiveness of the selected feature subsets. The first three indices namely, class separability, K-NN classification accuracy and naive Bayes classification accuracy do need class information of the samples while the remaining three namely, entropy, fuzzy feature evaluation index and representation entropy, do not. Before we discuss them, we mention, for convenience, the following notations: Let n be the number of sample points in the data set, M be the number of classes present in the data set, P be the number of features in the original feature set A, p be the number of features in the reduced feature set R, Ω_A be the original feature space with dimension P, and Ω_R be the transformed feature space with dimension p.

1. *Class separability* [30]: Class separability S of a data set is defined as $S = trace(S_b^{-1}S_w)$. S_w is the within class scatter matrix and S_b is the between class

scatter matrix, defined as:

$$
\begin{aligned}
S_w &= \sum_{j=1}^{M} \pi_j E\{(\mathbf{x}-\mu_j)(\mathbf{x}-\mu_j)^T|\omega_j\} = \sum_{j=1}^{M} \pi_j \Sigma_j \\
S_b &= \sum_{j=1}^{M} (\mu_j - \bar{\mathbf{x}})(\mu_j - \bar{\mathbf{x}})^T \\
\bar{\mathbf{x}} &= E\{\mathbf{x}\} = \sum_{j=1}^{M} \pi_j \mu_j
\end{aligned} \tag{3.1}
$$

where π_j is the a priori probability that a pattern belongs to class ω_j, $\mathbf{x}$ is the feature vector, μ_j is the sample mean vector of class ω_j, $\bar{\mathbf{x}}$ is the sample mean vector for the entire data points, Σ_j is the sample covariance matrix of class ω_j, and $E\{.\}$ is the expectation operator. A lower value of the separability criteria S ensures that the classes are well separated by their scatter means.

2. *K-NN classification accuracy*: Here we have used the K-NN rule for evaluating the effectiveness of the reduced set for classification. Cross-validation is performed in the following manner - we randomly select 90% of the data as training set and classify the remaining 10% points. Ten such independent runs are performed, and the average classification accuracy on test set is used. The value of K, chosen for the K-NN rule, is the square root of the number of data points in the training set.

3. *Naive Bayes classification accuracy*: A Bayes maximum likelihood classifier [30], assuming normal distribution of classes, is also used for evaluating the classification performance. Mean and covariance of the classes are estimated from a randomly selected 10% training sample, and the remaining 90% of the points are used as test set. Ten such independent runs are performed and the average classification accuracy on test set is provided.

4. *Entropy* [83]: Let the distance between two data points i, j be

$$
\mathcal{D}_{ij} = \left[\sum_{l=1}^{p} \left(\frac{x_{i,l} - x_{j,l}}{max_l - min_l} \right)^2 \right]^{1/2},
$$

where $x_{i,l}$ denotes feature value for i along lth direction, and max_l, min_l are the maximum and minimum values computed over all the samples along lth axis, p

is the number of features. Similarity between i, j is given by $\text{sim}(i,j) = e^{-\alpha \mathcal{D}_{ij}}$, where α is a positive constant. A possible value of α is $\frac{-\ln 0.5}{\bar{\mathcal{D}}}$. $\bar{\mathcal{D}}$ is the average distance between data points computed over the entire data set. Entropy is defined as:

$$E = -\sum_{i=1}^{n}\sum_{j=1}^{n}(\text{sim}(i,j) \times \log \text{sim}(i,j) + (1-\text{sim}(i,j)) \times \log (1-\text{sim}(i,j))) \quad (3.2)$$

where n is the number of sample points. If the data is uniformly distributed in the feature space entropy is maximum. When the data has well-formed clusters uncertainty is low and so is entropy.

5. *Fuzzy feature evaluation index* [113]: Fuzzy feature evaluation index (FFEI) is defined as:

$$FFEI = \frac{2}{n(n-1)} \sum_{i} \sum_{i \neq j} \frac{1}{2} \left[\mu_{ij}^{R}(1-\mu_{ij}^{A}) + \mu_{ij}^{A}(1-\mu_{ij}^{R})\right] \quad (3.3)$$

where μ_{ij}^{A} and μ_{ij}^{R} are the degrees that both patterns i and j belong to the same cluster in the feature spaces Ω_A and Ω_R respectively. Membership function μ_{ij} may be defined as

$$\begin{aligned} \mu_{ij} &= 1 - \tfrac{d_{ij}}{\mathcal{D}_{max}} && \text{if } d_{ij} \leq \mathcal{D}_{max} \\ &= 0, && \text{otherwise.} \end{aligned}$$

d_{ij} is the distance between patterns i and j, and $\mathcal{D}_{max}$ is the maximum separation between patterns in the respective feature spaces.

The value of FFEI decreases as the intercluster/intracluster distances increase/ decrease. Hence, the lower the value of FFEI, more crisp is the cluster structure.

Note that the first two indices, class separability and K-NN accuracy, measure the effectiveness of the feature subsets for classification, while the indices entropy and fuzzy feature evaluation index evaluate the clustering performance of the feature subsets. Let us now describe a quantitative index which measures the amount of redundancy present in the reduced subset.

6. *Representation entropy* [30]: Let the eigenvalues of the $p \times p$ covariance matrix of a feature set of size p be $\lambda_l, l = 1, \ldots, p$. Let $\tilde{\lambda}_l = \frac{\lambda_l}{\sum_{l=1}^{p} \lambda_l}$. $\tilde{\lambda}_l$ has similar

properties like probability, namely, $0 \leq \tilde{\lambda}_l \leq 1$ and $\sum_{l=1}^{p} \lambda_l = 1$. Hence, an entropy function can be defined as

$$H_R = -\sum_{l=1}^{p} \tilde{\lambda}_l \log \tilde{\lambda}_l. \tag{3.4}$$

The function H_R attains a minimum value (zero) when all the eigenvalues except one are zero, or in other words when all the information is present along a single co-ordinate direction. If all the eigenvalues are equal, i.e., information is equally distributed among all the features, H_R is maximum and so is the uncertainty involved in feature reduction.

The above measure is known as *representation entropy*. It is a property of the *data set as represented by a particular set of features*, and is a measure of the amount of information compression possible by dimensionality reduction. This is equivalent to the amount of redundancy present in that particular representation of the data set. Since the proposed algorithm involves partitioning of the original feature set into a number of homogeneous (highly compressible) clusters, it is expected that representation entropy of the individual clusters are as low as possible, while that of the final reduced set of features has low redundancy i.e., a high value of representation entropy.

It may be noted that among all the p dimensional subspaces of an original P dimensional data set, the one corresponding to the Karhunen-Loeve co-ordinates [30] (for the first p eigenvalues) has the highest representation entropy, i.e., is least redundant. However, for large dimensional data sets K-L transform directions are difficult to compute. Also, K-L transform results in general transformed variables and not exact subsets of the original features.

3.5 Experimental Results and Comparisons [101]

Organization of the experimental results is as follows: First the performance of the proposed algorithm in terms of the feature evaluation indices, discussed in Section 3.4, is compared with five other feature selection schemes. Then we study the redundancy reduction aspect of the algorithm quantitatively along with comparisons. Effect of varying the parameter k, used in feature clustering, is also studied.

Three categories of real life public domain data sets are used: low dimensional ($P \leq 10$) (e.g., Iris, Wisconsin cancer, and Forest cover type (considering numerical features only) data), medium dimensional ($10 < P \leq 100$) (e.g., Ionosphere, Waveform and Spambase data), and high dimensional ($P > 100$) (e.g., Arrhythmia, Multiple features and Isolet data), containing both large and relatively smaller number of points. Their characteristics are described in Appendix A.

3.5.1 Comparison: Classification and clustering performance

Four indices, *viz*, entropy (Equation 3.2), fuzzy feature evaluation index (Equation 3.3), class separability (Equation 3.1), K-NN and naive Bayes classification accuracy are considered to demonstrate the efficacy of the proposed methodology and for comparing it with other methods. Four unsupervised feature selection schemes considered for comparison are:

1. Branch and Bound Algorithm (BB) [30]: A search method in which all possible subsets are implicitly inspected without exhaustive search. If the feature selection criterion is monotonic BB returns the optimal subset.

2. Sequential Forward Search (SFS) [30]: A suboptimal search procedure where one feature at a time is added to the current feature set. At each stage, the feature to be included in the feature set is selected from among the remaining available features so that the new enlarged feature set yields a maximum value of the criterion function used.

3. Sequential Floating Forward Search (SFFS) [144]: A near optimal search procedure with lower computational cost than BB. It performs sequential forward search with provision for backtracking.

4. Step Wise Clustering (using correlation coefficient) (SWC) [69]: A non-search based scheme which obtains a reduced subset by discarding correlated features.

In our experiments we have mainly used entropy (Equation 3.2) as the feature selection criterion with the first three search algorithms.

Comparisons in terms of five indices are made for different sizes of the reduced feature subsets. Tables 3.1, 3.2 and 3.3 provide such a comparative result corresponding to

Table 3.1: Comparison of feature selection algorithms for large dimensional data sets

Data set	Method	Evaluation Criteria					CPU Time (sec)
		E	FFEI	S	KNNA (%)	BayesA (%)	
					Mean SD	Mean SD	
Isolet	SFS	0.52	0.41	1.09	95.02 0.89	92.03 0.52	14.01×10^4
p=310	SWC	0.71	0.55	2.70	72.01 0.71	68.01 0.44	431
P=617	Relief-F	0.70	0.52	2.24	95.81 0.81	95.52 0.47	5.03×10^3
$k = 305$	Proposed	0.50	0.40	1.07	96.00 0.78	95.01 0.52	440
Mult. Feat.	SFS	0.67	0.47	0.45	77.01 0.24	75.02 0.14	5.00×10^4
p=325	SWC	0.79	0.55	0.59	52.00 0.19	50.05 0.10	401
P=649	Relief-F	0.71	0.50	0.52	78.37 0.22	75.25 0.11	1.10×10^3
$k = 322$	Proposed	0.68	0.48	0.45	78.34 0.22	75.28 0.10	451
Arrhythmia	SFS	0.74	0.44	0.25	52.02 0.55	50.21 0.43	1511
p=100	SWC	0.82	0.59	0.41	40.01 0.52	38.45 0.38	70
P=195	Relief-F	0.78	0.55	0.27	56.04 0.54	54.55 0.40	404
$k = 95$	Proposed	0.72	0.40	0.17	58.93 0.54	56.00 0.41	74

E: Entropy, FFEI: Fuzzy Feature Evaluation Index, S: Class Separability, KNNA: k-NN classification accuracy, BayesA: naive Bayes classification accuracy, SD: standard deviation. SFS: Sequential Forward Search, SWC: Step Wise Clustering. p: number of selected features, P: number of original features, k: parameter used by the proposed method.

high, medium and low dimensional data sets when the size of the reduced feature subset is taken to be about half of the original size as an example. Comparison for other sizes of the reduced feature set is provided in Figure 3.3 considering one data set from each of the three categories, namely, multiple features (high), ionosphere (medium) and cancer (low). The CPU time required by each of the algorithms on a Sun UltraSparc 350 MHz workstation are also reported in Tables 3.1–3.3. Since the branch and bound (BB) and the sequential floating forward search (SFFS) algorithms require infeasibly high computation time for the large data sets, we could not provide the figures for them in Table 3.1. For the classification accuracies (using K-NN and Bayes), both mean and standard deviations (SD) computed for ten independent runs are presented.

Table 3.2: Comparison of feature selection algorithms for medium dimensional data sets

Data set	Method	Evaluation Criteria					CPU Time (sec)
		E	FFEI	S	KNNA (%)	BayesA (%)	
					Mean SD	Mean SD	
	BB	0.50	0.30	0.28	90.01 0.71	88.17 0.55	1579
Spambase	SFFS	0.50	0.30	0.28	90.01 0.72	88.17 0.55	1109
	SFS	0.52	0.34	0.29	87.03 0.68	86.20 0.54	121.36
p=29	SWC	0.59	0.37	0.41	82.04 0.68	79.10 0.55	11.02
P=57	Relief-F	0.59	0.36	0.34	87.04 0.70	86.01 0.52	70.80
$k = 27$	Proposed	0.50	0.30	0.28	90.01 0.71	88.19 0.52	13.36
	BB	0.67	0.47	0.29	78.02 0.47	62.27 0.41	1019
Waveform	SFFS	0.68	0.48	0.31	77.55 0.45	62.22 0.41	627
	SFS	0.69	0.49	0.37	74.37 0.44	59.01 0.42	71.53
p=20	SWC	0.72	0.55	0.41	62.03 0.40	47.50 0.40	8.01
P=40	Relief-F	0.73	0.54	0.38	74.88 0.41	62.88 0.40	50.22
$k = 17$	Proposed	0.68	0.48	0.30	75.20 0.43	63.01 0.40	8.28
	BB	0.65	0.44	0.07	75.96 0.35	65.10 0.28	150.11
Ionosphere	SFFS	0.65	0.44	0.08	74.73 0.37	65.08 0.31	50.36
	SFS	0.65	0.44	0.10	69.94 0.32	62.00 0.27	10.70
p=16	SWC	0.66	0.47	0.22	62.03 0.32	59.02 0.25	1.04
P=32	Relief-F	0.62	0.47	0.15	72.90 0.34	64.55 0.27	8.20
$k = 11$	Proposed	0.64	0.43	0.10	78.77 0.35	65.92 0.28	1.07

BB: Branch and Bound, SFFS: Sequential Floating Forward Search

Table 3.3: Comparison of feature selection algorithms for low dimensional data sets

Data set	Method	Evaluation Criteria					CPU Time (sec)
		E	FFEI	S	KNNA (%)	BayesA (%)	
					Mean SD	Mean SD	
	BB	0.65	0.40	0.90	64.03 0.41	63.55 0.40	4.01×10^4
Forest	SFFS	0.64	0.39	0.81	67.75 0.43	66.22 0.41	3.02×10^4
	SFS	0.64	0.41	0.98	62.03 0.41	61.09 0.40	7.00×10^3
p=5	SWC	0.68	0.45	1.00	54.70 0.37	53.25 0.35	50.03
P=10	Relief-F	0.65	0.40	0.90	64.03 0.41	63.55 0.40	2.80×10^4
$k = 5$	Proposed	0.65	0.40	0.90	64.03 0.41	63.55 0.40	55.50
	BB	0.59	0.36	1.84	94.90 0.17	94.45 0.14	3.39
Cancer	SFFS	0.59	0.36	1.84	94.90 0.17	94.45 0.14	6.82
	SFS	0.61	0.37	2.68	92.20 0.17	91.05 0.15	1.16
p=4	SWC	0.60	0.37	2.69	90.01 0.19	89.11 0.17	0.10
P=9	Relief-F	0.59	0.36	1.84	94.90 0.17	94.25 0.17	0.91
$k = 5$	Proposed	0.56	0.34	1.70	95.56 0.17	94.88 0.17	0.10
	BB	0.55	0.34	22.0	96.80 0.14	97.33 0.10	0.56
Iris	SFFS	0.55	0.34	22.0	96.80 0.14	97.33 0.10	0.71
	SFS	0.57	0.35	27.0	92.55 0.17	93.10 0.14	0.25
p=2	SWC	0.60	0.37	29.2	92.19 0.19	93.02 0.17	0.01
P=4	Relief-F	0.55	0.34	22.0	96.80 0.14	97.33 0.10	0.14
$k = 2$	Proposed	0.55	0.34	22.0	96.80 0.14	97.33 0.10	0.01

Compared to the search based algorithms (BB, SFFS and SFS), the performance of the proposed scheme is comparable or slightly superior, while the computational time requirement is much less for the proposed scheme. On the other hand, compared to the similarity based SWC method the performance of the proposed algorithm is much superior, keeping the time requirement comparable. It is further to be noted that the superiority in terms of computational time increases as the dimensionality and sample size increase. For example, in the case of low dimensional data sets speedup factor of the proposed scheme compared to BB and SFFS algorithms is about 30-50, for Forest data which is low dimensional but has large sample size the factor is about 100, for medium dimensional data sets, BB and SFFS are about 100 times slower and SFS about 10 times slower, while for the high dimensional data sets SFS is about 100 times slower, and BB and SFFS could not be compared as they require infeasibly high run time.

It may be noted that the aforesaid unsupervised feature selection algorithms (viz., BB, SFFS, SFS) usually consider 'entropy' as the selection criterion. Keeping this in mind detailed results are provided in Tables 3.1-3.3. However, we have also run the experiments using another unsupervised measure, namely, fuzzy feature evaluation index (FFEI) (Equation 3.3). Table 3.4 shows, as an illustration, the results only for the four large data sets (Isolet, Multiple features, Arrhythmia and Forest cover type). These results corroborate the findings obtained using entropy.

In a part of the experiment we have also compared the performance with a supervised method Relief-F, which is widely used. We have used 50% of the samples as design set for the Relief-F algorithm. Results are presented in Tables 3.1-3.3. The Relief-F algorithm provides classification performance comparable to the proposed scheme in spite of using class label information. Moreover, it has much higher time requirement, specially for data sets with large number of samples e.g., the Forest data. Its performance in terms of the unsupervised indices is also poorer.

Statistical significance of the classification performance of the proposed method compared to those of the other algorithms is tested. Means and SD values of the accuracies, computed over 10 independent runs, are used for this purpose. The test statistics described in Section 2.5.1 is used. It is observed that the proposed method has significantly better performance compared to the SWC algorithm for all the data sets, and the SFS algorithm for most of the data sets. For the other algorithms namely, Relief-F,

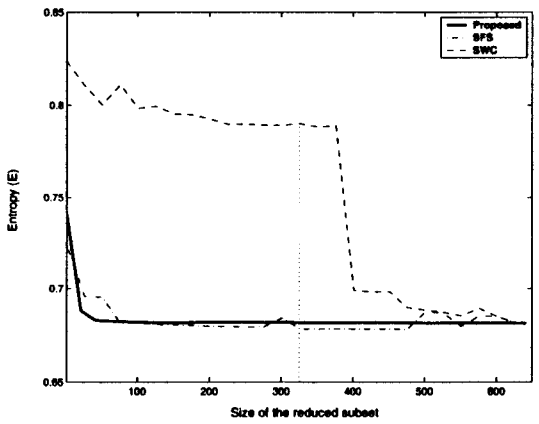
Table 3.4: Comparison of feature selection algorithms for large data sets when search algorithms use FFEI as the selection criterion

Data set	Method	Evaluation Criteria					CPU Time (sec)
		FFEI	E	S	KNNA (%)	BayesA (%)	
					Mean SD	Mean SD	
Isolet	SFS	0.40	0.54	0.98	95.81 0.82	92.19 0.72	28.01×10^4
p=310, P=617	Proposed	0.40	0.50	1.07	96.00 0.78	95.01 0.52	440
Mult. Feat.	SFS	0.44	0.67	0.44	77.71 0.44	75.81 0.17	9.20×10^4
p=325, P=649	Proposed	0.48	0.68	0.45	78.34 0.22	75.28 0.10	451
Arrhythmia	SFS	0.40	0.77	0.21	53.22 0.59	52.25 0.44	2008
p=100, P=195	Proposed	0.40	0.72	0.17	58.93 0.54	56.00 0.41	74
Forest	BB	0.40	0.65	0.90	64.03 0.41	63.55 0.40	9.21×10^4
	SFFS	0.40	0.66	0.83	67.01 0.45	66.00 0.44	7.52×10^4
	SFS	0.43	0.66	1.01	61.41 0.44	60.01 0.41	17.19×10^3
p=5, P=10	Proposed	0.40	0.65	0.90	64.03 0.41	63.55 0.40	55.50

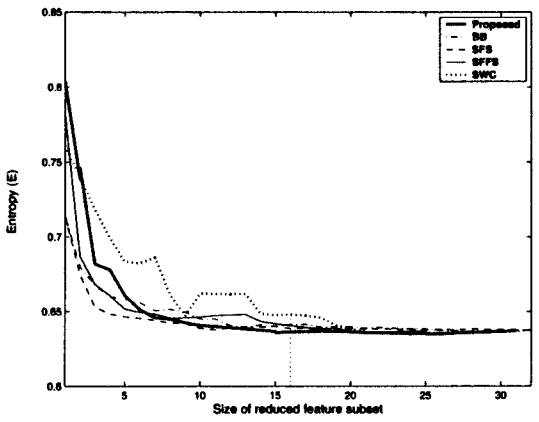
BB and SFFS, the performance is comparable, i.e., the difference of the mean values of the classification scores is statistically insignificant.

3.5.2 Redundancy reduction: Quantitative study

As mentioned before, the proposed algorithm involves partitioning the original feature set into certain number of homogeneous groups and then replacing each group by a single feature, thereby resulting in the reduced feature set. Representation entropy (H_R), defined in Section 3.4, is used to measure the redundancy in both the homogeneous clusters and the final selected feature subset. H_R when computed over the individual clusters should be as low as possible (indicating high redundancy among the features belonging to a single cluster), while giving as high value as possible for the selected subset (indicating minimum redundancy). Let us denote the average value of H_R computed over the homogeneous groups by H_R^g and the value of H_R for the final selected subset by H_R^s.



(a)



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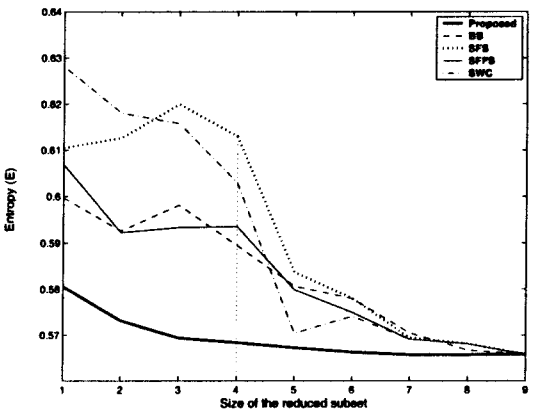


(c)

Figure 3.3: Variation in classification accuracy with size of the reduced subset for - (a) Multiple features, (b) Ionosphere, and (c) Cancer data sets. The vertical dotted line marks the point for which results are reported in Tables 3.1-3.3.

Table 3.5: Representation entropy H_R^s of subsets selected using some algorithms

Data set	BB	SFFS	SFS	SWC	Relief-F	Proposed
Isolet	-	-	2.91	2.87	2.89	3.50
Mult. Ftrs.	-	-	2.02	1.90	1.92	3.41
Arrhythmia	-	-	2.11	2.05	2.02	3.77
Spambase	2.02	1.90	1.70	1.44	1.72	2.71
Waveform	1.04	1.02	0.98	0.81	0.92	1.21
Ionosphere	1.71	1.71	1.70	0.91	1.52	1.81
Forest	0.91	0.82	0.82	0.77	0.91	0.91
Cancer	0.71	0.71	0.55	0.55	0.59	0.82
Iris	0.47	0.47	0.41	0.31	0.47	0.47

Table 3.5 shows the comparative results of the proposed method with other feature selection algorithms in terms of H_R^s. It is seen that the subset obtained by the proposed scheme is least redundant having the highest H_R^s values.

To demonstrate the superiority of the *maximal information compression index* λ_2, compared to the other two feature similarity measures (ρ and e) used previously, we provide Table 3.6, where we have compared both H_R^s and H_R^g values obtained using each of the similarity measures, in our clustering algorithm. It is seen from Table 3.6 that, λ_2 has superior information compression capability compared to the other two measures as indicated by the lowest and highest values of H_R^g and H_R^s respectively.

3.5.3 Effect of parameter k

In our algorithm the size of the reduced feature subset and hence the scale of details of data representation is controlled by the parameter k. Figure 3.4 illustrates such an effect for three data sets - multiple features, ionosphere and cancer, considering one data from each of the high, medium and low categories. As expected, the size of the reduced subset decreases overall with increase in k. However, for medium and particularly large dimensional data (Figure 3.4a) it is observed that for certain ranges of k at the lower side, there is no change in the size of the reduced subset i.e., no reduction in dimension occurs. Another interesting fact observed in all the data sets

Table 3.6: Redundancy reduction using different feature similarity measures

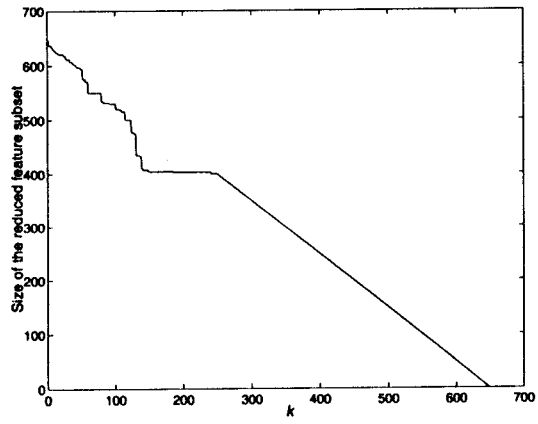
Data set	Similarity Measure: λ_2		Similarity Measure: e		Similarity Measure: ρ	
	H_R^g	H_R^s	H_R^g	H_R^s	H_R^g	H_R^s
Isolet	0.001	3.50	0.007	3.01	0.003	3.41
Mult. Ftrs.	0.002	3.41	0.008	2.95	0.007	3.01
Arrhythmia	0.007	3.77	0.017	2.80	0.010	3.41
Spambase	0.04	2.71	0.07	2.01	0.05	2.53
Waveform	0.10	1.21	0.14	1.04	0.11	1.08
Ionosphere	0.05	1.81	0.07	1.54	0.07	1.54
Forest	0.10	0.91	0.17	0.82	0.11	0.91
Cancer	0.19	0.82	0.22	0.71	0.19	0.82
Iris	0.17	0.47	0.22	0.31	0.17	0.47

H_R^g: average representation entropy of feature groups, H_R^s: representation entropy of selected subset, λ_2: maximal information compression index, e: least square regression error, ρ: correlation coefficients.

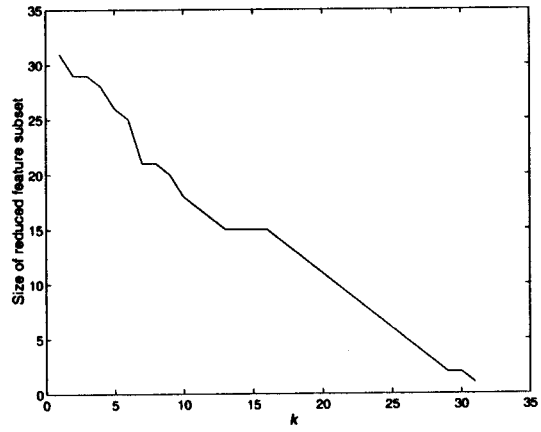
considered is that, for all values of k in the case of small dimensional data sets, and for high values of k in the case of medium and large dimensional data sets, the size of the selected subset varies linearly with k. Further, it is seen in those cases, $p + k \approx P$, where p is the size of the reduced subset and P is the size of the original feature set.

3.6 Conclusions and Discussion

An algorithm for unsupervised feature selection using feature similarity measures is described. The novelty of the scheme, as compared to other conventional feature selection algorithms, is the absence of search process which contributes to the high computational time requirement of those feature selection algorithms. Our algorithm is based on pairwise feature similarity measures, which are fast to compute. It is found to require several orders less CPU time compared to other schemes. Unlike other approaches which are based on optimizing either classification or clustering performance explicitly, here we determine a set of maximally independent features by discarding the redundant ones. This enhances the applicability of the resulting features to compres-



(a)



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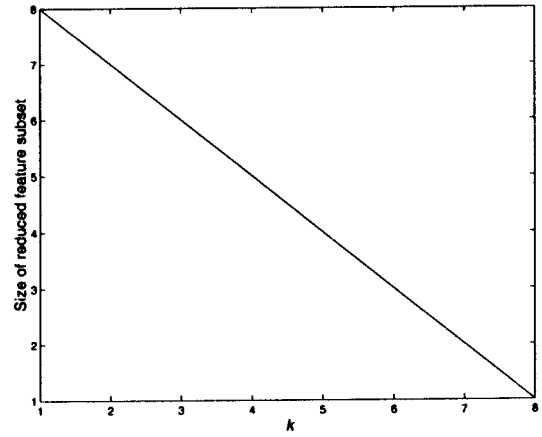


(c)

Figure 3.4: Variation in size of the reduced subset with parameter k for - (a) Multiple features, (b) Ionosphere, and (c) Cancer Data.

sion and other tasks like forecasting, summarization, association mining in addition to classification/clustering. Another characteristics of the proposed algorithm is its capability of multiscale representation of data sets. The scale parameter k used for feature clustering efficiently parametrizes the trade-off between representation accuracy and feature subset size. All these make it suitable for a wide variety of data mining tasks involving large (in terms of both dimension and size) data sets.

Besides formulating the novel clustering algorithm, we have defined a feature similarity measure called, *maximal information compression index*. One may note that the definition of the said parameter is not new, it is its use in feature subset selection framework which is novel. The superiority of this measure for feature selection is established experimentally. It is also demonstrated through extensive experiments that *representation entropy* can be used as an index for quantifying both redundancy reduction and information loss in a feature selection method.

We have measured the information loss in terms of second order statistics. The similarity measure used for the feature selection algorithm is selected/defined accordingly. One may modify these measures suitably in case even higher order statistics are used. In this regard modifications of correlation indices [148] which measure higher order polynomial dependency between variables may be considered. Also the similarity measure is valid only for numeric features; its extension to accommodate other kinds of variables (e.g., symbolic, categorical, hybrid) may also be investigated.

Chapter 4

Active Support Vector Learning

4.1 Introduction

In the previous two chapters we have dealt with some preprocessing tasks of data mining. The present chapter is concerned with its classification/learning aspect. Here we present two active learning strategies [99, 102] for handling the large quadratic programming problem of designing support vector machine classifier.

The support vector machine (SVM) [20, 163] has been successful as a high performance classifier in several domains including pattern recognition, data mining and bioinformatics. It has strong theoretical foundations and good generalization capability. Another advantage of SVM is that, as a by-product of learning, it obtains a set of support vectors (SVs) which characterizes a given classification task or compresses a labeled data set. Often the number of the SVs is only a small fraction of that of the original data set.

A limitation of the SVM design algorithm, particularly for large data sets, is the need to solve a quadratic programming (QP) problem involving a dense $n \times n$ matrix, where n is the number of points in the data set. Since most QP routines have quadratic complexity, SVM design requires huge memory and computational time for large data applications. Several approaches exist for circumventing the above shortcomings. These include simpler optimization criterion for SVM design, e.g., the linear SVM [17] and the kernel adatron [40], specialized QP algorithms like the conjugate gradient method [65], decomposition techniques which break down the large QP problem into a series of smaller QP sub-problems [110], and sequential minimal optimization (SMO) algorithm [140] and its various extensions.

A simple method to solve the SVM QP problem has been described by Vapnik [163], which is known as 'chunking'. The chunking algorithm uses the fact that the solution of the SVM problem remains the same if one removes the points that correspond to zero Lagrange multipliers of the QP problem (the non-SV points). The large QP problem can thus be broken down into a series of smaller QP problems, whose ultimate goal is to identify all of the non-zero Lagrange multipliers (SVs) while discarding the zero Lagrange multipliers (non-SVs). At every step, chunking solves a QP problem that consists of the non-zero Lagrange multiplier points from the previous step, and a chunk of q other points. At the final step, the entire set of non-zero Lagrange multipliers has been identified; thereby solving the large QP problem. Several variations of chunking

algorithm exist depending upon the method of forming the chunks [20, 153]. Chunking greatly reduces the training time compared to batch learning of SVMs. However, it may not handle large-scale training problems due to slow convergence of the chunking steps when q new points are chosen randomly.

Recently, active learning has become a popular paradigm for reducing the sample complexity of large scale learning tasks [6, 25]. Here, instead of learning from samples selected randomly, the learner has the ability to select its own training data. This is done iteratively, and the output of a step is used to select the examples for the next step. Several active learning strategies exist in practice, e.g., error driven techniques, uncertainty sampling, version space reduction and adaptive resampling.

In the context of support vector machine, active learning can be used to speed up chunking algorithms. In [21], a query learning strategy for large margin classifiers is presented which iteratively requests the label of the data point closest to the current separating hyperplane. This accelerates the learning drastically compared to random sampling. An active learning strategy based on version space splitting is presented in [161]. The points which split the current version space into two halves having equal volumes are selected at each step, as they are likely to be the actual support vectors. Three heuristics for approximating the above criterion are described, the simplest among them selects the point closest to the current hyperplane as in [21]. A greedy optimal strategy for active SV learning is described in [154]. Here, logistic regression is used to compute the class probabilities, which is further used to estimate the expected error after adding an example. The example that minimizes this error is selected as a candidate SV. Here also two heuristics are suggested for practical implementation by focusing only on the informative dimensions and selecting examples based on their proximity to the separating hyperplane. Although these active learning strategies query only for a single point at each step, several studies have noted that the gain in computational time can be obtained by querying multiple instances at a time. This motivates the formulation of active learning strategies which query for multiple points.

Another major limitation of all the above strategies is that they are essentially greedy methods where the selection of a new point is influenced only by the current hypothesis (separating hyperplane) available. In the above setup, learning may be severely hampered in two situations: a 'bad' example is queried which drastically worsens the current hypothesis, and the current hypothesis itself is far from the optimal hypothesis

(e.g., in the initial phase of learning). As a result, the examples queried are less likely to be the actual support vectors.

The model of *learning from statistical queries* captures the natural notion of learning algorithms that construct a hypothesis based on statistical properties of large samples rather than the idiosyncrasies of a particular sample [66]. Such a model of active learning seems intuitively more robust than those that are willing to make radical alterations to their hypothesis on the basis of individual examples. Here, instead of the original oracle which provides random examples of the target hypothesis, the learner interacts with an intermediate oracle whose goal is to enforce restriction on the learner's use of the examples. The intermediate oracle provides an estimate of the probability (with an allowed approximation error) that an example belongs to the target hypothesis *i.e.*, provides answers to statistical queries rather than exact membership queries. The probability of a point being selected for learning may be set equal to that answer. The statistical query model has been theoretically demonstrated to provide efficient and robust learning in noisy environments [66].

The chapter has two parts. First we present an error driven incremental method [99] for active support vector learning. The method involves selecting a chunk of q new points, having equal number of correctly classified and misclassified points, at each iteration by resampling the data set, and using it to update the current SV set. The resampling strategy is computationally superior to random chunk selection, while achieving higher classification accuracy. Since, it allows for querying multiple instances at each iteration, it is computationally more efficient than those that are querying for a single example at a time.

The second part of this chapter provides a method for active support vector learning in statistical query framework [102]. Like the previous algorithm, it also involves queries for multiple instances at each iteration. The intermediate statistical query oracle, involved in the learning process, returns the value of the probability that a new example belongs to the actual support vector set. A set of q new points is selected according to the above probability, and is used along with the current SVs to obtain the new SVs. The probability is estimated using a combination of two factors: the margin of the particular example with respect to the current hyperplane, and the degree of confidence that the current set of SVs provides the actual SVs. The degree of confidence is quantified by a measure which is based on the local properties of each

of the current support vectors and is computed using the nearest neighbor estimates.

The methodology in the second part has some more advantages. It not only queries for the error points (or points having low margin) but also a number of other points far from the separating hyperplane (interior points). Thus, even if a current hypothesis is erroneous there is a scope for it being corrected owing to the interior points. If only error points were selected the hypothesis might have actually been worse. The ratio of selected points having low margin and those far from the hyperplane is decided by the confidence factor, which varies adaptively with iteration. If the current SV set is close to the optimal one, the algorithm focuses only on the low margin points and ignores the redundant points that lie far from the hyperplane. On the other hand, if the confidence factor is low (say, in the initial learning phase) it explores a higher number of interior points. Thus, the trade-off between efficiency and robustness of performance is adequately handled in this framework. Also, the efficiency of most of the existing active SV learning algorithms depends on the sparsity ratio (*i.e.*, the ratio of the number of support vectors to the total number of data points) of the data set. Due to the adaptive nature of the query in the proposed algorithm, it is likely to be efficient for a wide range of sparsity ratio.

Experiments have been performed on five real life classification problems. The sample size ranges from 351 to 495141, dimension from 9 to 34, and the sparsity ratio from 0.01 to 0.51. Our algorithms are found to provide superior performance and faster convergence compared to several related algorithms for incremental and active SV learning.

The organization of the chapter is as follows. In the next section we describe briefly the basic support vector machine algorithm for classification. Then we describe the algorithm of incremental support vector learning in Section 4.3. In Section 4.4 we provide a formal description of the learning with statistical query framework along with a methodology for estimating the associated confidence factor. The algorithm for active learning with statistical queries is described in Section 4.5. Experimental results are presented in Section 4.6, and finally conclusions and discussion are provided in Section 4.7.

4.2 Support Vector Machine

Support vector machines are a general class of learning architectures inspired from statistical learning theory that performs *structural risk minimization* on a nested set structure of separating hyperplanes [163]. Given a training data, the SVM training algorithm obtains the optimal separating hyperplane in terms of generalization error. Though SVMs may also be used for regression and multiclass classification, in this study we concentrate only on two-class classification problem.

Algorithm: Suppose we are given a set of labelled examples $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_i, y_i)$ $\ldots, (\mathbf{x}_n, y_n), \mathbf{x}_i \in R^P, y_i \in \{-1, +1\}$. We consider functions of the form $sgn((\mathbf{w}\cdot\mathbf{x})+b)$, in addition we impose the condition

$$\inf_{i=1,\ldots,n} |(\mathbf{w} \cdot \mathbf{x}_i) + b| = 1. \tag{4.1}$$

We would like to find a decision function $f_{\mathbf{w},b}$ with the properties $f_{\mathbf{w},b}(\mathbf{x}_i) = y_i;\ i = 1, \ldots, n$. If such a function exists, condition (4.1) implies

$$y_i((\mathbf{w} \cdot \mathbf{x}_i) + b) \geq 1, \quad \forall\ i = 1, \ldots, n. \tag{4.2}$$

In many practical situations, a separating hyperplane does not exist. To allow for possibilities of violating Equation 4.2, slack variables are introduced like

$$\xi_i \geq 0, \quad i = 1, \ldots, n \tag{4.3}$$

to get

$$y_i((\mathbf{w} \cdot \mathbf{x}_i) + b) \geq 1 - \xi_i, \quad i = 1, \ldots, n. \tag{4.4}$$

The support vector approach for minimizing the generalization error consists of the following:

$$\textbf{Minimize}: \qquad \Phi(\mathbf{w}, \xi) = (\mathbf{w} \cdot \mathbf{w}) + C \sum_{i=1}^{n} \xi_i \tag{4.5}$$

subject to the constraints (4.3) and (4.4).

It can be shown that minimizing the first term in Equation 4.5, amounts to minimizing the VC-dimension or maximizing the margin (Figure 4.1), while minimizing the second

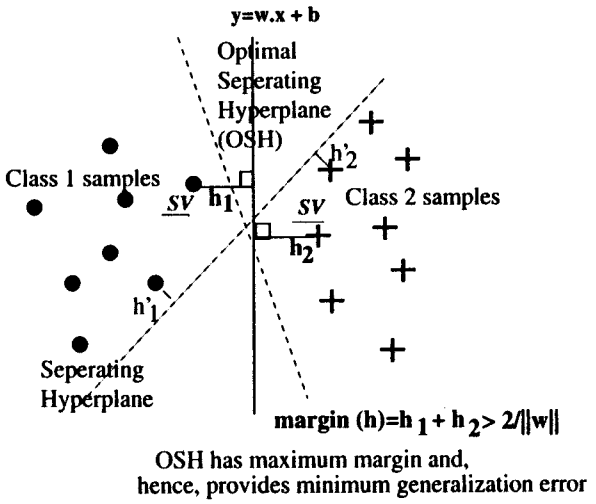


Figure 4.1: SVM as maximum margin classifier (linearly separable case)

term corresponds to minimizing the misclassification error [20]. SVM's provide the maximum margin classifiers for a given misclassification on the training set. This is illustrated in Figure 4.1.

The above minimization problem can be posed as a constrained quadratic programming (QP) problem. The solution gives rise to a decision function of the form:

$$f(\mathbf{x}) = sgn\left[\sum_{i=1}^{n} y_i \alpha_i (\mathbf{x} \cdot \mathbf{x_i}) + b\right],$$

where α_i's are positive numbers. Only a small fraction of the α_i coefficients are non-zero. The corresponding pairs of $< \mathbf{x_i}, y_i >$ entries are known as *support vectors* and they fully define the decision function. The support vectors are geometrically the points lying near the class boundaries as illustrated in [20]. We use linear kernels for SVM. However, nonlinear kernels like polynomial, sigmoidal and radial basis functions may also be used.

We briefly mention below an alternate explanation of SVM learning, applicable to hard margin case, which provides a better insight of the incremental SV learning procedure. The approach is due to Tong and Koller [161]. Consider a feature space $\mathcal{F}$ and the parameter space $\mathcal{W}$. If the training data is linearly separable in the feature space, the set of hyperplanes that separate the data is called the *version space* $\mathcal{V}$, defined as

$$\mathcal{V} = \{\mathbf{w} \in \mathcal{W} | \ ||\mathbf{w}|| = 1, y_i(\mathbf{w} \cdot \mathbf{x}_i) > 0, \ i = 1, \ldots, n\}. \tag{4.6}$$

There exists a duality between the feature space $\mathcal{F}$ and the parameter space $\mathcal{W}$: points in $\mathcal{F}$ correspond to hyperplanes in $\mathcal{W}$ and *vice versa.* Also, the version space is a connected region on the surface of a hypersphere in parameter space. Using the above facts and considering the SVM optimality criterion, it can be shown that SVMs find the center of the largest hypersphere whose center can be placed in version space and whose surface does not intersect with the hyperplanes corresponding to the training instances. The hyperplanes that are touched by the maximal radius hypersphere correspond to support vectors and the radius of the hypersphere is the margin of the SVM. Thus if one queries for the training instances which maximally reduce the size of the current version space, the SVM obtained would eventually lie close to the actual SVM. It can be shown that maximal reduction in size of the version space takes place if $\mathcal{V}_i^- = \mathcal{V}_i^+$, where $\mathcal{V}_i^-$ and $\mathcal{V}_i^+$ denote the resulting version spaces if instance i is added and has labels -1 and $+1$ respectively.

4.3 Incremental Support Vector Learning with Multiple Points [99]

The objective of the algorithm is to select a minimal subset of support vectors such that the corresponding SVM would provide minimum misclassification on the remaining points in the sample set. The methodology is motivated from the condensation technique proposed by Hart [54] for reducing the computational complexity and storage requirements of k-NN classifiers.

Algorithm 1:

Set up data bins called STORE and GRABBAG. Initially, k randomly selected samples are placed in STORE, all other samples are placed in GRABBAG. k is chosen arbitrarily, such that STORE contains at least one point from each class.

Step 1: Design a SVM using the samples in STORE. Retain the *support vectors* in STORE, and discard other points in STORE.

Step 2: Resample GRABBAG. From GRABBAG select $q/2$ points which are correctly classified and $q/2$ points which are misclassified by the SVM obtained in Step 1. Append the (q) resampled points to STORE obtained after Step 1. Repeat Step 1, till

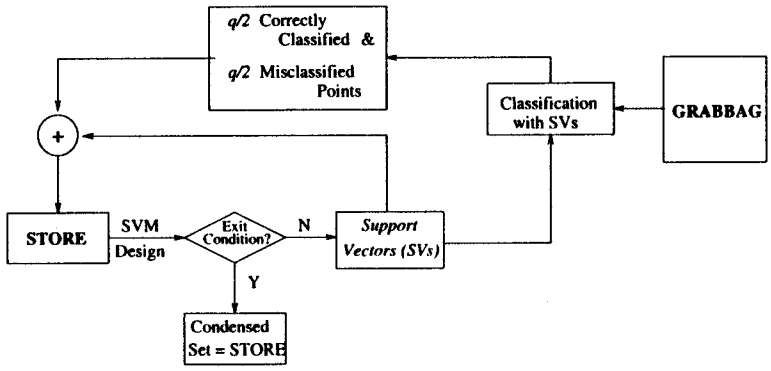


Figure 4.2: Incremental support vector learning with multiple points (Algorithm 1)

the required accuracy is achieved on a test set, or GRABBAG is exhausted. □

The algorithm is illustrated in Figure 4.2. ♦

In the next section we describe briefly the model of learning using statistical queries. This is useful in understanding the second algorithm (Algorithm 2) for active support vector learning, described in Section 4.5.

4.4 The Statistical Query Model of Learning

Let $\mathcal{C}$ be a (concept) class of $\{0,1\}$ valued functions over an input space X. In trying to design a learning algorithm for the class $\mathcal{C}$, we assume that there is a fixed but arbitrary and unknown target probability distribution $\mathcal{P}$ over X that governs the generation of random examples. The standard supervised learning model (PAC model [163]), when executed on the target concept $f \in \mathcal{C}$, a learning algorithm will be given access to an oracle $EX(f,\mathcal{P})$ that on each call draws an input $\mathbf{x}$ randomly and independently according to $\mathcal{P}$, and returns the labeled example $< \mathbf{x}, f(\mathbf{x}) >$.

In the statistical query model [66] the standard examples oracle $EX(f,\mathcal{P})$ is replaced by a new oracle $STAT(f,\mathcal{P})$. The oracle $STAT(f,\mathcal{P})$ takes as input a statistical query of the form (χ,α). Here χ is any mapping of a labeled example to $\{0,1\}$, and $\alpha \in [0,1]$. A query (χ,α) is interpreted as a request for the value $P_\chi = \mathbf{Pr}_{\mathbf{x}\in\mathcal{P}}(\chi(\mathbf{x},f(\mathbf{x})) = 1)$, which can be abbreviated as $\mathbf{Pr}_{EX(f,\mathcal{P})}(\chi = 1)$. Thus, each query is a request for the probability of some event on the distribution generated by $EX(f,\mathcal{P})$. However, the oracle $STAT(f,\mathcal{P})$ will not return the exact value of P_χ but only an approximation,

and the role of α is to quantify the amount of error the learning algorithm is willing to tolerate in this approximation.

In the context of support vector machines, the target of the learning algorithm is to learn the set of all support vectors. This is done by incrementally training a SVM on a set of examples consisting of the previous SVs and a new set of points. In the proposed algorithm the new set of points, instead of being randomly generated by $EX(f, \mathcal{P})$, is generated according to $\mathbf{Pr}_\chi$ returned by the oracle $STAT(f, \mathcal{P})$. $\chi(\mathbf{x}, f(\mathbf{x}))$ denotes the event that the example $\mathbf{x}$ is a SV. $f(\mathbf{x})$ is the optimal separating hyperplane. Let $< \mathbf{w}, b >$ be the current separating hyperplane available to the learner. We define the probability $\mathbf{Pr}_\chi$ returned by the oracle $STAT(f, \mathcal{P})$ as follows:

$$\begin{aligned} P_\chi = &\quad c \quad \text{if } y(\mathbf{w} \cdot \mathbf{x} + b) \leq 1 \\ = &\quad 1 - c \quad \text{otherwise.} \end{aligned} \tag{4.7}$$

Here c is a *confidence parameter* which denotes how close the current hyperplane $< \mathbf{w}, b >$ is to the optimal one, and y is the label of $\mathbf{x}$.

The significance of P_χ is as follows: if c is high, which signifies that the current hyperplane is close to the optimal one, points lying within the margin band of the current hyperplane are highly likely to be the actual SVs. Hence, the probability P_χ returned to the corresponding query is set to a high value c. When the value c is low, the probability of selecting a point lying within the margin decreases, and a high probability value $(1 - c)$ is then assigned to an interior point. Let us now describe a method for estimating the confidence factor c.

Estimating the confidence factor for a SV set

Let the current set of support vectors be denoted by $S = \{\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_l\}$. Also, consider a test set $T = \{\mathbf{x}'_1, \mathbf{x}'_2, \ldots, \mathbf{x}'_m\}$ and an integer k (say, $k = \sqrt{m}$). For every $\mathbf{s}_i \in S$ compute the set of k nearest points in T. Among the k nearest neighbors let k_i^+ and k_i^- number of points have labels $+1$ and -1 respectively. The confidence factor c is then defined as

$$c = \frac{2}{kl} \sum_{i=1}^{l} \min(k_i^+, k_i^-). \tag{4.8}$$

Note that the maximum value of the confidence factor c is unity when $k_i^+ = k_i^-$

$\forall i = 1, \ldots, l$, and the minimum value is zero when $\min(k_i^+, k_i^-) = 0 \ \forall i = 1, \ldots, l$. The first case implies that all the support vectors lie near the class boundaries and the set $S = \{\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_l\}$ is close to the actual support vector set. (It may be noted that support vectors are points lying near the class boundaries). The second case, on the other hand, denotes that the set S consists only of interior points and is far from the actual support vector set. Thus, the confidence factor c measures the degree of closeness of S to the actual support vector set. Higher the value of c is, the closer is the current SV set to the actual SV set.

The use of the factor c can also be justified from the point of view of Bayes classification rule. It is known that for overlapping classes the support vector set consists of the error points and the points lying within a margin band of the decision boundary. Bayes classification rule states that posteriori probabilities of each of the classes are equal along the decision boundary and on the error region. The ratios k_i^+/k and k_i^-/k are nearest neighbor estimates of the posteriori probabilities for the classes $+1$ and -1 respectively. Hence, they attain almost equal values for both error points and points lying near the class boundaries. It may also be mentioned that the support vector set, when used for k nearest neighbor classification, is known to provide high classification accuracy [31].

A version space explanation of the factor c may also be provided. It is evident from the discussion in Section 4.2, that points which split the version space into two equal halves are considered to be the likely candidates for being support vectors. Volumes of the version spaces $\mathcal{V}^+$ and $\mathcal{V}^-$, as obtained after adding those points with labels $+1$ and -1, are equal [161]. Examination of the SVM objective function reveals that, if a neighborhood of a point $\mathbf{s}_i$ contains equal number of examples having labels $+1$ and -1, then addition of the point $\mathbf{s}_i$ with labels $+1$ and -1 results in version spaces $\mathcal{V}^+$ and $\mathcal{V}^-$ respectively with equal volumes. Hence, as the value of c (Equation 4.8) increases, the probability that $\mathbf{s}_i$'s are the candidate support vectors increases.

4.5 Learning Support Vectors with Statistical Queries [102]

Here we describe a method for active learning of support vectors with statistical queries. The active support vector learning algorithm obtains a new SV set at each step by minimizing the objective function of Equation 4.5 for a set of points consisting of the SVs of the previous step and q new points. These new q points are obtained from the training set using the statistical query strategy, as discussed in the previous section. The algorithm is presented below and the block diagram is shown in Figure 4.3.

Algorithm 2:

Let $A = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ denote the entire training set used for SVM design. $SV(B)$ denotes the set of support vectors, of the set B, obtained using the methodology described in Section 4.2. $S_t = \{\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_l\}$ is the support vector set obtained after tth iteration, and $< \mathbf{w}_t, b_t >$ is the corresponding separating hyperplane. $V_t = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_q\}$ is the set of q points actively queried for at step t. c is the confidence factor obtained using Equation 4.8. The learning steps involved are given below:

Initialize: Randomly (without replacement) select an initial starting set V_0 of q instances from the training set A. Set $t = 0$ and $S_0 = SV(V_0)$. Let the parameters of the corresponding hyperplane be $< \mathbf{w}_0, b_0 >$.

While *Stopping Criterion* is not satisfied:
  $V_t = \emptyset$.
  While Cardinality$(V_t) \leq q$:
    Randomly (without replacement) select an instance $\mathbf{x} \in A$.
    Let y be the label of $\mathbf{x}$.
    If $y(\mathbf{w}_t \cdot \mathbf{x} + b) \leq 1$:
      Select $\mathbf{x}$ with probability c. Set $V_t = V_t \cup \{\mathbf{x}\}$.
    Else:
      Select $\mathbf{x}$ with probability $1 - c$. Set $V_t = V_t \cup \{\mathbf{x}\}$.
    End If
  End While
  $S_t = SV(S_t \cup V_t)$, $t = t + 1$.
End While

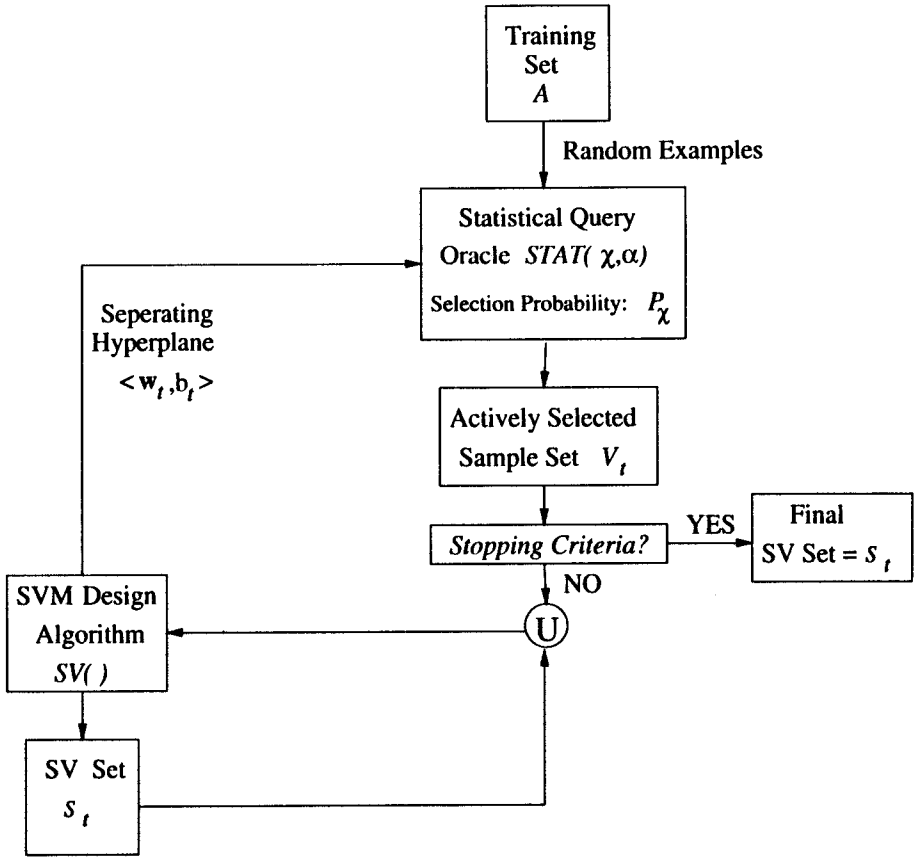


Figure 4.3: Active support vector learning with statistical queries (Algorithm 2)

The set S_{t^*}, where t^* is the iteration at which the algorithm terminates, contains the final SV set. □

Stopping Criterion: Among the q points actively queried at each step t, let q' points have margin greater than unity ($y(\mathbf{w}_t \cdot \mathbf{x} + b) > 1$). Learning is stopped if the quantity $\frac{c \cdot q'}{q}$ exceeds a threshold Th (say, $= 0.9$).

Remarks:

1. The selection probability P_χ (Equation 4.7) returned by the statistical query oracle is a two level function of the margin ($y(\mathbf{w} \cdot \mathbf{x} + b)$) of a point $\mathbf{x}$. Continuous functions of margin of $\mathbf{x}$ may also be used. Such an algorithm can be considered to be statistical query based extensions of the existing methods of active support vector learning which query for the nearest point to the separating hyperplane.

2. The stopping criteria may be interpreted as follows. A high value of the quantity $\frac{q'}{q}$ implies that the query set contains a few number of points with margin less than unity. No further gain can be thus achieved by the learning process. The value of q' may also be large when the value of c is low in the initial phase of learning. However, if both c and q' have high values, the current SV set is close to the actual one (*i.e.*, a good classifier is obtained) and also the margin band is empty (*i.e.*, the learning process is saturated); hence, the learning may be terminated.

4.6 Experimental Results and Comparison

Organization of the experimental results is as follows. First, the performance of the two algorithms, presented in Sections 4.3 and 4.5, is compared with two other incremental support vector learning algorithms as well as the batch SVM, in terms of generalization capability, training time and $\mathcal{D}$ (Equation 4.9). The effectiveness of the confidence factor c, used for active querying by the second algorithm, is then studied. Finally, we investigate the nature of the margin distribution, obtained by the second algorithm, as compared to those obtained by some other related large margin classifiers.

Five data sets are used, namely, Wisconsin cancer, Ionosphere, Heart, Twonorm and Forest cover type. They are described in Appendix A. The first four data sets have two overlapping classes. The fifth one (Forest cover type) contains seven classes; but 80% of the points belong to classes one and two. We consider here only the points belonging to those two classes.

4.6.1 Comparison: Classification accuracy and training time

The algorithms for incremental SV learning with multiple points (Algorithm 1, denoted by IncrSVM in Table 4.1) and active SV learning with statistical queries (Algorithm 2, denoted by StatQSVM in Table 4.1) are compared with (i) incremental SV learning with random chunk selection [20] (denoted by RandSVM in Table 4.1), and (ii) a recently proposed method for active SV learning which queries for the point closest to the current separating hyperplane [21] (denoted by QuerySVM in Table 4.1). Note

that the QuerySVM is identical to the 'simple margin' strategy described in [161]. A comparison with the actual batch SVM algorithm (denoted by BatchSVM in Table 4.1) is also provided, since this is the ideal one. The batch SVM algorithm could not provide results for the Forest cover type data, due to its large size.

Comparison is made on the basis of the following quantities:

1. Classification accuracy on training set ($a_{training}$): The training set is obtained by sampling 90% of the points from the entire data set. Mean of the accuracy, computed over 10 such random selection, is reported.

2. Classification accuracy on test set (a_{test}): The test set has size 10% of that of the entire data set, and contains points which do not belong to the training set. Here also means over 10 independent runs are reported.

3. Closeness of the SV set: We measure closeness of the SV set ($\tilde{S}$), obtained by an algorithm, to the actual one (S) which is obtained by the batch SVM algorithm. This is measured by the distance $\mathcal{D}$ defined as follows [91]:

$$\mathcal{D} = \frac{1}{n_{\tilde{S}}} \sum_{\mathbf{x}_1 \in \tilde{S}} \delta(\mathbf{x}_1, S) + \frac{1}{n_S} \sum_{\mathbf{x}_2 \in S} \delta(\mathbf{x}_2, \tilde{S}) + Dist(\tilde{S}, S), \tag{4.9}$$

where

$$\delta(\mathbf{x}_1, S) = \min_{\mathbf{x}_2 \in S} d(\mathbf{x}_1, \mathbf{x}_2), \ \delta(\mathbf{x}_2, \tilde{S}) = \min_{\mathbf{x}_1 \in \tilde{S}} d(\mathbf{x}_1, \mathbf{x}_2),$$

and

$$Dist(\tilde{S}, S) = \max\{\max_{\mathbf{x}_1 \in \tilde{S}} \delta(\mathbf{x}_1, S), \max_{\mathbf{x}_2 \in S} \delta(\mathbf{x}_2, \tilde{S})\}.$$

$n_{\tilde{S}}$ and n_S are the number of points in $\tilde{S}$ and S respectively. $Dist(\tilde{S}, S)$ is the Hausdorff distance between sets $\tilde{S}$ and S. $d(\mathbf{x}_1, \mathbf{x}_2)$ is the Euclidean distance between points $\mathbf{x}_1$ and $\mathbf{x}_2$. The distance measure $\mathcal{D}$ has been used for quantifying the errors of set approximation algorithms [91], and is related to the ϵ-cover of a set.

4. CPU time (t_{cpu}) required on a Sun UltraSparc 350MHz Workstation.

It is observed from the results shown in Table 4.1 that all the incremental algorithms, as expected, require significantly less training time as compared to the batch SVM

Table 4.1: Comparison of performance of SVM design algorithms

Data	Algorithm	$a_{training}(\%)$	$a_{test}(\%)$	$\mathcal{D}$	t_{cpu} (sec)
Cancer	BatchSVM	97.44	96.32	*Zero*	1291
	RandSVM	87.19	86.10	10.92	302
	QuerySVM	97.10	96.21	9.91	262
	IncrSVM	92.10	91.01	10.40	221
	StatQSVM	97.40	96.43	7.82	171
Ionosphere	BatchSVM	88.87	84.57	*Zero*	271
	RandSVM	78.10	77.17	8.92	81
	QuerySVM	78.19	77.02	8.01	95
	IncrSVM	79.50	78.22	9.10	78
	StatQSVM	84.09	82.20	7.01	68
Heart	BatchSVM	78.80	77.35	*Zero*	2702
	RandSVM	72.52	70.82	0.37	94
	QuerySVM	75.04	74.01	280	72
	IncrSVM	74.05	72.11	410	55
	StatQSVM	75.82	74.91	168	25
Twonorm	BatchSVM	98.58	97.46	*Zero*	8.01×10^4
	RandSVM	93.40	92.01	12.70	770
	QuerySVM	95.01	93.04	12.75	410
	IncrSVM	95.22	93.10	12.52	520
	StatQSVM	97.02	96.01	12.01	390
Forest cover type	RandSVM	59.22	57.90	-	4.70×10^4
	QuerySVM	66.01	65.77	-	3.20×10^4
	IncrSVM	64.02	61.02	-	2.90×10^4
	StatQSVM	75.44	74.83	-	2.01×10^4

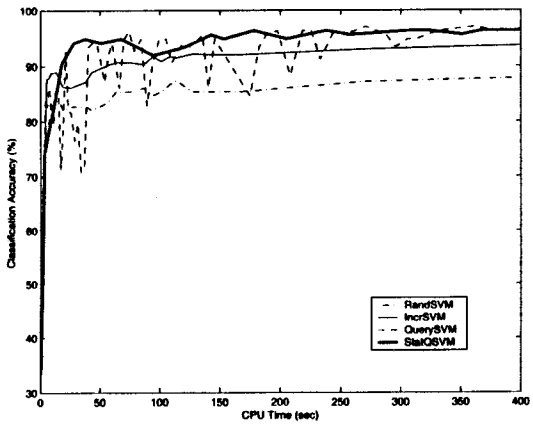
- The value of $\mathcal{D}$ corresponding to BatchSVM is *Zero* by definition.
- Since BatchSVM could not be obtained for the *large* Forest cover type data, $\mathcal{D}$ could not be computed, and is denoted by '-'.

with little degradation in classification accuracy. Comparing the three active learning algorithms (namely, QuerySVM, IncrSVM, and StatQSVM) with RandSVM shows that the use of active learning strategy enhances the performance in terms of both classification accuracy and training time, for all the data sets. Again, among the active learning techniques, StatQSVM achieves the highest classification score with minimum $\mathcal{D}$ value in least time for all the cases. This superiority of StatQSVM becomes more apparent for the Forest cover type data, where it significantly outperforms the other three incremental learning methods. When tested for statistical significance (using the methodology described in Section 2.5.1), the classification accuracy of StatQSVM was found to be significantly higher, compared to the other three incremental methods, for all the data sets except the Cancer data, where significance could not be established while comparing with QuerySVM. It may be further noted that QuerySVM provides higher classification accuracy compared to IncrSVM; this is expected since QuerySVM involves complex queries requiring more CPU time.

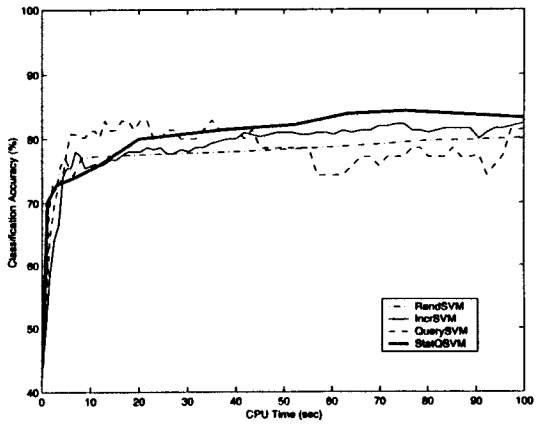
The nature of convergence of the classification accuracy on test set a_{test} is shown in Figure 4.4 for all the data sets. It is observed that the convergence curve for the StatQSVM algorithm dominates over those of RandSVM, IncrSVM and QuerySVM. Since the RandSVM algorithm selects the chunks randomly, the corresponding curve is smooth and almost monotonic, although its convergence rate is much slower. On the other hand, the QuerySVM algorithm selects only the point closest to the current separating hyperplane and achieves a high classification accuracy in few iterations. However, its convergence curve is oscillatory and the classification accuracy falls significantly after certain iterations. This is expected as querying for points close to the current separating hyperplane may often result in gain in performance if the current hyperplane is close to the optimal one. While querying for interior points reduces the risk of performance degradation, it achieves poor convergence rate. StatQSVM, on the other hand, selects an optimal proportion of low margin and interior points, and hence, maintains a fast convergence rate without oscillatory performance degradation.

4.6.2 Effectiveness of the confidence factor c

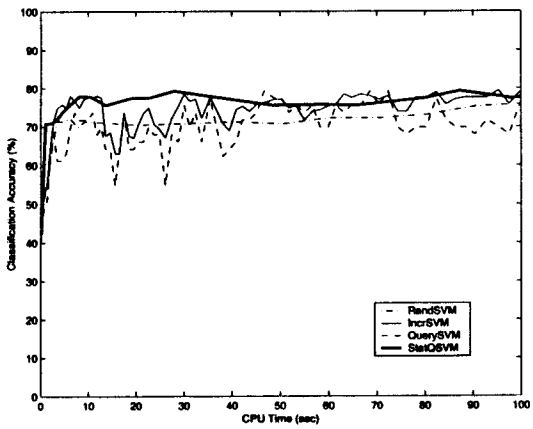
Figure 4.5 shows the variation of c (Equation 4.8), for the SV sets obtained in StatQSVM, with distance $\mathcal{D}$. It is observed that for all the data sets c is (negatively) correlated



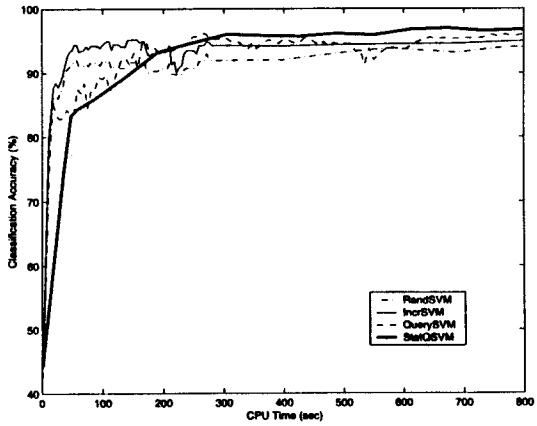
(a)



(b)



(c)



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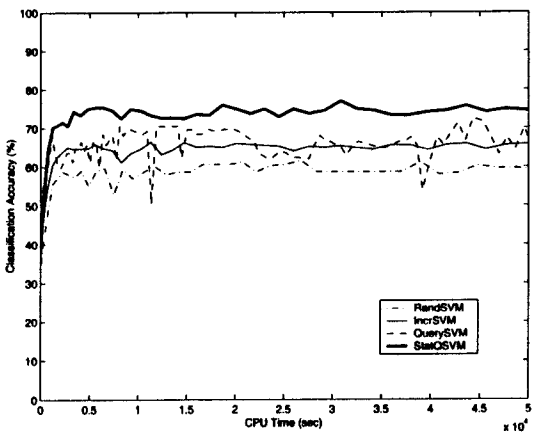


(e)

Figure 4.4: Variation of a_{test} with CPU time for (a) Cancer, (b) Ionosphere, (c) Heart, (d) Twonorm, and (e) Forest cover type data

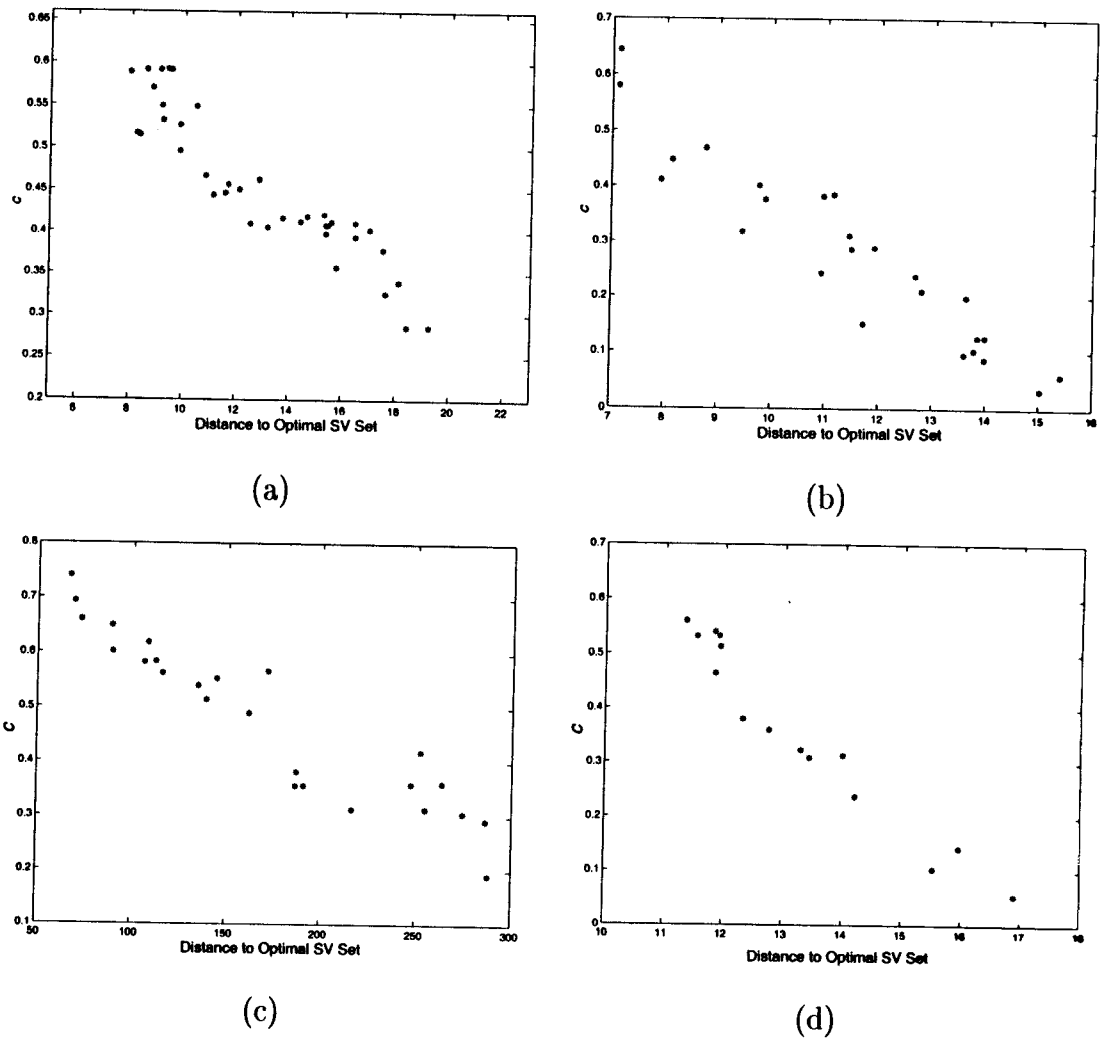


Figure 4.5: Variation of confidence factor c and distance $\mathcal{D}$ for (a) Cancer, (b) Ionosphere, (c) Heart, and (d) Twonorm data

with $\mathcal{D}$. As the current SV set approaches the optimal one, the value of $\mathcal{D}$ decreases and the value of confidence factor c increases. Hence, c also provides an effective measure of the closeness of the SV set to the actual one. Variation of c with iteration for the StatQSVM algorithm is shown in Figure 4.6. For all the data sets, the value of the confidence factor c is low in the initial phases of learning, and subsequently it increases to attain a value closer to unity when learning converges.

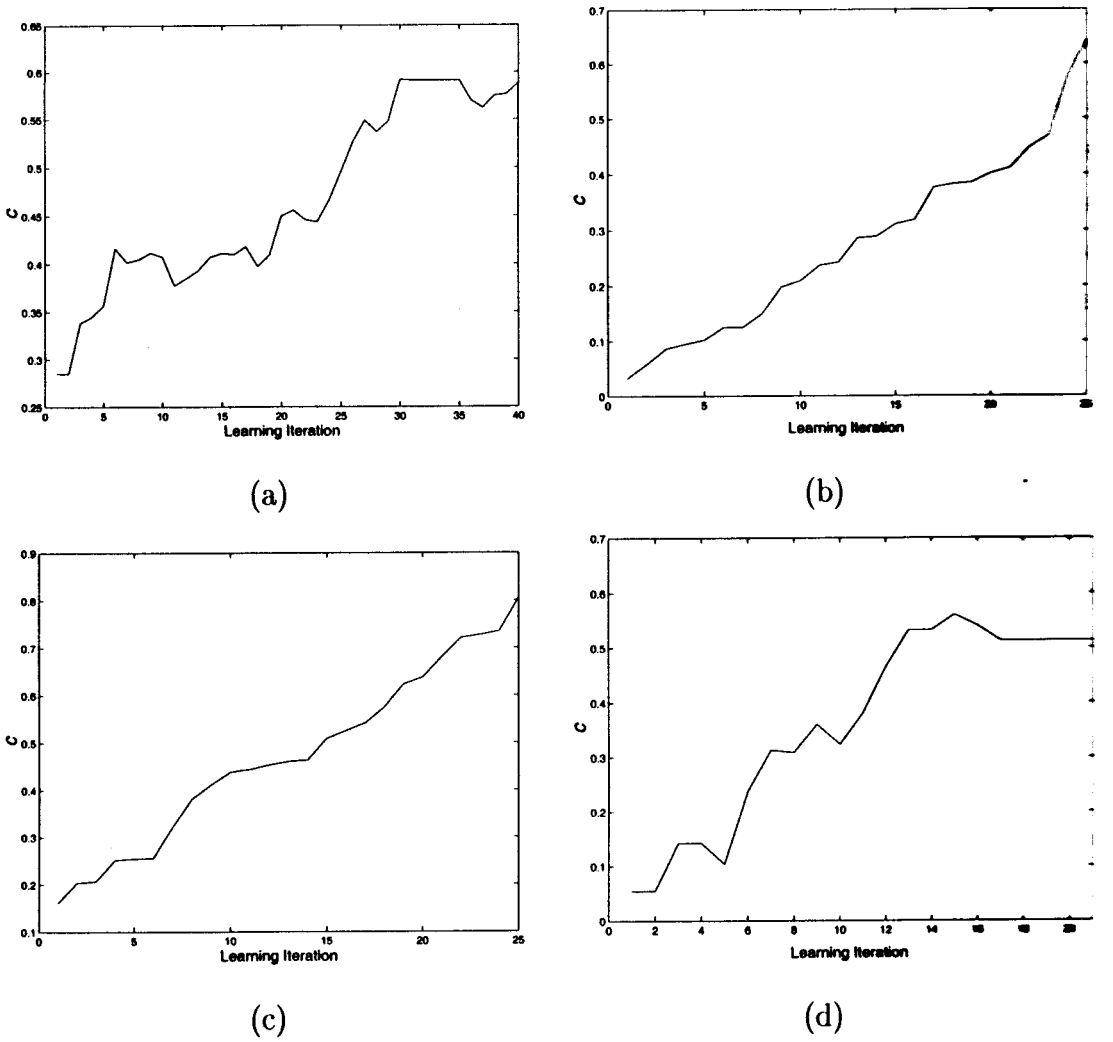


Figure 4.6: Variation of confidence factor c with iterations of StatQSVM **algorithm for** (a) Cancer, (b) Ionosphere, (c) Heart, and (d) Twonorm data

4.6.3 Margin distribution

Recently it has been shown that the generalization capability of a classifier can be characterized not only by the minimum margin, but also by more general parameters that can be estimated from the margin distribution. Some such parameters were studied in [39]. In our experiments we also investigate the nature of the margin distribution in terms of the cumulative distribution of the quantity $y(\mathbf{w} \cdot \mathbf{x} + b)$. In Figure 4.7 we show the variation of the margin distribution, obtained at different learning iterations of the StatQSVM algorithm, for the Twonorm data set only, as an example. It is seen that with iteration the distribution shifts to the right with more number of points having high margin. In Figure 4.8 we present a comparison among all the four aforesaid SVM learning algorithms, as well as a SVM designed using boosting [130], in terms of their final margin distributions. (Note that boosting SVM is considered in Figure 4.8 because it is well known for providing large margin classifiers, though it is computationally demanding for large data sets. Since it is not an incremental learning method, we did not consider it in Table 4.1 for comparison.) It is observed that for most data points a higher margin value is achieved for both boosting SVM and StatQSVM as compared to batch SVM, RandSVM and QuerySVM. This may be due to the fact that both the former ones incrementally use a set of points which are obtained by sampling from a distribution that varies with iteration. In the case of StatQSVM the statistical query oracle generates this distribution, while for boosting SVM the distribution is obtained from the probability values which are stored for all the points and updated with iteration. Both these distributions drift towards the actual separating hyperplane with iteration.

4.7 Conclusions and Discussion

Two methods for active SVM learning are presented to overcome the large QP problem arising in SVM design. The effectiveness of the algorithms is experimentally demonstrated for some real life data sets. Among the two algorithms presented, the second one, based on statistical query model of learning, provides better performance. This is because of the use of an adaptive query strategy whose novelty is as follows. Most of the algorithms for incremental SV learning either query for points close to the current

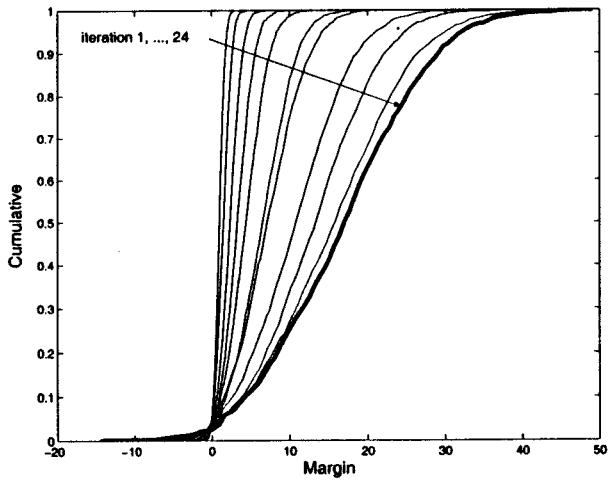


Figure 4.7: Margin distribution obtained at each iteration by the proposed algorithm for the Twonorm data. The bold line denotes the final distribution obtained

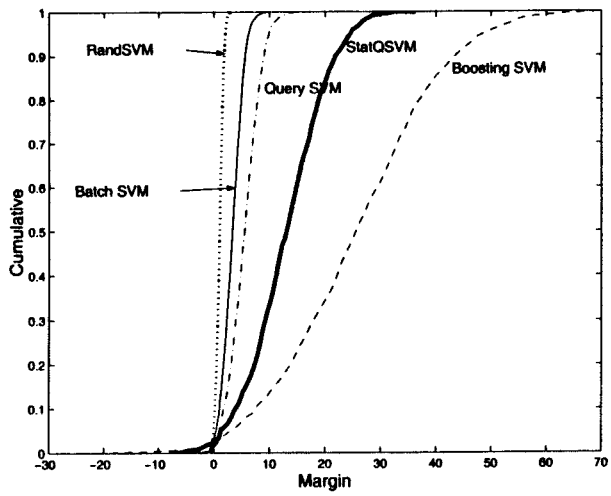


Figure 4.8: Margin distribution obtained by some SVM design algorithms for the Twonorm data set.

separating hyperplane or select random chunks consisting mostly of interior points. Both these strategies represent extreme cases; the former one is fast but unstable, while the latter one is robust but slowly converging. The former strategy is useful in the final phase of learning, while the latter one is more suitable in the initial phase. The concept of a statistical query oracle which uses an adaptive confidence factor handles the above trade-off and thereby achieves faster convergence.

In Algorithm 1, we have selected equal number of correctly classified ($n_c = q/2$) and misclassified ($n_m = q/2$) points in the resampling step. One may use other values of n_c/n_m. In that case for data sets having substantial overlap (high sparsity ratio), the choice of n_c and n_m influences the nature of the convergence curve. If more misclassified points, compared to correctly classified points, are chosen (*i.e.*, $n_c/n_m < 1$) the convergence curve is oscillatory in nature. On the other hand, choosing a larger number of correctly classified points compared to misclassified points (*i.e.*, $n_c/n_m > 1$) leads to smoother but slower convergence. ♦

So far we have used, in Chapters 2-4, classical approach for developing methodologies for data condensation, feature selection and active learning. The next two chapters (Chapters 5 and 6) emphasize on demonstrating the effectiveness of integrating different soft computing tools, e.g., fuzzy logic, artificial neural networks, rough sets and genetic algorithms for performing tasks like case (class prototypes) generation, clustering/classification, and rule generation/evaluation for mining and knowledge discovery.

Chapter 5

Rough-fuzzy Case Generation and Clustering

5.1 Introduction

Granular computing (GrC) may be regarded as a unified framework for theories, methodologies and techniques that make use of granules in the process of problem solving. A granule is a clump of objects (points), in the universe of discourse, drawn together by indistinguishability, similarity, proximity, or functionality. Granulation leads to information compression/summarization. Therefore computing with granules, rather than points, provides gain in computation time; thereby making the role of granular computing significant in data mining.

Granulation may be crisp or fuzzy, depending on whether the boundaries of granules do or do not lend themselves to precise definition. Fuzzy granulation (*f-granulation*) may be obtained using the concepts of linguistic variable, fuzzy if-then rule, and fuzzy graph [168]. Recently, rough set theory [131, 132] has become a popular mathematical framework for granular computing. While fuzzy set theory assigns to each object a grade of belongingness to represent an imprecise set, the focus of rough set theory is on the ambiguity caused by limited discernibility of objects in the domain of discourse. The key concepts in rough set theory are those of 'indiscernibility' and 'reducts'. Indiscernibility formalizes the concept of finite precision representation of objects in real life situations, and reducts represent the 'core' of an information system (both in terms of objects and features) in a granular universe. Recently, rough sets and fuzzy sets are being integrated in soft computing framework, the aim being to develop a model of uncertainty stronger than either [127]. In the present chapter we exploit the merits of the aforesaid integration for performing two tasks, namely, case generation and clustering.

A case may be defined as a contextualized piece of knowledge representing an experience that teaches a lesson fundamental to achieving goals of the system [74]. Selection and generation of cases (*i.e.*, representative class prototypes) are two important components of a case based reasoning (CBR) system. While case selection deals with selecting informative prototypes from the data, case generation concerns with construction of 'cases' that need not necessarily include any of the given data points.

Early CBR systems mainly used case selection mechanisms based on the nearest neighbor principle. These algorithms involve case pruning/growing methodologies, as exemplified by the popular IB3 algorithm [5]. A summary of the above approaches may

be found in [164]. Recently, fuzzy logic and other soft computing tools have been integrated with CBR for developing efficient methodologies and algorithms [114]. For case selection and retrieval, the role of fuzzy logic has been mainly in providing similarity measures and modeling ambiguous situations [114]. A neuro-fuzzy method for selecting cases has been proposed in [113], where a fuzzy case similarity measure is used, with repeated growing and pruning of cases, until the case base becomes stable. All the operations are performed using a connectionist model with adaptive link structure. Use of fuzzy feature vectors and neural networks for case retrieval has been studied in [90]. It may be noted that, cases (class prototypes) represent the informative and irreducible part of a problem. Rough set theory, which also deals with 'information granules' and 'reducts', is therefore a natural choice for case generation in domains which are data rich, contain uncertainties and allow tolerance for imprecision. Additionally, rough sets have the capability of handling complex objects (e.g., proofs, hierarchies, frames, rule bases); thereby strengthening further the necessity of rough-CBR systems. Some of the attempts being made in this regard are available in [142].

In the first part of this chapter, we use rough-fuzzy hybridization for designing a methodology for case generation. Each pattern (object) is represented by its fuzzy membership values with respect to three overlapping linguistic property sets 'low', 'medium' and 'high'; thereby generating a fuzzy granulation of the feature space which contains granules with ill-defined boundaries. Discernibility of the granulated objects in terms of attributes is then computed in the form of a discernibility matrix. Using rough set theory a number of decision rules are generated from the discernibility matrix. The rules represent *rough clusters* of points in the original feature space. The fuzzy membership functions corresponding to the region, modeled by a rule, are then stored as a case. A strength factor, representing the *a priori* probability (size) of the cluster, is associated with each case. In other words, each case has three components, namely, the membership functions of the fuzzy sets appearing in the reducts, the class labels and the strength factor. In the *retrieval* phase, these fuzzy membership functions are utilized to compute the similarity of the stored cases with an unknown pattern.

It may be noted that unlike most case selection schemes, the cases generated by our algorithm need not be any of the objects (patterns) encountered, rather they represent regions having dimensions equal to or less than that of the input feature space. That is, all the input features (attributes) may not be required to represent a case. This

type of variable and reduced length representation of cases results in the decrease in retrieval time. Furthermore, the proposed algorithm deals only with the information granules, not the actual data points. Because of these characteristics its significance to data mining applications is evident.

The effectiveness of the methodology is demonstrated on some real life data sets, large both in dimension and size. Cases are evaluated in terms of the classification accuracy obtained using 1-NN rule. Comparison is made with the conventional IB3 and IB4 algorithms [5], and random case selection method. The proposed methodology is found to perform better in terms of 1-NN accuracy, average number of features per case, case generation time and average case retrieval time.

The second part of this chapter describes a method for non-convex clustering using expectation maximization (EM) algorithm initialized by crude clusters which are obtained by fuzzy discretization along with rough set rule generation. As discussed in Chapter 1, clustering is an important task in several data mining applications including document retrieval, image/spatial data segmentation, market analysis [149]. Data mining applications place the following two primary requirements on clustering algorithms: scalability to large data sets (or, the issue of computation time) [16] and non-presumption of any canonical data properties like convexity.

Clustering algorithms can be grouped broadly into two categories. One is based on iterative refinement of cluster parameters, optimizing some criterion function or likelihood of some probabilistic model (e.g., k-means [149], mixture of Gaussians [28]). The second is graph-theoretic clustering, where each cluster represents a subgraph of a graph of the entire data. One of the well known graph-theoretic clustering is based on the construction of the minimal spanning tree (MST) of the data [170]. Both the approaches have their advantages and disadvantages and cannot directly be applied for data mining. While the iterative refinement schemes like k-means and expectation maximization (EM) are fast and easily scalable to large databases [16], they can only produce convex clusters and are sensitive to initialization of the parameters. The graph-theoretic methods can model arbitrary shaped clusters, but are slow and sensitive to noise. It may be noted that, the advantages of one are complementary in overcoming the limitations of the other, and vice versa.

A general method of clustering using statistical principles is to represent the probability

density function of the data as a *mixture model*, which asserts that the data is a combination of k individual component densities (commonly Gaussians), corresponding to k clusters. The task is to identify, given the data, a set of k populations in the data, and provide a model (density distribution) for each of the populations. The EM algorithm is an effective and popular technique for estimating the mixture model parameters [28]. It iteratively refines an initial cluster model to better fit the data and terminates at a solution which is locally optimal for the underlying clustering criterion [28]. Log-likelihood is used as the objective function which measures how well the model fits the data. Like other iterative refinement clustering methods, including the popular k-means algorithm, the EM algorithm is fast and its scalable versions are available [16]. An advantage of EM over k-means is that it provides a statistical model of the data and is capable of handling the associated uncertainties. However, a problem arising due to its iterative nature is convergence to a local rather than the global optima. It is sensitive to initial conditions and is not robust. To overcome the initialization problem, several methods for determining 'good' initial parameters for EM have been suggested, mainly based on subsampling, voting and two stage clustering [94]. However, most of these methods have heavy computational requirement and/or are sensitive to noise.

In our clustering algorithm, rough set theoretic logical rules are used to obtain initial approximate mixture model parameters. As in the first part of the chapter, linguistic representation of patterns is used for fuzzy granulation. The crude mixture model, after refinement through EM, leads to accurate clusters. Here, rough set theory offers a fast and robust (noise insensitive) solution to the initialization and local minima problem of iterative refinement clustering. Also the problem of choosing the number of mixtures is circumvented, since the number of Gaussian components to be used is automatically decided by rough set theory.

The problem of modeling non-convex clusters is addressed by constructing a minimal spanning tree (MST) with each Gaussian as nodes and Mahalanobis distance between them as edge weights. Since graph-theoretic clustering is performed on the Gaussian models rather than the individual data points and the number of models are much less than the data points, the computational time requirement is significantly small. A (non-convex) cluster obtained from the graph is a particular subset of all the Gaussians used to model the data.

Experiments are performed on some real life and artificially generated non-convex data sets. It is found that rough set with fuzzy discretization enhances the performance of EM algorithm both in terms of cluster quality and computational time. Integration of minimal spanning tree with rough-fuzzy initialized EM, results in further improvement of performance with a slight increase in computational time. The merits of the proposed algorithm are also demonstrated, in another part of the experiment, for the problem of segmentation of multispectral satellite images.

The organization of the chapter is as follows. Section 5.2 presents the basic features of rough set theory which are relevant to this chapter. In Section 5.3, the methodology for fuzzy granulation and linguistic representation of patterns is described. The rough-fuzzy case generation methodology is described in Section 5.4, along with experimental results and comparison. The non-convex clustering algorithm is stated in Section 5.5 together with experimental results and comparison. Application of the clustering algorithm to multispectral remote sensing image segmentation is demonstrated in Section 5.6.

5.2 Rough Sets

Let us present here some preliminaries of rough set theory which are relevant to this chapter. For details one may refer to [132] and [157].

5.2.1 Information systems

An *information system* is a pair $\mathcal{S} =< U, A >$, where U is a non-empty finite set of *objects* called the *universe* and A a non-empty finite set of *attributes* such that $a : U \rightarrow V_a$ for every $a \in A$. The set V_a is called the *value set* of a.

In many situations there is an outcome of classification that is known. This *a posteriori* knowledge is expressed by one distinguished attribute called decision attribute. Information systems of this kind are called decision systems. A *decision system* is any information system of the form $\mathcal{A} = (U, A \cup \{d\})$, where $d \notin A$ is the *decision attribute*. The elements of A are called *conditional attributes*. An information (decision) system may be represented as an *attribute-value (decision) table*, in which rows are labeled by

Table 5.1: *Hiring*: An example of a decision table

	Diploma (i)	*Experience* (e)	*French* (f)	*Reference* (r)	*Decision*
$\mathbf{x}_1$	MBA	Medium	Yes	Excellent	Accept
$\mathbf{x}_2$	MBA	Low	Yes	Neutral	Reject
$\mathbf{x}_3$	MCE	Low	Yes	Good	Reject
$\mathbf{x}_4$	MSc	High	Yes	Neutral	Accept
$\mathbf{x}_5$	MSc	Medium	Yes	Neutral	Reject
$\mathbf{x}_6$	MSc	High	Yes	Excellent	Reject
$\mathbf{x}_7$	MBA	High	No	Good	Accept
$\mathbf{x}_8$	MCE	Low	No	Excellent	Reject

objects of the universe and columns by the attributes. Table 5.1 is an example of representing a decision system $\mathcal{A}' = (U, \{Diploma,\ Experience,\ French,\ Reference\} \cup \{Decision\})$, for hiring personnel.

5.2.2 Indiscernibility and set approximation

A decision system (*i.e.*, a decision table) expresses all the knowledge available about a system. This table may be unnecessarily large because it could be redundant at least in two ways. The same or indiscernible objects may be represented several times, or some attributes may be superfluous. The notion of equivalence relation is used to tackle this problem.

With every subset of attributes $B \subseteq A$, one can easily associate an *equivalence relation* I_B on U: $I_B = \{(\mathbf{x}_1, \mathbf{x}_2) \in U : \text{for every a} \in \text{B, a}(\mathbf{x}_1) = \text{a}(\mathbf{x}_2)\}$. I_B is called *B-indiscernibility relation.* If $(\mathbf{x}_1, \mathbf{x}_2) \in I_B$, then objects $\mathbf{x}_1$ and $\mathbf{x}_2$ are indiscernible from each other by attributes B. The equivalence classes of the partition induced by the B-indiscernibility relation are denoted by $[\mathbf{x}]_B$. These are also known as *granules.* For example, in the case of the decision system represented by Table 5.1, if we consider the attribute set $B = \{Diploma,\ Experience\}$, the relation I_B defines the following partition of the universe,

$$I_B = I_{\{Diploma,\ Experience\}} = \{\{\mathbf{x}_3, \mathbf{x}_8\}, \{\mathbf{x}_4, \mathbf{x}_6\}, \{\mathbf{x}_5\}, \{\mathbf{x}_1\}, \{\mathbf{x}_2\}, \{\mathbf{x}_7\}\}.$$

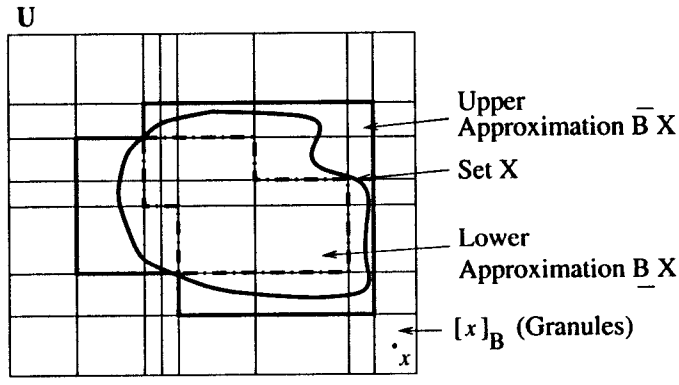


Figure 5.1: Rough representation of a set with upper and lower approximations

Here $\{x_3, x_8\}, \{x_4, x_6\}, \{x_5\}, \{x_1\}, \{x_2\}, \{x_7\}$ are the granules obtained by the relation I_B.

The partition induced by the equivalence relation I_B can be used to build new subsets of the universe. Subsets that are most often of interest have the same value of the outcome attribute *i.e.*, belong to the same class. It may happen, however, that a concept (e.g., '*Reject*' in Table 1) cannot be defined crisply using the attributes available. It is here that the notion of rough set emerges. Although we cannot delineate the concept crisply, it is possible to delineate the objects which definitely 'belong' to the concept and those which definitely 'do not belong' to the concept. These notions are formally expressed as follows.

Let $\mathcal{A} = (U, A)$ be an information system and let $B \subseteq A$ and $X \subseteq U$. We can approximate X using only the information contained in B by constructing the lower and upper approximations of X. If $X \subseteq U$, the sets $\{x \in U : [x]_B \subseteq X\}$ and $\{x \in U : [x]_B \cap X \neq \emptyset\}$, where $[x]_B$ denotes the equivalence class of the object $x \in U$ relative to I_B, are called the *B-lower* and *B-upper approximation* of X in $\mathcal{S}$ and denoted by $\underline{B}X, \overline{B}X$ respectively. The objects in $\underline{B}X$ can be certainly classified as members of X on the basis of knowledge in B, while objects in $\overline{B}X$ can only be classified as possible members of X on the basis of B. This is illustrated in Figure 5.1. Considering the decision system *Hiring* (Table 5.1), if $B = \{Diploma,\ Experience\}$ and X is the concept *Reject*, then: $\underline{B}X = \{x_2, \{x_3, x_8\}, x_5\}$ and $\overline{B}X = \{x_2, \{x_3, x_8\}, \{x_4, x_6\}, x_5\}$.

5.2.3 Reducts

Indiscernibility relation reduces the data by identifying equivalence classes, *i.e.*, objects that are indiscernible, using the available attributes. Only one element of the equivalence class is needed to represent the entire class. Reduction can also be done by keeping only those attributes that preserve the indiscernibility relation and consequently, set approximation. So one is, in effect, looking for *minimal* sets of attributes taken from the initial set A, so that the minimal sets induce the *same* partition on the domain as done by A. In other words, the essence of the information remains intact, and superfluous attributes are removed. The above sets of attributes are called *reducts.* Depending on the nature of information preserved, there may be four important categories of reducts. They are:

1. Reducts not relative to a particular case (or object) and not relative to the decision attribute. The full discernibility relation is preserved. Reducts of this type are minimal attribute subsets that enable us to discern all cases from each other, upto the same degree as the full set of attribute does.

2. Reducts not relative to a particular case (or object) but relative to the decision attribute. All regions with the same value of the generalized decision are preserved. Reducts of this type are minimal conditional attribute subsets $B \subseteq A$ that for all classes enable us to make the same classifications as the full set of attributes does.

3. Reducts relative to case (or object) $\mathbf{x}$ but not relative to the decision attribute. Reducts of this type are minimal conditional attribute subsets that enable us to discern case $\mathbf{x}$ from all other cases upto the same degree as the full set of conditional attributes does.

4. Reducts relative to case (or object) $\mathbf{x}$ and relative to the decision attribute. Our ability to discern case $\mathbf{x}$ from cases with different generalized decision than $\mathbf{x}$ is preserved. Reducts B of this type are minimal conditional attribute subsets that enable us to determine the outcome of case $\mathbf{x}$, upto the same degree as the full set of attribute does.

Reducts have been nicely characterized in [157] by *discernibility matrices* and *discernibility functions*. Consider $U = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ and $A = \{a_1, \ldots, a_p\}$ in the information system $\mathcal{S} =< U, A >$. By the discernibility matrix $\mathbf{M}(\mathcal{S})$ of $\mathcal{S}$ is meant an $n \times n$-matrix (symmetrical with empty diagonal) such that

$$c_{ij} = \{a \in A : a(\mathbf{x}_i) \neq a(\mathbf{x}_j)\}. \tag{5.1}$$

A discernibility function $f_{\mathcal{S}}$ is a function of m boolean variables $\bar{a}_1, \ldots, \bar{a}_p$ corresponding to the attributes $a_1, \ldots, a_p$ respectively and defined as follows:

$$f_{\mathcal{S}}(\bar{a}_1, \ldots, \bar{a}_p) = \bigwedge\{\bigvee(c_{ij}) : 1 \leq i, j \leq n,\ j < i,\ c_{ij} \neq \emptyset\}\ , \tag{5.2}$$

where $\bigvee(c_{ij})$ is the disjunction of all variables $\bar{a}$ with $a \in c_{ij}$. It is seen in [157] that $\{a_{i_1}, \ldots, a_{i_r}\}$ is a reduct in $\mathcal{S}$ if and only if $a_{i_1} \wedge \ldots \wedge a_{i_r}$ is a prime implicant (constituent of the disjunctive normal form) of $f_{\mathcal{S}}$.

5.2.4 Dependency rule generation

A principal task in the method of rule generation is to compute reducts relative to a particular kind of information system, the decision system. Relativized versions of discernibility matrices and functions shall be the basic tools used in the computation. *d*-reducts and *d*-discernibility matrices are used for this purpose [157]. The methodology is described below.

Let $\mathcal{S} =< U, A >$ be a decision table, with $A = C \cup d$, and d and C its sets of decision and condition attributes respectively. Let the value set of d be of cardinality M, *i.e.*, $V_d = \{d_1, d_2, \ldots, d_M\}$, representing M classes. Divide the decision table $\mathcal{S} =< U, A >$ into M tables $\mathcal{S}_i = < U_i, A_i >$, $i = 1, ..., M$, corresponding to the M decision attributes $d_1, ..., d_M$, where $U = U_1 \cup ... \cup U_M$ and $A_i = C \cup \{d_i\}$.

Let $\{\mathbf{x}_{i1}, ..., \mathbf{x}_{ir}\}$ be the set of those objects of U_i that occur in $\mathcal{S}_i, i = 1, ..., M$. Now for each d_i-reduct $B = \{b_1, ..., b_k\}$ (say), a discernibility matrix (denoted by $\mathbf{M}_{d_i}(B)$) can be derived from the d_i-discernibility matrix as follows:

$$c_{ij} = \{a \in B : a(\mathbf{x}_i) \neq a(\mathbf{x}_j)\}, \tag{5.3}$$

for $i, j = 1, ..., n$.

For each object $\mathbf{x}_j \in \mathbf{x}_{i_1}, \ldots, \mathbf{x}_{i_r}$, the discernibility function $f_{d_i}^{\mathbf{x}_j}$ is defined as

$$f_{d_i}^{\mathbf{x}_j} = \bigwedge\{\bigvee(c_{ij}) : 1 \leq i, j \leq n,\ j < i,\ c_{ij} \neq \emptyset\}\ , \tag{5.4}$$

where $\bigvee(c_{ij})$ is the disjunction of all members of c_{ij}. Then $f_{d_i}^{\mathbf{x}_j}$ is brought to its disjunctive normal form (d.n.f). One thus obtains a dependency rule $\mathbf{r}_i$, *viz.* $d_i \leftarrow P_i$, where P_i is the disjunctive normal form (d.n.f) of $f_{d_i}^{\mathbf{x}_j}, j \in i_1, \ldots, i_r$.

The dependency factor df_i for $\mathbf{r}_i$ is given by

$$df_i = \frac{card(POS_{B_i}(d_i))}{card(U_i)}\ , \tag{5.5}$$

where $POS_{B_i}(d_i) = \bigcup_{X \in I_{d_i}} \underline{B_i}(X)$, and $\underline{B_i}(X)$ is the lower approximation of X with respect to B_i. B_i is the set of condition attributes occurring in the rule $\mathbf{r}_i$: $d_i \leftarrow P_i$. $POS_{B_i}(d_i)$ is the positive region of class d_i with respect to attributes B_i, denoting the region of class d_i that can be surely described by attributes B_i. Thus, df_i measures the information about decision attributes d_i derivable from the condition attributes of a rule B_i. df_i has values in the interval $[0, 1]$, with the maximum and minimum values corresponding to complete dependence and independence of d_i on B_i respectively.

Example 1:

The methodology for rough set rule generation is illustrated here. Let us consider the *Hiring* decision system $\mathcal{A}' = (U, \{Diploma(i),\ Experience(e),\ French(f),\ Refer ence(r)\} \cup \{Decision\})$ of Table 5.1. $V_{Decision} = \{Accept, Reject\}$ is the value set of the attribute *Decision*; $V_{Decision}$ is of cardinality two. The original decision table (Table 5.1) is thus split into two decision tables $\mathcal{S}_{Accept}$ (Table 5.2(a)), and $\mathcal{S}_{Reject}$ (Table 5.2(b)). Since all the objects in each table are distinct, they could not be reduced further. Next, for each decision table the discernibility matrices $\mathbf{M}_{Accept}(C)$ and $\mathbf{M}_{Reject}(C)$ are obtained using Equation 5.3. Among them only the matrix $\mathbf{M}_{Accept}(C)$ is shown in Table 5.3, as an illustration. The discernibility function obtained from $\mathbf{M}_{Accept}(C)$ is

$$\begin{aligned} f_{Accept} &= (i \vee e \vee r) \wedge (e \vee f \vee r) \wedge (i \vee f \vee r) \\ &= (e \wedge i) \vee (e \wedge f) \vee (i \wedge f) \vee r \qquad \text{(disjunctive normal form)} \end{aligned}$$

The following dependency rules are obtained from f_{Accept}

$$
\begin{aligned}
\mathit{Accept} &\leftarrow e \wedge i \\
\mathit{Accept} &\leftarrow e \wedge f \\
\mathit{Accept} &\leftarrow i \wedge f \\
\mathit{Accept} &\leftarrow r
\end{aligned}
$$

Table 5.2: Two decision tables obtained by splitting the *Hiring* table $\mathcal{S}$ (Table 5.1)

(a) $\mathcal{S}_{Accept}$

	i	e	f	r	*Decision*
$\mathbf{x}_1$	MBA	Medium	Yes	Excellent	Accept
$\mathbf{x}_4$	MSc	High	Yes	Neutral	Accept
$\mathbf{x}_7$	MBA	High	No	Good	Accept

(b) $\mathcal{S}_{Reject}$

	i	e	f	r	*Decision*
$\mathbf{x}_2$	MBA	Low	Yes	Neutral	Reject
$\mathbf{x}_3$	MCE	Low	Yes	Good	Reject
$\mathbf{x}_5$	MSc	Medium	Yes	Neutral	Reject
$\mathbf{x}_6$	MSc	High	Yes	Excellent	Reject
$\mathbf{x}_8$	MCE	Low	No	Excellent	Reject

Table 5.3: Discernibility matrix $\mathbf{M}_{Accept}$ for the split *Hiring* decision table $\mathcal{S}_{Accept}$ (Table 5.2(a))

Objects	$\mathbf{x}_1$	$\mathbf{x}_4$	$\mathbf{x}_7$
$\mathbf{x}_1$		i, e, r	e, f, r
$\mathbf{x}_4$			i, f, r
$\mathbf{x}_7$			

5.3 Linguistic Representation of Patterns and Fuzzy Granulation

As is evident from the previous section, rough set theory deals with a set of objects in a granular universe. In the present section we describe a way of obtaining the granular feature space using fuzzy linguistic representation of patterns. Only the case of numeric features is mentioned here. (Features in descriptive and set forms can also be handled in this framework.) The details of the methodologies involved may be found in [122, 123].

Let a pattern (object) $\mathbf{F}$ be represented by p numeric features (attributes), *i.e.*, $\mathbf{F} = [\mathrm{F}_1, \mathrm{F}_2, \ldots, \mathrm{F}_\mathrm{p}]$. Note that, $\mathbf{F}$ is equivalent to a p-dimensional feature vector $\mathbf{x}$. Each feature is described in terms of its fuzzy membership values corresponding to three linguistic fuzzy sets, namely *low* (L), *medium* (M) and *high* (H). Thus a p-dimensional pattern vector is represented as a $3p$-dimensional vector [122, 123]

$$\begin{aligned}\mathbf{F} \;=\; & [\mu^1_{low}(F_1), \mu^1_{medium}(F_1), \mu^1_{high}(F_1); \mu^2_{low}(F_2), \mu^2_{medium}(F_2), \mu^2_{high}(F_2); \\ & \ldots; \mu^p_{low}(F_p), \mu^p_{medium}(F_p), \mu^p_{high}(F_p)] \end{aligned} \tag{5.6}$$

where $\mu^j_{low}(.), \mu^j_{medium}(.)$ and $\mu^j_{high}(.)$ indicate the membership values of (.) to the fuzzy sets *low, medium* and *high* along feature axis j. $\mu(.) \in [0, 1]$.

For each input feature F_j, the fuzzy sets *low, medium* and *high* are characterized individually by a π-membership function whose form is [166]

$$\mu(F_j) = \pi(F_j; c, \lambda) = \begin{cases} 2(1 - \frac{|F_j - c|}{\lambda})^2, & \text{for } \frac{\lambda}{2} \leq |F_j - c| \leq \lambda \\ 1 - 2(\frac{|F_j - c|}{\lambda})^2, & \text{for } 0 \leq |F_j - c| \leq \frac{\lambda}{2} \\ 0\ , & \text{otherwise}\ , \end{cases} \tag{5.7}$$

where $\lambda(> 0)$ is the radius of the $\pi-$function with c as the central point. For each of the fuzzy sets *low, medium* and *high*, λ and c take different values. These values are chosen so that the membership functions for these three fuzzy sets have overlapping nature (intersecting at membership value 0.5), as shown in Figure 5.2.

Let us now explain the procedure for selecting the centers (c) and radii (λ) of the overlapping $\pi-$functions. Let m_j be the mean of the pattern points along j^{th} axis. Then m_{j_l} and m_{j_h} are defined as the mean (along j^{th} axis) of the pattern points

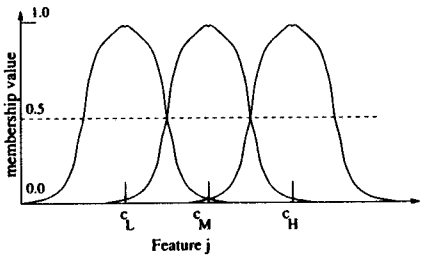


Figure 5.2: $\pi-$Membership functions for linguistic fuzzy sets *low* (L), *medium* (M) and *high* (H) for each feature axis.

having co-ordinate values in the range $[F_{j_{min}}, m_j)$ and $(m_j, F_{j_{max}}]$ respectively, where $F_{j_{max}}$ and $F_{j_{min}}$ denote the upper and lower bounds of the dynamic range of feature F_j. The centers and the radii of the three π-functions are defined as

$$\begin{aligned} c_{low(F_j)} &= m_{j_l} \\ c_{medium(F_j)} &= m_j \\ c_{high(F_j)} &= m_{j_h} \\ \lambda_{low(F_j)} &= c_{medium(F_j)} - c_{low(F_j)} \\ \lambda_{high(F_j)} &= c_{high(F_j)} - c_{medium(F_j)} \\ \lambda_{medium(F_j)} &= 0.5\ (c_{high(F_j)} - c_{low(F_j)}). \end{aligned} \tag{5.8}$$

Here we take into account the distribution of the pattern points along each feature axis while choosing the corresponding centers and radii of the linguistic fuzzy sets.

The aforesaid three overlapping functions along each axis generate the fuzzy granulated feature space in p-dimension. The granulated space contains 3^p granules with fuzzy boundaries among them. Here the granules (clumps of similar objects or patterns) are attributed by the three fuzzy linguistic values 'low', 'medium' and 'high'. The degree of belongingness of a pattern to a granule (or the degree of possessing a property low, medium or high by a pattern) is determined by the corresponding membership function.

Furthermore, if one wishes to obtain crisp granules (or crisp subsets), α-cut, $0 < \alpha < 1$, [166] of these fuzzy sets may be used. (α-cut of a fuzzy set is a crisp set of points for which membership value is greater than or equal to α.) Note that the concept of fuzzy granulation has been explained earlier in different ways and effectively used in rough-fuzzy framework [137, 138, 168].

Note that we have used three fuzzy property sets 'low', 'medium' and 'high'. One may consider hedges like 'very', 'more or less' to generate more granules *i.e.*, finer granulated space. However, this will enhance the computational requirement for both case generation and retrieval.

5.4 Rough-fuzzy Case Generation Methodology [119, 120]

Here we describe a methodology for case generation on the fuzzy granulated space as obtained in the previous section. This involves two tasks, namely, (a) generation of fuzzy rules using rough set theory, and (b) mapping the rules to cases. Since rough set theory operates on crisp granules (*i.e.*, subsets of the universe) we need to convert the fuzzy membership values of the patterns to binary ones or, to convert the fuzzy membership functions to binary functions in order to represent the crisp granules (subsets) for application of rough set theory. This conversion can be done using an α-cut. This is illustrated in Figure 5.3, where 0.5-cut is used to obtain $3^2 = 9$ crisp granules (subsets) of the 2-dimensional feature space from the linguistic representation of the input features.

The schematic diagram for the generation of case is shown in Figure 5.4. One may note that, the inputs to the case generation process are fuzzy membership functions, the output 'cases' are also fuzzy membership functions, but the intermediate rough set theoretic processing is performed on binary functions representing crisp sets (granules). For example, the inputs to Block 2 are fuzzy membership functions. Its outputs are binary membership functions which are used for rough processing in Block 3 and Block 4. Finally, the outputs of Block 4, representing cases, are again fuzzy membership functions. Each task is discussed below.

5.4.1 Thresholding and rule generation

Consider the $3p$ fuzzy membership values of a p dimensional pattern $\mathbf{F}_i$. Then select only those attributes having values greater than or equal to Th ($= 0.5$, say). In other words, we obtain a 0.5-cut of all the fuzzy sets to obtain binary membership values

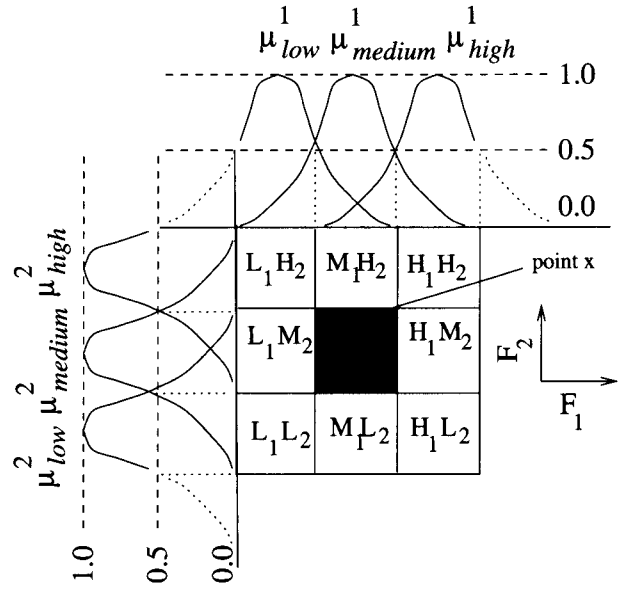


Figure 5.3: Generation of crisp granules from linguistic (fuzzy) representation of the features F_1 and F_2. Dark region (M_1, M_2) indicates a crisp granule obtained by 0.5-cuts on the μ^1_{medium} and μ^2_{medium} functions

corresponding to the sets *low, medium* and *high.*

For example, consider the point **x** in Figure 5.3. Its $3p$ dimensional fuzzy representation is $\mathbf{F} = [0.4, 0.7, 0.1, 0.2, 0.8, 0.4]$. After binarization it becomes $\mathbf{F}_b = [0, 1, 0, 0, 1, 0]$, which denotes the crisp granule (or subset) at the center of the 3×3 granulated space.

After the binary membership values are obtained for all the patterns we constitute the decision table for rough set rule generation. As the method considers multiple objects in a class a separate $n_k \times 3p$-dimensional attribute-value decision table is generated for each class d_k (where n_k indicates the number of objects in d_k). Let there be m sets $O_1, ..., O_m$ of objects in the table having identical attribute values, and $card(O_i) = n_{k_i}, i = 1, ..., m$, such that $n_{k_1} \geq \ldots \geq n_{k_m}$ and $\sum_{i=1}^{m} n_{k_i} = n_k$. The attribute-value table can now be represented as an $m \times 3p$ array. Let $n_{k'_1}, n_{k'_2}, \ldots, n_{k'_m}$ denote the distinct elements among $n_{k_1}, \ldots, n_{k_m}$ such that $n_{k'_1} > n_{k'_2} > \ldots > n_{k'_m}$. Let a heuristic threshold function be defined as [10]

$$Tr = \left\lceil \frac{\sum_{i=1}^{m} \frac{1}{n_{k'_i} - n_{k'_{i+1}}}}{Th} \right\rceil, \tag{5.9}$$

so that all entries having frequency less than Tr are eliminated from the table, resulting

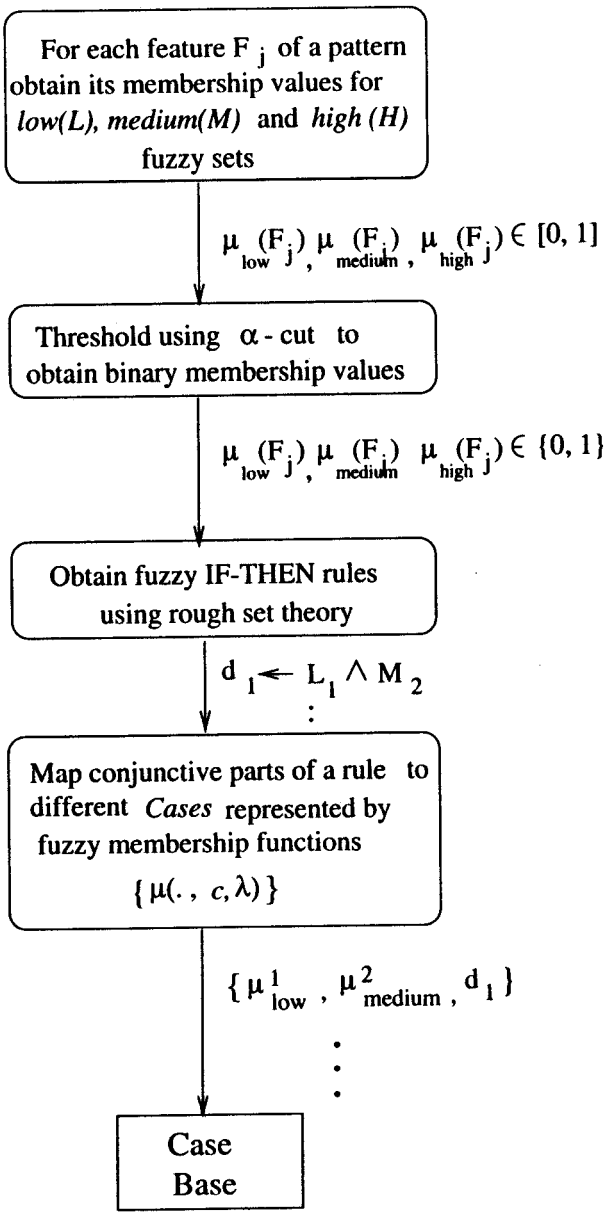


Figure 5.4: Schematic diagram of rough-fuzzy case generation

in the reduced attribute-value table. The main motive of introducing this threshold function lies in reducing the size of the case base and in eliminating the noisy patterns. From the reduced attribute-value table, thus obtained, rough dependency rules are generated using the methodology described in Section 5.2.4.

5.4.2 Mapping dependency rules to cases

We now describe the technique for mapping rough dependency rules to cases. The algorithm is based on the observation that each dependency rule (having frequency above some threshold) represent a cluster in the feature space. It may be noted that only a subset of features appears in each of the rules, this indicates the fact that the entire feature set is not always necessary to characterize a cluster. A *case* is constructed out of a *dependency rule* in the following manner:

1. Consider the antecedent part of a rule; Split it into atomic formulas containing only conjunction of literals.
2. For each atomic formula, generate a case - containing the centers and radii of the fuzzy linguistic variables ('low', 'medium' and 'high') which are present in the formula. (Thus, multiple cases may be generated from a rule.)
3. Associate with each such case generated, the precedent part of the rule and the case strength equal to the dependency factor of the rule (Equation 5.5). The strength factor reflect the size of the corresponding cluster and the significance of the case

Thus a case has the following structure:

case{
Feature i: $fuzzset_i$: center, radius;
.....
Class k
Strength
}

where $fuzzset$ denote the fuzzy sets 'low', 'medium' or 'high'. The method is explained below with the help of an example.

One may note that while 0.5-cut is used to convert the $3n$ fuzzy membership functions of a pattern to binary ones for rough set rule generation (Section 5.4.1), the original fuzzy functions are retained in order to use them in for representing the generated cases (Section 5.4.2). These are also illustrated in Figure 5.4, where the outputs μ^1_{low}, μ^2_{medium} are fuzzy sets (membership functions).

Example 2:

Consider a data having two features F_1, F_2 and two classes as shown in Figure 5.5. The granulated feature space has $3^2 = 9$ granules. These granules are characterized by three membership functions along each axis, and have ill-defined boundaries. Let the following two dependency rules be obtained from the reduced attribute table:

$$class_1 \leftarrow L_1 \wedge H_2,\ df = 0.5$$

$$class_2 \leftarrow H_1 \wedge L_2,\ df = 0.4$$

Let the parameters of the fuzzy sets 'low', 'medium' and 'high' be as follows:
Feature 1: c_L=0.1, λ_L=0.5, c_M=0.5, λ_M=0.7, c_H=0.7, λ_H=0.4.
Feature 2: c_L=0.2, λ_L=0.5, c_M=0.4, λ_M=0.7, c_H=0.9, λ_H=0.5.

Therefore, we have the following two cases:

case 1{
Feature No: 1, *fuzzset*(L): center=0.1, radius=0.5
Feature No: 2, *fuzzset* (H): center=0.9, radius=0.5
Class=1
Strength=0.5
}

case 2{
Feature No: 1, *fuzzset* (H): center=0.7, radius=0.4
Feature No: 2, *fuzzset* (L): center=0.2, radius=0.5
Class=2
Strength=0.4
}

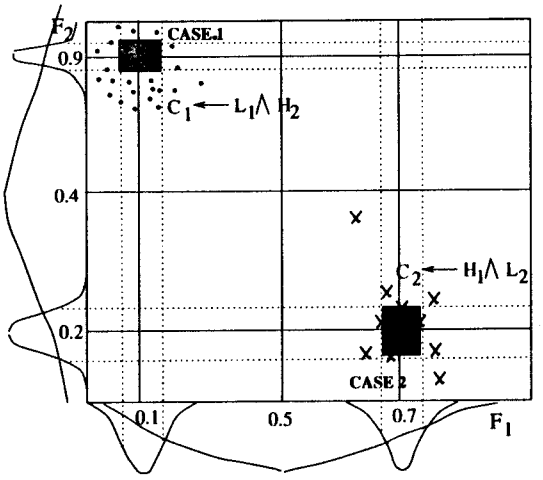


Figure 5.5: Rough-fuzzy case generation for a two dimensional data

5.4.3 Case retrieval

Each case thus obtained in the previous section is a collection of fuzzy sets $\{fuzzsets\}$ described by a set of one dimensional π-membership functions with different c and λ values. To compute the similarity of an unknown pattern $\mathbf{F}$ (of dimension p) to a case $\mathbf{p}$ (of variable dimension p_m, $p_m \leq p$), we use

$$sim(\mathbf{F}, \mathbf{p}) = \sqrt{\frac{1}{p_m} \sum_{j=1}^{p_m} \left(\mu^j_{fuzzset}(F_j)\right)^2} \tag{5.10}$$

where $\mu^j_{fuzzset}(F_j)$ is the degree of belongingness of the j^{th} component of $\mathbf{F}$ to $fuzzset$ representing the case $\mathbf{p}$. When $\mu^j = 1$ for all j, $sim(\mathbf{F}, \mathbf{p}) = 1$ (maximum) and when $\mu^j = 0$ for all j, $sim(\mathbf{F}, \mathbf{p}) = 0$ (minimum). Therefore Equation 5.10 provides a collective measure computed over the degree of similarity of each component of the unknown pattern with the corresponding one of a stored case. Higher the value of the similarity, the closer is the pattern $\mathbf{F}$ to the case $\mathbf{p}$. Note that fuzzy membership functions in Equation 5.10 take care of the distribution of points within a granule; thereby providing a better similarity measure between $\mathbf{F}$ and $\mathbf{p}$ than the conventional Euclidean distance between two points.

For classifying (or to provide a label to) an unknown pattern, the case closest to the pattern, in terms of $sim(\mathbf{F}, \mathbf{p})$ measure, is retrieved and its class label is assigned to that pattern. Ties are resolved using the parameter *Case Strength*.

5.4.4 Results and comparison

Experiments are performed on three real life data sets, namely, Iris data, Forest cover type data and Multiple features data sets. The last two data sets have large number of samples and features. The characteristics of the data sets are described in Appendix A.

The cases generated using the rough-fuzzy methodology are compared with those obtained using the following three case selection methodologies:

(i) Instance based learning algorithm, IB3 [5],

(ii) Instance based learning algorithm with reduced number of features, IB4 [2]. The feature weighting is learned by random hill climbing in IB4. A specified number of features having high weights is selected, and

(iii) Random case selection.

Comparison is made on the basis of the following:

(a) 1-NN classification accuracy using the generated/selected cases. For all the data 10% of the samples are used as training set for case generation and 90% of the samples are used as test set. Mean of the accuracy computed over 10 such random split is reported.

(b) Number of cases stored in the case base.

(c) Total CPU time required (on a DEC Alpha 400 MHz Workstation) for case generation.

(d) Average CPU time required (on a DEC Alpha 400 MHz Workstation) to retrieve a case for the patterns in test set.

For the purpose of illustration, we present the rough dependency rules and the corresponding generated cases in Tables 5.4 and 5.5 respectively for the Iris data, as an example. Comparative results of the rough-fuzzy case generation methodology with other case selection algorithms are presented in Tables 5.6, 5.7 and 5.8 for the Iris, Forest cover type and Multiple features data respectively in terms of number of cases, 1-NN classification accuracy, average number of features per case (p_{avg}), and case generation (t_{gen}) and retrieval (t_{ret}) times. It can be seen from the tables that the cases obtained using the proposed rough-fuzzy methodology are much superior to random selection method and IB4, and close to IB3 in terms of classification accuracy. (The superiority

over random selection and IB4 was found to be statistically significant, when tested using the statistics described in Section 2.5.1.) The method requires significantly less time compared to IB3 and IB4 for case generation. As is seen from the tables, the average number of features stored per case (p_{avg}) by the rough-fuzzy technique is much less than the original data dimension (p). As a consequence, the average retrieval time required is very low. IB4 also stores cases with a reduced number of features and has a low retrieval time, but its accuracy is much less compared to the proposed method. Moreover, all the cases involve equal number of features, unlike ours.

Table 5.4: Rough dependency rules for the Iris data

$$
\begin{array}{lcll}
C_1 & \leftarrow & L_1 \wedge H_2 \wedge L_3 & df = 0.81 \\
C_2 & \leftarrow & M_1 \wedge L_2 \wedge M_4 & df = 0.81 \\
C_3 & \leftarrow & H_1 \wedge H_4 & df = 0.77
\end{array}
$$

Table 5.5: Cases generated for the Iris data

case 1{
Feature No: 1, *fuzzset*(L): center=5.19, radius=0.65
Feature No: 2, *fuzzset* (H): center=3.43, radius=0.37
Feature No: 3, *fuzzset* (L): center=0.37, radius=0.82
Class=1
Strength=0.81
}
case 2{
Feature No: 1, *fuzzset*(M): center=3.05, radius=0.34
Feature No: 2, *fuzzset* (L): center=1.70, radius=2.05
Feature No: 4, *fuzzset* (M): center=1.20, radius=0.68
Class=2
Strength=0.81
}
case 3{
Feature No: 1, *fuzzset*(H): center=6.58, radius=0.74
Feature No: 4, *fuzzset* (H): center=1.74, radius=0.54
Class=3
Strength=0.77
}

Table 5.6: Comparison of case selection algorithms for Iris data

Algorithm	No. of Cases	p_{avg}	Classification accuracy (%)	t_{gen} (sec)	t_{ret} (sec)
Rough-fuzzy	3	2.67	98.17	0.2	0.005
IB3	3	4	98.00	2.50	0.01
IB4	3	4	90.01	4.01	0.01
Random	3	4	87.19	0.01	0.01

Table 5.7: Comparison of case selection algorithms for Forest cover type data

Algorithm	No. of Cases	p_{avg}	Classification accuracy (%)	t_{gen} (sec)	t_{ret} (sec)
Rough-fuzzy	542	4.10	67.01	244	4.4
IB3	545	10	66.88	4055	52.0
IB4	545	4	50.05	7021	4.5
Random	545	10	41.02	17	52.0

Table 5.8: Comparison of case selection Algorithms for Multiple features data

Algorithm	No. of Cases	p_{avg}	Classification accuracy (%)	t_{gen} (sec)	t_{ret} (sec)
Rough-fuzzy	50	20.87	77.01	1096	10.05
IB3	52	649	78.99	4112	507
IB4	52	21	41.00	8009	20.02
Random	50	649	50.02	8.01	507

5.5 Clustering [121]

In Section 5.4 we have demonstrated how fuzzy granulation along with rough set theoretic rule generation can be used to efficiently generate cases (class prototypes). Note

that, these logical rules correspond to different important regions of the feature space, and represent crude clusters. We now exploit the above capability of rough-fuzzy computing for fast clustering via the expectation maximization (EM) algorithm and minimal spanning tree (MST).

5.5.1 Mixture model estimation via the EM algorithm

The mixture model approximates the data distribution by fitting k component density functions f_h, $h = 1, \ldots, k$ to a data set D having n patterns and p features. Let $\mathbf{x} \in D$ be a pattern, the mixture model probability density function evaluated at $\mathbf{x}$ is:

$$\mathrm{p}(\mathbf{x}) = \sum_{h=1}^{k} w_h f_h(\mathbf{x}|\phi_h). \tag{5.11}$$

The weights w_h represent the fraction of data points belonging to model h, and they sum to one ($\sum_{h=1}^{k} w_h = 1$). The functions $f_h(\mathbf{x}|\phi_h)$, $h = 1, \ldots, k$ are the component density functions modeling the points of the hth cluster. ϕ_h represents the specific parameters used to compute the value of f_h (e.g., for a Gaussian component density function, ϕ_h is the mean and covariance matrix).

For continuous data, Gaussian distribution is the most common choice for component density function. This is motivated by a result from density estimation theory stating that any distribution can be effectively approximated by a mixture of Gaussians with weights w_h. The multivariate Gaussian with p-dimensional mean vector μ_h and $p \times p$ covariance matrix Σ_h is:

$$f_h(\mathbf{x}|\mu_h, \Sigma_h) = \frac{1}{\sqrt{(2\pi)^p |\Sigma_h|}} exp\left(-\frac{1}{2}(\mathbf{x} - \mu_h)^T (\Sigma_h)^{-1}(\mathbf{x} - \mu_h)\right) \tag{5.12}$$

The quality of a given set of parameters $\Phi = \{(w_h, \mu_h, \Sigma_h), h = 1, \ldots, k\}$ is determined by how well the corresponding mixture model fits the data. This is quantified by the log-likelihood of the data, given the mixture model:

$$L(\Phi) = \sum_{\mathbf{x} \in D} \log\left(\sum_{h=1}^{k} w_h f_h(\mathbf{x}|\mu_h, \Sigma_h)\right). \tag{5.13}$$

The EM begins with an initial estimation of Φ and iteratively updates it such that $L(\Phi)$ is non-decreasing. .We next outline the EM algorithm.

EM Algorithm:

Given a data set D with n patterns and p continuous features, a stopping tolerance $\epsilon > 0$ and mixture parameters Φ^j at iteration j, compute Φ^{j+1} at iteration $j+1$ as follows:

Step 1. *(E-Step)* For pattern $\mathbf{x} \in D$:
Compute the membership probability $w_h(\mathbf{x})$ of $\mathbf{x}$ in each cluster $h = 1, \ldots, k$:

$$w_h^j(\mathbf{x}) = \frac{w_h^j f_h(\mathbf{x}|\mu_h^j, \Sigma_h^j)}{\sum_i w_i^j f_i(\mathbf{x}|\mu_i^j, \Sigma_i^j)}.$$

Step 2. *(M-Step)* Update mixture model parameters:

$$w_h^{j+1} = \sum_{\mathbf{x} \in D} w_h^j(\mathbf{x}),$$

$$\mu_h^{j+1} = \frac{\sum_{\mathbf{x} \in D} w_h^j(\mathbf{x})\mathbf{x}}{\sum_{\mathbf{x} \in D} w_h^j(\mathbf{x})},$$

$$\Sigma_h^{j+1} = \frac{\sum_{\mathbf{x} \in D} w_h^j(\mathbf{x}) \left(\mathbf{x} - \mu_h^{j+1}\right) \left(\mathbf{x} - \mu_h^{j+1}\right)^T}{\sum_{\mathbf{x} \in D} w_h^j(\mathbf{x})}, \quad h = 1, \ldots, k.$$

Stopping Criterion: If $|L(\Phi^j) - L(\Phi^{j+1})| \leq \epsilon$, Stop. Else set $j \leftarrow j+1$ and Go To Step 1. $L(\Phi)$ is as given in Equation 5.13.

5.5.2 Rough set initialization of mixture parameters

In this section we describe the methodology for obtaining crude initial values of the parameters (Φ) of the mixture of Gaussians used to model the data. The parameters are refined further using EM algorithm described in the previous section. The methodology is based on the observation that 'reducts' obtained using rough set theory represent crude clusters in the feature space.

Reducts are computed using the methodology for fuzzy granulation and rule generation described in Sections 5.3 and 5.2.4. Note that, case generation (studied in Section 5.4) is a supervised task while clustering involves unsupervised data analysis. Hence, unlike Section 5.4.1, where decision relative reducts are used, here we use reducts which are

not relative to decision attributes. In addition a 'support factor' is defined to measure the strength of a reduct.

Support factor sf_i for the rule $\mathbf{r}_i$ is defined as

$$sf_i = \frac{n_{k_i}}{\sum_{i=1}^{r} n_{k_i}}, \tag{5.14}$$

where $n_{k_i}, i = 1, \ldots, r$ are the cardinality of the sets O_i of identical objects belonging to the reduced attribute value table.

5.5.3 Mapping reducts to mixture parameters

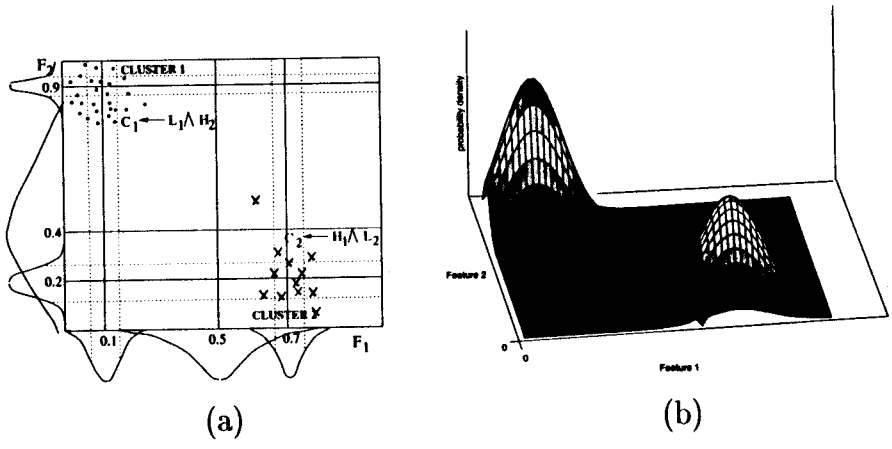
The mixture model parameters consists of the number of component Gaussian density functions (k) and weights (w_h), means (μ_h) and variances (Σ_h) of the components. We describe below the methodology for obtaining them.

1. Number of Gaussians (k): Consider the antecedent part of a rule $\mathbf{r}_i$; Split it into atomic formulas containing only conjunction of literals. For each such atomic formula, assign a component Gaussian. Let the number of such formula be k.

2. Component weights (w_h): Weight of each Gaussian is set equal to the normalized support factor sf_i (obtained using Equation 5.14) of the rule ($\mathbf{r}_i$) from which it is derived, $w_h = \frac{sf_i}{\sum_{i=1}^{k} sf_i}$.

3. Means (μ_h): An atomic formula consists of conjunction of a number of literals. The literals are linguistic fuzzy sets 'low', 'medium' and 'high' along some feature axes. The component of the mean vector along that feature is set equal to the center (c) of the π-membership function of the corresponding fuzzy linguistic set. Note that all features do not appear in a formula, implying those features are not necessary to characterize the corresponding cluster. The component of the mean vector along those features which do not appear are set to the mean of the entire data along those features.

4. Variances (Σ_h): A diagonal covariance matrix is considered for each component Gaussian. As in the case of means, the variance for feature j is set equal to radius λ of the corresponding fuzzy linguistic set. For those features not appearing in a formula the variance is set to small random value.



(a) (b)

Figure 5.6: Rough-fuzzy generation of crude clusters for a two dimensional data (a) data distribution and rough set rules, (b) probability density function for the initial mixture model.

Example:

Consider the following two reducts obtained from a reduced attribute value table of a data having two dimensions F_1 and F_2. The example is illustrated in Figure 5.6.

$$cluster_1 \leftarrow L_1 \wedge H_2,\ sf_1 = 0.50$$

$$cluster_2 \leftarrow H_1 \wedge L_2,\ sf_2 = 0.40$$

Let the parameters of the fuzzy linguistic sets 'low', 'medium' and 'high' be as follows:
Feature 1: c_L=0.1, λ_L=0.5, c_M=0.5, λ_M=0.7, c_H=0.7, λ_H=0.4.
Feature 2: c_L=0.2, λ_L=0.5, c_M=0.4, λ_M=0.7, c_H=0.9, λ_H=0.5.

Then we have two component Gaussians with parameters as follows:

$w_1 = 0.56$, $\mu_1 = [0.1, 0.9]$ and $\Sigma_1 = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$

$w_2 = 0.44$, $\mu_2 = [0.7, 0.2]$ and $\Sigma_2 = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$ ♦

We summarize below all the steps for rough set initialization of mixture models.

1. Represent each pattern in terms of its membership to fuzzy linguistic sets *low*, *medium* and *high* along each axis. Thus an p dimensional pattern is now represented by a $3p$-dimensional vector.

2. Threshold each $3p$-dimensional vector containing fuzzy membership values to obtain $3p$-dimensional binary vector. Retain only those vectors which are distinct and appear with frequency above a threshold.

3. Construct an attribute-value table from the reduced set of binary vectors.

4. Construct discernibility matrix from the attribute value table. Generate discernibility functions (rules) for each object in the matrix. Consider atomic formula of the rules which are conjunction of literals (linguistic variables 'low', 'medium' and 'high', in this case)

5. Map each atomic formula to parameters w_h, μ_h and Σ_h of corresponding component Gaussian density functions.

5.5.4 Graph-theoretic clustering of Gaussian components

In this section we describe the methodology for obtaining the final clusters from the Gaussian components used to represent the data. A minimal spanning tree (MST) based approach is adopted for this purpose. The MST is a graph that connects a data set of N points so that a complete 'tree' of N-1 edges is built. (A tree is a connected graph without cycles.) The tree is 'minimal' when the total length of the edges is the minimum necessary to connect all the points. A MST may be constructed using either Kruskal's or Prim's algorithm. Desired number of clusters of points may be obtained from a MST by deleting the edges having highest weights. For example for the set of 9 points {A, B, C, D. E, F, G, H, I} illustrated in Figure 5.7, two clusters can be obtained by deleting the edge CD having highest weight 6. The two subgraphs represent the clusters. It may be mentioned that arbitrary shaped clusters may be obtained using the above algorithm.

Instead of using individual points, we construct a MST whose vertices are the Gaussian components of the mixture model and the edge weights are the Mahalanobis distance (D_M) between them defined as:

$$D_M^2 = (\mu_1 - \mu_2)^T(\Sigma_1 + \Sigma_2)^{-1}(\mu_1 - \mu_2) \tag{5.15}$$

where μ_1, μ_2 and Σ_1, Σ_2 are the means and variances of the pair of Gaussians. To obtain k clusters, $k-1$ edges having the highest weights are deleted, and components

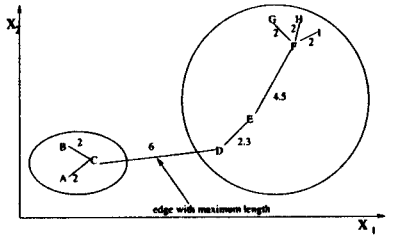


Figure 5.7: Using minimal spanning tree to form clusters

belonging to a single connected subgraph after deletion are considered to represent a single cluster.

Note that each cluster obtained as above is a mixture model in itself. The number of its component Gaussians being equal to the number of vertices of the corresponding subgraph. For assigning a point ($\mathbf{x}$) to a cluster, probability of belongingness of $\mathbf{x}$ to each of the clusters (sub-mixture models) is computed using Equation 5.11, and the cluster giving the highest probability $p(\mathbf{x})$ is assigned to $\mathbf{x}$, *i.e.*, we follow the Bayesian classification rule.

5.5.5 Results and comparison

Experiments are performed on two real life data sets (Forest cover type and Multiple features) with large number of samples and dimension. An artificial non-convex data set (Pat) is also considered for the convenience of demonstrating some features of the algorithm along with visualization of the performance. The data sets are described in Appendix A.

The clustering results of the proposed methodology are compared with those obtained using -

1. k-means algorithm with random initialization (KM).

2. k-means algorithm with rough set initialization (of centers) and graph-theoretic clustering (RKMG).

3. EM algorithm with random initialization and graph-theoretic clustering (EMG).

4. EM algorithm with means initialized with the output of k-means algorithm and with graph-theoretic clustering (KEMG).

5. BIRCH [171], a clustering algorithm suitable for large data sets.

Among the algorithms mentioned above, methods 2, 3 and 4 have the capability for obtaining non-convex clusters, while method 1 can obtain convex clusters only. It may be mentioned that, in the proposed algorithm, we use EM algorithm with rough set initialization and graph-theoretic clustering. For the purpose of comparison, in addition to rough set theoretic initialization, we have also considered EM algorithms with random initialization (method 3) and another popular method for initialization (method 4). Besides these, to demonstrate the effect of rough set theoretic initialization on another hybrid iterative refinement-graph theoretic clustering method, we consider method 2, which is the k-means algorithm with graph theoretic clustering. We could not present the comparisons with purely graph-theoretic techniques (*i.e.*, on the original data) as they require infeasibly large time for the data sets used.

Comparison is performed on the basis of cluster quality index β [116] and CPU time. CPU time is obtained on an Alpha 400 MHz workstation. β is defined as [116]:

$$\beta = \frac{\sum_{i=1}^{k}\sum_{j=1}^{n_i}(X_{ij}-\bar{X})^T(X_{ij}-\bar{X})}{\sum_{i=1}^{k}\sum_{j=1}^{n_i}(X_{ij}-\bar{X}_i)^T(X_{ij}-\bar{X}_i)} \tag{5.16}$$

where n_i is the number of points in the ith ($i = 1,\ldots,k$) cluster, X_{ij} is the feature vector of the jth pattern ($j = 1,\ldots,n_i$) in cluster i, $\bar{X}_i$ the mean of n_i patterns of the ith cluster, n is the total number of patterns, and $\bar{X}$ is the mean value of the entire set of patterns. Note that β is nothing but the ratio of the total variation and within-cluster variation. This type of measure is widely used for feature selection and cluster analysis [116]. For a given data and k (number of clusters) value, the higher the homogeneity within the clustered regions, higher would be the β value.

For the purpose of visualization of the partitioning, and illustration of several characteristics of the algorithm, we first present the results on the artificial Pat data set which is of smaller dimension (=2). The non-convex character of the data is shown in Figure 5.8. The reducts obtained using rough set theory, and the parameters of the corresponding four Gaussians are as follows:

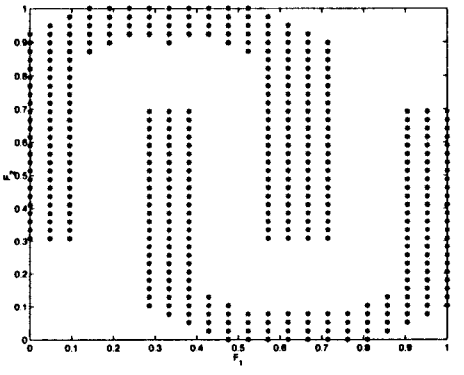


Figure 5.8: Scatter plot of the artificial data Pat

$$cluster_1 \leftarrow L_1 \wedge M_2; \quad w_1 = 0.15,\ \mu_1 = [0.223, 0.511],\ \Sigma_1 = \begin{bmatrix} 0.276 & 0 \\ 0 & 0.240 \end{bmatrix}$$

$$cluster_2 \leftarrow H_1 \wedge M_2; \quad w_2 = 0.16,\ \mu_2 = [0.753, 0.511],\ \Sigma_2 = \begin{bmatrix} 0.233 & 0 \\ 0 & 0.240 \end{bmatrix}$$

$$cluster_3 \leftarrow M_1 \wedge H_2; \quad w_3 = 0.35,\ \mu_3 = [0.499, 0.744],\ \Sigma_3 = \begin{bmatrix} 0.265 & 0 \\ 0 & 0.233 \end{bmatrix}$$

$$cluster_4 \leftarrow M_1 \wedge L_2; \quad w_4 = 0.34,\ \mu_4 = [0.499, 0.263],\ \Sigma_4 = \begin{bmatrix} 0.265 & 0 \\ 0 & 0.248 \end{bmatrix}$$

The distribution of points belonging to each component Gaussian, obtained after refining the parameters using EM, is plotted in Figure 5.9. These are indicated by symbols: +, o, $\diamond$, and $\triangle$. The variation of log-likelihood with EM iteration is presented in Figure 5.10 for both random initialization and rough set initialization. It is seen that for rough set initialization log-likelihood attains a higher value at the start of EM. The final clusters (two in number) obtained by our method after graph-theoretic partitioning of the Gaussians are shown in Figure 5.11(a). The algorithm is seen to produce the same natural non-convex partitions, as in the original data. It may be noted that the conventional k-means algorithm, which is capable of generating convex clusters efficiently, fails to do so (Figure 5.11(b)), as expected.

Table 5.9 provides comparative results (in terms of β and CPU time) of the proposed algorithm with other four, as mentioned before, for three different data sets. It is seen that the proposed methodology produces clusters having the highest β value for all the cases. Note that, since no training/test set selection is involved, the concept of statistical significance is not applicable here. The CPU time required is less than that

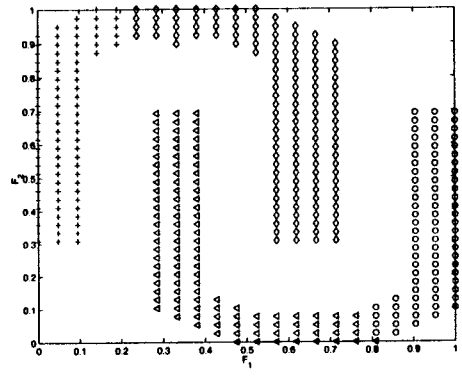


Figure 5.9: Scatter plot of points belonging to four different component Gaussians for the Pat data. Each Gaussian is represented by a separate symbol (+, o, $\diamond$ and Δ).

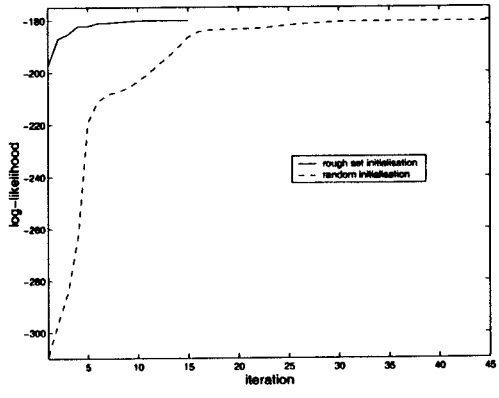
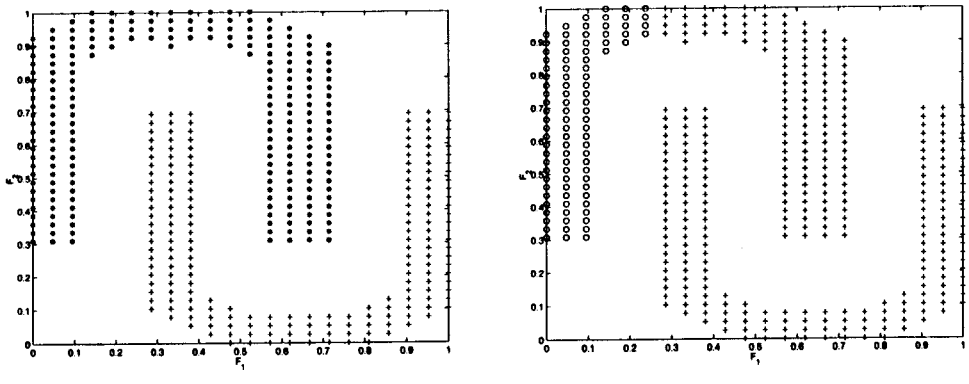


Figure 5.10: Variation of log-likelihood with EM iterations for the Pat data



(a) (b)

Figure 5.11: Final clusters obtained using (a) proposed algorithm (b) k-means algorithm for the Pat data (clusters are marked by '+' and 'o').

of the other two EM based algorithms (EMG and KEMG). For the k-means algorithm (KM) although the CPU time requirement is very low, its performance is significantly poorer. The BIRCH algorithm requires the least CPU time, but has performance poorer than the proposed algorithm, KEMG, EMG and RKMG.

Rough set theoretic initialization is found to improve the β value as well as reduce the time requirement of both EM and k-means. It is also observed that k-means with rough set theoretic initialization (RKMG) performs better than EM with random initialization (EMG), though it is well known that EM is usually superior to k-means in partitioning.

Table 5.9: Comparative performance of clustering algorithms

Algorithm	Cluster quality (β)	CPU time (sec)
Forest cover type data		
Proposed	7.10	1021
KEMG	6.21	2075
EMG	5.11	1555
RKMG	5.90	590
KM	3.88	550
BIRCH	4.21	104
Multiple features data		
Proposed	11.20	721
KEMG	10.90	881
EMG	10.40	810
RKMG	10.81	478
KM	7.02	404
BIRCH	8.91	32
Pat data		
Proposed	18.10	1.04
KEMG	15.40	2.10
EMG	10.90	1.80
RKMG	15.30	0.91
KM	8.10	0.80
BIRCH	9.02	0.55

5.6 Multispectral Image Segmentation [121]

In the present section, we describe an application of the aforesaid clustering algorithm to another real life problem, namely, segmentation of multispectral satellite images into different landcover types. Merits of the methodology as depicted in the previous section are also found to hold good. Before we provide the results of investigations, we describe, in brief, the relevance of the methodology for multispectral image segmentation and the implementation procedure. Note that the process of fuzzy discretization used here is different from that used in the previous section.

Segmentation is a process of partitioning an image space into some nonoverlapping meaningful homogeneous regions. The success of an image analysis system depends on the quality of segmentation. Two broad approaches to segmentation of remotely sensed images are gray level thresholding and pixel classification. In thresholding [116] one tries to get a set of thresholds $\{T_1, T_2, \ldots, T_k\}$ such that all pixels with grey values in the range $[T_i, T_{i+1})$ constitute the ith region type. On the other hand in pixel classification, homogeneous regions are determined by clustering the feature space of multiple image bands. Both thresholding and pixel classification algorithms may be either local *i.e.*, context dependent or global *i.e.*, blind to the position of a pixel. Multispectral nature of most remote sensing images make pixel classification the natural choice for segmentation.

Statistical methods are widely used in unsupervised pixel classification framework because of their capability of handling uncertainties arising from both measurement error and the presence of mixed pixels. In most statistical approaches, an image is modeled as a 'random field' consisting of collections of two random variables $Y = (Y_s)_{s \in S}, X = (X_s)_{s \in S}$. The first one takes values in the field of 'classes', while the second one deals with the field of 'measurements' or 'observations'. The problem of segmentation is to estimate Y from X. A general method of statistical clustering is to represent the probability density function of the data as a *mixture model*, which asserts that the data is a combination of k individual component densities (commonly Gaussians), corresponding to k clusters. The task is to identify, given the data, a set of k populations in it, and provide a model (density distribution) for each of the populations. The EM algorithm is an effective and popular technique for estimating the mixture model parameters. It iteratively refines an initial cluster model to better fit the data and

terminates at a solution which is locally optimal for the underlying clustering criterion [28]. An advantage of EM is that it is capable for handling uncertainties due to mixed pixels and helps in designing multivalued recognition systems. The EM algorithm has following limitations, (i) the number of clusters needs to be known, (ii) the solution depends strongly on initial conditions, and (iii) can only model convex clusters.

The first limitation is a serious handicap in satellite image processing; since in real images the number of classes is frequently difficult to determine *a priori*. To overcome the second, several methods for determining 'good' initial parameters for EM have been suggested, mainly based on subsampling, voting and two stage clustering [94]. However, most of these methods have high computational requirement and/or are sensitive to noise. The stochastic EM (SEM) algorithm [93] for segmentation of images is another attempt in this direction which provides an upper bound on the number of classes, robustness to initialization and fast convergence.

The clustering algorithm, described in Section 5.5, circumvents many of the above problems. Block diagram of the integrated segmentation methodology is shown in Figure 5.12. Discretization of the feature space, for the purpose of rough set rule generation, is performed by gray level thresholding of the image bands individually. Thus, each attribute (band) now takes on values in $\{1, 2, ., k+1\}$, where k is the number of threshold levels for that band. The fuzzy correlation $(C(\mu_1, \mu_2))$ between a fuzzy representation of an image (μ_1) and its nearest two-tone version (μ_2) is used. Fuzzy correlation $C(\mu_1, \mu_2)$ is defined as [115]

$$C(\mu_1, \mu_2) = 1 - \frac{4}{X_1 + X_2}\left(\sum_{i=0}^{T}\{[\mu_1(i)]^2 h(i)\} + \sum_{i=T+1}^{L-1}\{[1-\mu_1(i)]^2 h(i)\}\right) \qquad (5.17)$$

with $X_1 = \sum_{i=0}^{L-1}[2\mu_1(i) - 1]^2 h(i)$ and $X_2 = \sum_{i=0}^{L-1}[2\mu_2(i) - 1]^2 h(i) =$ constant, $L-1$ is the maximum grey level and $h(i)$ is the frequency of the ith grey level. The *maximas* of the $C(\mu_1, \mu_2)$ represent the threshold levels. For details of the above method one may refer to [115]. We have considered correlation as a measure of thresholding, since it is found recently to provide good segmentation in less computational time compared to similar methods [116]. However, any other grey level thresholding technique may be used. Note that, we have not used fuzzy linguistic granulation of the feature space here, since histogram based thresholding provides a natural mean of discretization of images.

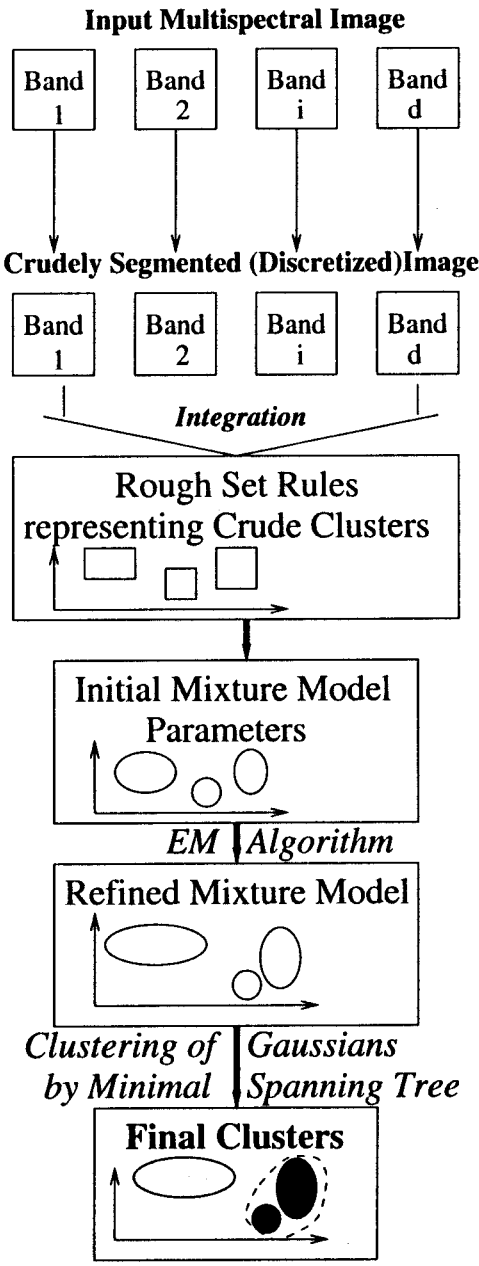


Figure 5.12: Block diagram of the proposed image segmentation algorithm

Results are presented on two IRS-1A (4 bands) images. The images were taken using LISS-II scanner in the wavelength range $0.77 - 0.86\mu m$ and it has a spatial resolution of $36.25m \times 36.25m$. The images are of size 512×512. They cover areas around the city of Calcutta and Bombay respectively.

For the Calcutta image the grey level thresholds obtained using the correlation based methodology are band 1: {34,47}, band 2: {20,29}, band 3: {24,30} and band 4: {31,36}. For Bombay image the corresponding values are {36,60}, {22,51}, {23,68} and {11,25}. After discretization, the attribute value table is constructed. Eight rough set rules (for Calcutta image) and seven rules (for Bombay image), each representing a crude cluster, is obtained. The rules are then mapped to initial parameters of the component Gaussians and refined using EM algorithm. The Gaussians are then merged using the minimal spanning tree based technique discussed in Section 5.5.4; thereby resulting in five clusters (from original eight and seven Gaussians). For both the images progressive improvement was observed from the initial grey level thresholding of the individual bands, clustering using crude mixture model obtained from rough set rules, clustering using refined mixture model obtained by EM, and finally to graph theoretic clustering of the component Gaussians.

The performance of the proposed hybrid method is compared extensively with that of various other related ones, as mentioned in Section 5.5.5. These involve different combinations of the individual components of the proposed scheme namely, rough set initialization, EM and MST, with other related schemes e.g., random initialization and k-means algorithm. The algorithms compared are (a) randomly initialized EM and k-means algorithm (EM, KM) (best of 5 independent random initializations), (b) rough set initialized EM and k-means (centers) algorithm (REM, RKM), (c) EM initialized with the output of k-means algorithm (KMEM), (d) EM with random initialization and MST clustering (EMMST), and (e) fuzzy k-means (FKM) algorithm.

For the purpose of qualitative comparison of the segmentation results we have considered the index β (Equation 5.16). We also present the total CPU time required by these algorithms on a DEC Alpha 400 MHz Workstation. It may be noted that except for the algorithms involving rough set, the number of clusters is not automatically determined.

Comparative results are presented in Tables 5.10 and 5.11. Segmented images of the

city of Calcutta obtained by these algorithms are also presented in Figure 5.13, for visual inspection. For Bombay image we show the segmented versions only for the proposed method and KM algorithm having the highest and lowest β values. The following conclusions can be arrived at from the results:

1. *EM vs k-means*: It is observed that EM is superior to k-means (KM) both with random and rough set initialization. However, k-means requires considerably less time compared to EM. The performance of fuzzy k-means (FKM) is intermediate between k-means and EM, though its time requirement is more than EM.

2. *Effect of rough set initialization*: Rough set theoretic initialization (REM, RKM) is found to improve the β value as well as reduce time requirement substantially for both EM and k-means. Rough set initialization is also superior to k-means initialization (KMEM).

3. *Contribution of MST*: Use of MST adds a small computational load to the EM algorithms (EM, REM), however, the corresponding integrated methods (EMMST and the Proposed algorithm) show a definite increase in β value.

4. Integration of all the three components, EM, rough set and MST, in the proposed algorithm, produces the best segmentation in terms of β value in the least computation time. This is also supported visually if we consider Figs. 5.15 and 5.16 which demonstrate the zoomed image of two man made structures viz, river bridge and airport strips of Calcutta image corresponding to the proposed method and KM algorithm providing the highest and lowest β values respectively.

5. *Computation time*: It is observed that the proposed algorithm requires significantly less time compared to other algorithms having comparable performance. Reduction in time is achieved due to two factors. Rough set initialization reduces the convergence time of the EM algorithm considerably compared to random initialization. Also, the MST being designed on component Gaussians rather than individual data points adds very little load to the overall time requirement while improving the performance significantly.

Table 5.10: Comparative performance of different clustering methods for the Calcutta image

Algorithm	No. of clusters	Index β	Time (sec)
EM	5	5.91	1720
KM	5	5.25	801
REM	8	6.97	470
RKM	8	5.41	301
KMEM	8	6.21	1040
EMMST	5	6.44	1915
FKM	5	5.90	2011
Proposed	5	7.37	505

Table 5.11: Comparative performance of different clustering methods for the Bombay image

Algorithm	No. of clusters	Index β	Time (sec)
EM	5	9.11	1455
KM	5	8.45	701
REM	7	10.12	381
RKM	7	10.00	277
KMEM	7	12.71	908
EMMST	5	14.04	1750
FKM	5	9.20	1970
Proposed	5	17.10	395

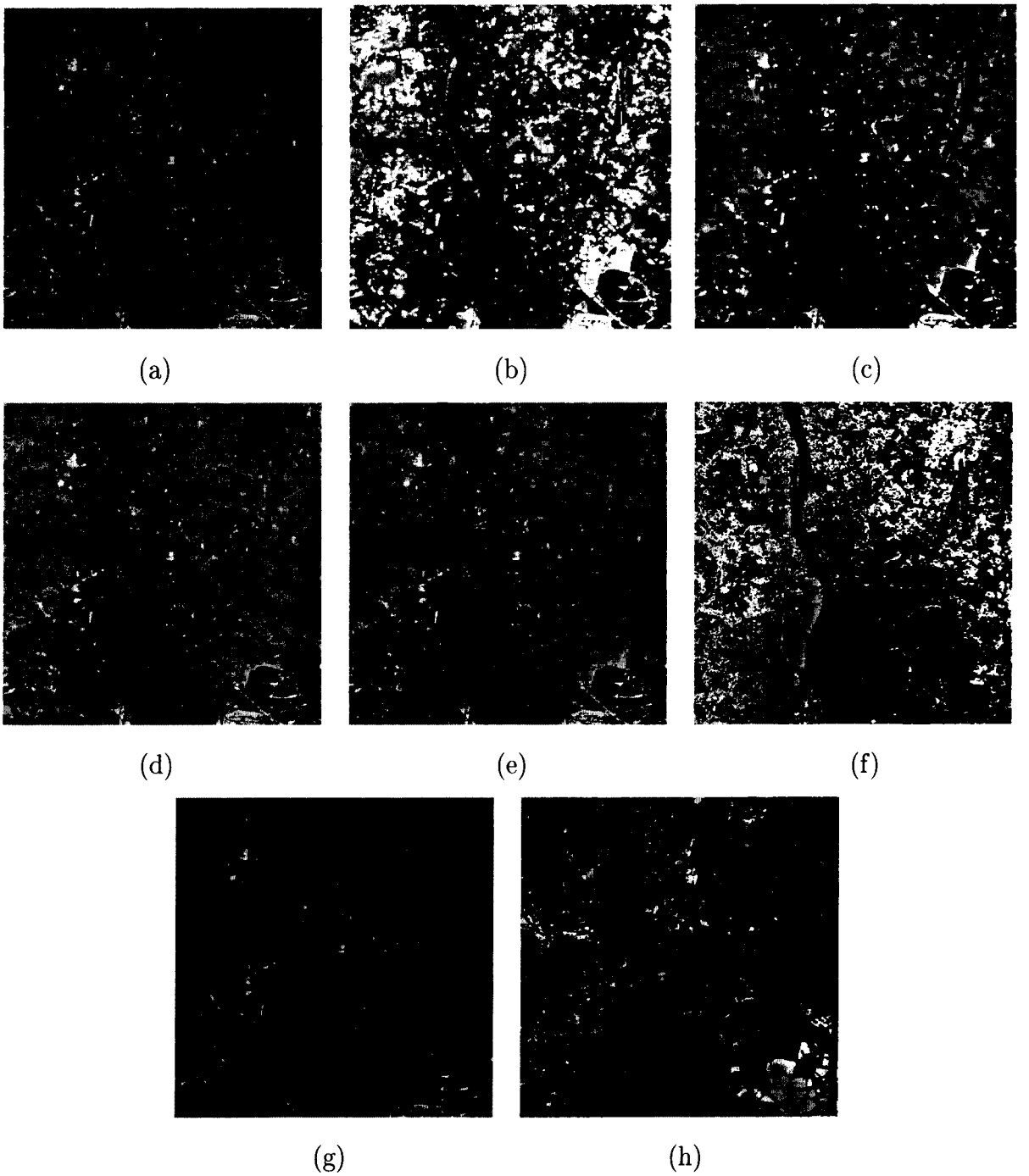
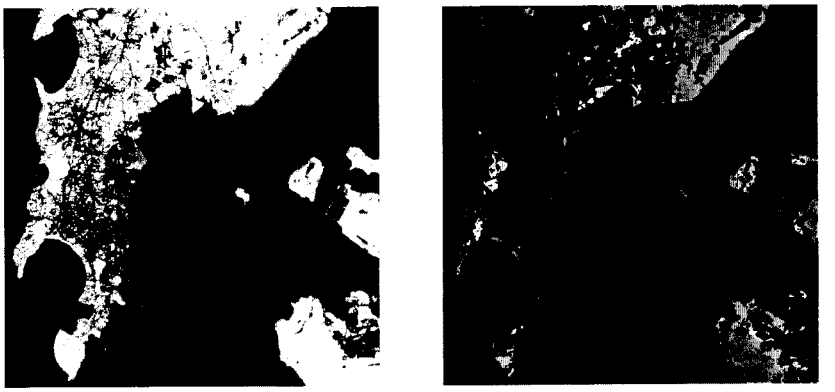
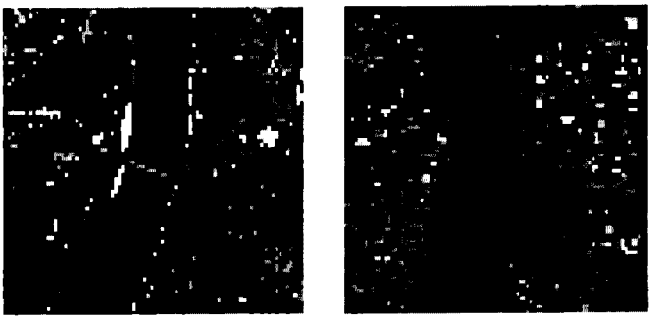


Figure 5.13: Segmented IRS image of Calcutta using (a) proposed method, (b) EM with MST (EMMST), (c) fuzzy k-means algorithm (FKM), (d) rough set initialized EM (REM), (e) EM with k-means initialization (KMEM), (f) rough set initialized k-means (RKM), (g) EM with random initialization (EM), (h) k-means with random initialization (KM)



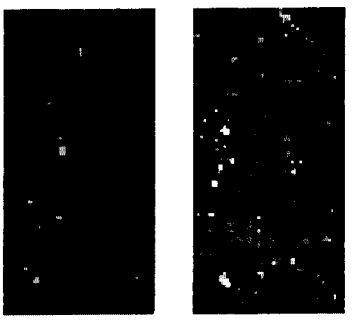
(a) (b)

Figure 5.14: Segmented IRS image of Bombay using (a) proposed method, (b) k-means with random initialization (KM)



(a) (b)

Figure 5.15: Zoomed images of a bridge on the river Ganges in Calcutta for (a) proposed method, (b) k-means with random initialization (KM)



(a) (b)

Figure 5.16: Zoomed images of two parallel airstrips of Calcutta airport for (a) proposed method, (b) k-means with random initialization (KM)

5.7 Conclusions and Discussion

We have presented new methodologies for case generation and clustering by exploiting the merits of rough-fuzzy hybridization. Fuzzy set theory is used to represent a pattern in terms of its membership to linguistic variables. This gives rise to efficient fuzzy granulation of the feature space. On the granular universe thus obtained, rough sets are used to form reducts which contain *informative* and *irreducible* information both in terms of features and patterns. The fuzzy linguistic rules obtained from the reducts represent different clusters in the granular feature space. Granular clusters (regions), modeled by the rules, are mapped to different cases, represented by fuzzy membership functions.

Since rough set theory is used to obtain cases through crude rules (*i.e.*, it deals with information granules, and not the original data), case generation time is reduced. Also, since only the informative regions and the relevant subset of features are stored (*i.e.*, the generated cases are represented by different reduced number of features), case retrieval time decreases significantly. Therefore, the case generation algorithm is suitable for mining data sets, large both in dimension and size.

Rough-fuzzy computing is also found to be successful in effectively circumventing the initialization and local minima problems of iterative refinement clustering algorithms (like EM and k-means). In addition, this improves the clustering performance, as measured by β value.

The contribution of the second part of the chapter also lies in the development of a methodology integrating the merits of graph-theoretic clustering (e.g., capability of generating non-convex clusters) and iterative refinement clustering (such as low computational time requirement). At the local level the data is modeled by Gaussians, *i.e.*, as combination of convex sets, while globally these Gaussians are partitioned using graph-theoretic technique; thereby enabling the efficient detection of the non-convex clusters present in the original data. Since the number of Gaussians is much less than the total number of data points, the computational time requirement for this integrated method is much less than that required by a conventional graph theoretic clustering.

Chapter 6

Modular Rough-fuzzy MLP: Evolution, Rule Generation and Evaluation

6.1 Introduction

In the previous chapter we have demonstrated a judicious integration of fuzzy sets and rough sets for providing an efficient granular computing paradigm useful for data mining applications. This chapter provides a synergistic integration of four soft computing components, namely, fuzzy sets, rough sets, neural networks and genetic algorithms along with modular decomposition strategy, for generating a modular rough-fuzzy multilayer perceptron (MLP). The resulting connectionist system achieves gain in terms of performance, learning time and network compactness for classification and linguistic rule generation. Different quantitative indices are used for evaluating the linguistic rules, and to reflect the knowledge discovery aspect.

There are ongoing efforts during the past decade to integrate fuzzy logic, artificial neural networks (ANN) and genetic algorithms (GAs) to build efficient systems in soft computing paradigm. Recently, the theory of rough sets [131, 132] has emerged as another mathematical tool for dealing with uncertainty arising from inexact or incomplete information, and is also being used in soft computing [127]. The rough-fuzzy MLP [10], developed in 1998 for pattern classification, is such an example combining both rough sets and fuzzy sets with neural networks for building an efficient connectionist system. In this hybridization, fuzzy sets help in handling linguistic input information and ambiguity in output decision, while rough sets extract the domain knowledge for determining the network parameters. Some other attempts in using rough sets (either individually or in combination with fuzzy set) for designing neural network systems are available in [109] where rough sets are used mainly for generating the network parameters, and in [139] where roughness at the neuronal level has been incorporated. One may also note the utility of GAs in determining the network parameters as well as the topology (growing/pruning of links), as has been noticed during the past decade [112]. Several algorithms have been developed for extracting embedded knowledge, in the form of symbolic rules, from these hybrid networks [68, 159, 160].

Two important issues which have not been adequately addressed by the above methodologies are those of lengthy training time and poor interpretability of the networks. A major disadvantage in neural networks learning of large scale tasks is the high computational time required (due to local minima and slow convergence). Use of knowledge based networks offers only a partial solution to the problem. Also, in most of the

above methodologies the link weights of the network are rather uniformly distributed and the network is not suitable for extracting crisp (certain) rules. Compact networks with structure imposed on the weight values are more desirable in this respect for network interpretation. We introduce here the concept of modular learning (in an evolutionary framework) to deal with these problems.

A recent trend in neural network design for large scale problems is to split the original task into simpler subtasks, and to co-evolve the subnetwork modules for each of the subtasks [53]. The modules are then combined to obtain the final solution. Some of the advantages of this modular approach include decomplexification of the task, and its meaningful and clear neural representation. The *divide and conquer* strategy leads to super-linear speedup in training. It also avoids the 'temporal crosstalk problem' and interference while learning. In addition, the number of parameters (*i.e.*, weights) can be reduced using modularity; thereby leading to a better generalization performance of the network [147], compactness in size and crispness in extracted rules.

In the present chapter a modular evolutionary approach is adopted for designing a hybrid connectionist system in soft computing framework for both classification and rule generation. The basic building block used is the rough-fuzzy MLP [10], mentioned earlier. The original classification task is split into several subtasks and a number of rough-fuzzy MLPs are obtained for each subtask. The subnetwork modules are integrated in a particular manner so as to preserve the crude domain knowledge which was encoded in them using rough sets. The pool of integrated networks is then evolved using a GA with a restricted (adaptive/variable) mutation operator that utilizes the domain knowledge to accelerate training and preserves the localized rule structure as potential solutions. The parameters for input and output fuzzy membership functions of the network are also tuned using GA together with the link weights. We have modified the existing procedure for generation of rough set dependency rules for handling directly the real valued attribute table containing fuzzy membership values. This helps in preserving all the class representative points in the dependency rules by adaptively applying a threshold that automatically takes care of the shape of membership functions. Unlike previous attempts of knowledge based network design [10, 162], here all possible inference rules, and not only the best rule, contribute to the final solution. The use of GAs in this context is beneficial for modeling multi-modal distributions, since all major representatives in the population are given fair chance during network

synthesis. Superiority of the proposed model, over some related ones, is experimentally demonstrated in terms of classification accuracy, network size and training time when both real life (speech and medical) and artificially generated data sets, with dimension ranging from two to twenty one and class boundaries overlapping as well as non-linear, are considered as input.

In the second part of the investigation, an algorithm for extracting linguistic rules, based on this hybrid model, is presented. The performance of the rules is evaluated quantitatively. Two new measures are accordingly defined indicating the *certainty* and *confusion* in a decision. These new indices are used along with some existing measures to evaluate the quality of the rules. A quantitative comparison of the rule extraction algorithm is made with some existing ones like *Subset* [42], *M of N* [162] and X2R [85]. It is observed that the proposed methodology extracts rules which are less in number, yet accurate, and have high certainty factor and low confusion with less computation time.

The organization of the chapter is as follows: Section 6.2 explains, in brief, the rough-fuzzy MLP [10]. The design procedure of the modular evolutionary algorithm is described in Section 6.3. The rule extraction method and the quantitative performance measures are presented in Section 6.4. The effectiveness of the proposed model and its comparison with some related ones are provided in Section 6.5. Finally, Section 6.6 concludes the chapter.

6.2 Rough-fuzzy MLP

The rough-fuzzy MLP [10] is described briefly in this section. First we explain the fuzzy MLP, for convenience. This is followed by the knowledge encoding algorithm for mapping the rules to the parameters of a fuzzy MLP.

6.2.1 Fuzzy MLP

The fuzzy MLP model [122] incorporates fuzziness at the input and output levels of the MLP, and is capable of handling exact (numerical) and/or inexact (linguistic) forms of input data. Any input feature value is described in terms of some combination of

membership values to the linguistic property sets *low* (L), *medium* (M) and *high* (H). Class membership values (μ) of patterns are represented at the output layer of the fuzzy MLP. During training, the weights are updated by backpropagating errors with respect to these membership values such that the contribution of uncertain vectors is automatically reduced.

A three-layered feedforward MLP is used. The output of a neuron in any layer (h) other than the input layer ($h = 0$) is given as

$$y_j^h = \frac{1}{1 + exp(-\sum_i y_i^{h-1} w_{ji}^{h-1})} \quad , \tag{6.1}$$

where y_i^{h-1} is the state of the ith neuron in the preceding $(h-1)$th layer and w_{ji}^{h-1} is the weight of the connection from the ith neuron in layer $h-1$ to the jth neuron in layer h. For nodes in the input layer, y_j^0 corresponds to the jth component of the input vector. Note that $x_j^h = \sum_i y_i^{h-1} w_{ji}^{h-1}$.

Input vector

An p-dimensional pattern $\mathbf{F_i} = [\mathrm{F_{i1}}, \mathrm{F_{i2}}, \ldots, \mathrm{F_{ip}}]$ is represented as a $3p$-dimensional vector

$$\mathbf{F_i} = [\mu_{\mathrm{low(F_{i1})}}(\mathbf{F_i}), \ldots, \mu_{\mathrm{high(F_{ip})}}(\mathbf{F_i})] = [\mathrm{y_1^0}, \mathrm{y_2^0}, \ldots, \mathrm{y_{3p}^0}] \quad , \tag{6.2}$$

where the μ values indicate the membership functions of the corresponding linguistic π-sets *low, medium* and *high* along each feature axis and $y_1^0, \ldots, y_{3p}^0$ refer to the activations of the $3p$ neurons in the input layer.

When the input feature is numerical, we use $\pi-$fuzzy sets (in the one dimensional form), with range [0,1], as represented by Equation 5.7. Note that features in linguistic and set forms can also be handled in this framework [122].

Output representation

Consider an M-class problem domain such that we have M nodes in the output layer. Let the p-dimensional vectors $\mathbf{o_k} = [o_{k1} ... o_{kp}]$ and $\mathbf{v_k} = [v_{k1}, ..., v_{kp}]$ denote the mean and standard deviation respectively of the numerical training data for the kth class c_k.

The weighted distance of the training pattern $\mathbf{F}_i$ from kth class c_k is defined as

$$z_{ik} = \sqrt{\sum_{j=1}^{p} \left[\frac{F_{ij} - o_{kj}}{v_{kj}}\right]^2} \quad for \quad k = 1, \ldots, M \ , \tag{6.3}$$

where F_{ij} is the value of the jth component of the ith pattern point.

The membership of the ith pattern in class k, lying in the range $[0, 1]$ is defined as [118]

$$\mu_k(\mathbf{F}_i) = \frac{1}{1 + (\frac{z_{ik}}{f_d})^{f_e}} \ , \tag{6.4}$$

where positive constants f_d and f_e are the denominational and exponential fuzzy generators controlling the amount of fuzziness in the class membership set.

6.2.2 Rough set knowledge encoding

Rough set knowledge encoding involves two steps: generating rough set dependency rules, and mapping the rules to initial network parameters. The basic principle of rough set rule generation is already discussed in Section 5.2. The following paragraphs describe, in brief, the steps used here to obtain the dependency rules, and the methodology for mapping the rules to the weights of a fuzzy MLP.

Consider the case of feature F_j for class c_k in the M-class problem domain. The inputs for the i^{th} representative sample $\mathbf{F}_i$ are mapped to the corresponding three-dimensional feature space of $\mu_{low(F_{ij})}(\mathbf{F}_i)$, $\mu_{medium(F_{ij})}(\mathbf{F}_i)$ and $\mu_{high(F_{ij})}(\mathbf{F}_i)$. Let these be represented by L_j, M_j and H_j respectively. These values are then used to construct the attribute value table. As the method considers multiple objects in a class, a separate $n_k \times 3p$-dimensional attribute-value decision table is generated for each class c_k (where n_k indicates the number of objects in c_k).

For constructing the discernibility matrix, the absolute distance between each pair of objects is computed along each attribute L_j, M_j, H_j for all j. We modify Equation 5.3 to directly handle a real-valued attribute table consisting of fuzzy membership values. We define

$$c_{ij} = \{a \in B : \ \mid a(\mathbf{x}_i) - a(\mathbf{x}_j) \mid > Th\} \tag{6.5}$$

for $i, j = 1, \ldots, n_k$, where Th is an adaptive threshold. Note that the adaptivity of this threshold is in-built, depending on the inherent shape of the membership function.

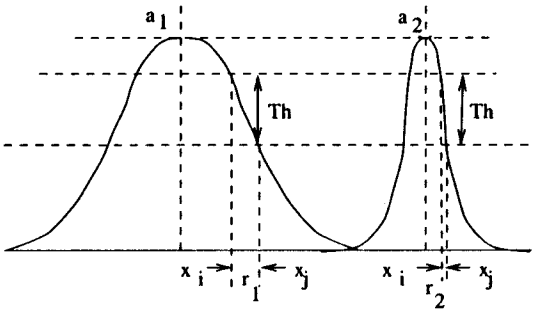


Figure 6.1: Illustration of adaptive thresholding of membership functions

Dependency rules are generated from the discernibility matrix using the methodology described in Section 5.2.4.

Consider Figure 6.1. Let a_1, a_2 correspond to two membership functions (attributes) with a_2 being steeper as compared to a_1. It is observed that $r_1 > r_2$. This results in an implicit adaptivity of Th while computing c_{ij} in the discernibility matrix directly from the real-valued attributes. Here lies the novelty of the proposed method. Moreover, this type of thresholding also enables the discernibility matrix to contain all the representative points/clusters present in a class. This is particularly useful in modeling multi-modal class distributions. Note that the above notion of adaptive thresholding, for constructing the discernibility matrix, is similar to that used in [135] related to *shadowed sets.*

Dependency rules are generated from the discernibility matrix, obtained as above, using the methodology described in Section 5.2.4.

While designing the initial structure of the rough-fuzzy MLP, the union of the rules of the M classes is considered. The input layer consists of $3p$ attribute values while the output layer is represented by M classes. The hidden layer nodes model the first level (innermost) operator in the antecedent part of a rule, which can be either a conjunct or a disjunct. The output layer nodes model the outer level operands, which can again be either a conjunct or a disjunct. For each inner level operator, corresponding to one output class (one dependency rule), one hidden node is dedicated. Only those input attributes that appear in this conjunct/disjunct are connected to the appropriate hidden node, which in turn is connected to the corresponding output node. Each outer level operator is modeled at the output layer by joining the corresponding hidden

nodes. Note that a single attribute (involving no inner level operators) is directly connected to the appropriate output node via a hidden node, to maintain uniformity in rule mapping.

Let the dependency factor for a particular dependency rule for class c_k be $df = \alpha = 1$ by Equation 5.5. The weight w_{ki}^1 between a hidden node i and output node k is set at $\frac{\alpha}{fac} + \varepsilon$, where fac refers to the number of outer level operands in the antecedent of the rule and ε is a small random number taken to destroy any symmetry among the weights. Note that $fac \geq 1$ and each hidden node is connected to only one output node. Let the initial weight so clamped at a hidden node be denoted as β. The weight $w_{ia_j}^0$ between an attribute a_j (where a corresponds to *low* (L), *medium* (M) or *high* (H)) and hidden node i is set to $\frac{\beta}{facd} + \varepsilon$, such that $facd$ is the number of attributes connected by the corresponding inner level operator. Again $facd \geq 1$. Thus for an M-class problem domain there are at least M hidden nodes. It is to be mentioned that the number of hidden nodes is determined directly from the dependency rules. It depends on the form in which the antecedents are present in the rules.

6.3 Modular Evolution of Rough-fuzzy MLP [96, 124, 103]

The design procedure of Modular Neural Networks (MNN) involves two broad steps - effective decomposition of the problem such that the subproblems can be solved with compact networks, and efficient combination and training of the networks such that there is gain in terms of training time, network size and accuracy. These are described in detail in the following section along with the steps involved and the characteristics features.

6.3.1 Algorithm

We use two phases. First an M-class classification problem is split into M two-class problems. Let there be M sets of subnetworks, with $3p$ inputs and one output node each. Rough set theoretic concepts are used to encode domain knowledge into each of the subnetworks, using Equations 5.4 and 6.5. As explained in Section 6.2.2 the number

of hidden nodes and connectivity of the knowledge-based subnetworks is automatically determined. Each two-class problem leads to the generation of one or more crude subnetworks, each encoding a particular decision rule. Let each of these constitute a pool. So we obtain $m \geq M$ pools of knowledge-based modules. Each pool k is perturbed to generate a total of n_k subnetworks, such that $n_1 = \ldots = n_k = \ldots = n_m$. These pools constitute the initial population of subnetworks, which are then evolved independently using genetic algorithms.

At the end of the above phase, the modules/subnetworks corresponding to each two-class problem are concatenated to form an initial network for the second phase. The inter module links are initialized to small random values as depicted in Figure 6.2. A set of such concatenated networks forms the initial population of the GA. The mutation probability for the inter-module links is now set to a high value, while that of intra-module links is set to a relatively lower value. This sort of *restricted* mutation helps preserve some of the localized rule structures, already extracted and evolved, as potential solutions. The initial population for the GA of the entire network is formed from all possible combinations of these individual network modules and random perturbations about them. This ensures that for complex multi-modal pattern distributions all the different representative points remain in the population. The algorithm then searches through the reduced space of possible network topologies. The steps are summarized below followed by an example.

Steps

Step 1: For each class, generate rough set dependency rules using the methodology described in Section 5.2.4.

Step 2: Map each of the dependency rules to a separate subnetwork modules (fuzzy MLPs) using the methodology described in Section 6.2.2.

Step 3: Partially evolve each of the subnetworks using conventional GA.

Step 4: Concatenate the subnetwork modules to obtain the complete network. For concatenation the intra-module links are left unchanged while the inter-module links are initialized to low random values (Figure 6.2). Note that each of the subnetworks solves a 2-class classification problem, while the concatenated network solve the actual

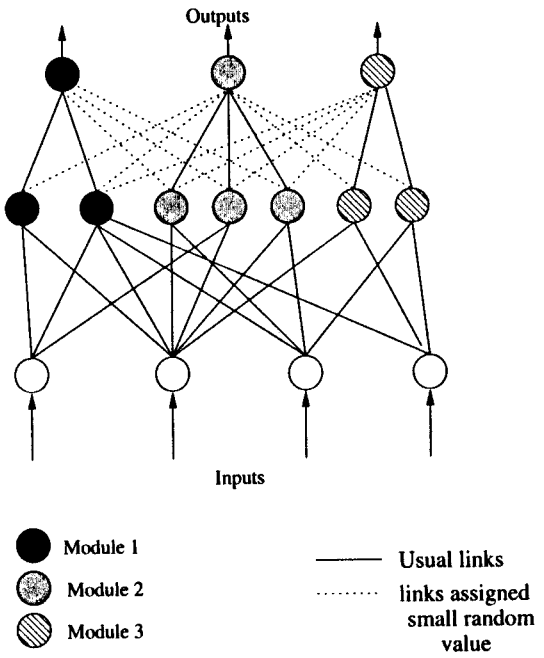


Figure 6.2: Intra and Inter module links

M-class problem. Every possible combination of subnetwork modules is generated to form a pool of networks.

Step 5: The pool of networks is evolved using a *modified* GA with an adaptive/variable mutation operator. The mutation probability is set to a low value for the intra-module links and to a high value for the inter-module links.

Example:

Consider a problem of classifying a two dimensional data into two classes. The input fuzzifier maps the features into a six dimensional feature space. Let a sample set of rules obtained from rough set theory be

$$c_1 \leftarrow (L_1 \wedge M_2) \vee (H_2 \wedge M_1),\ c_2 \leftarrow M_2 \vee H_1,\ c_2 \leftarrow L_2 \vee L_1,$$

where L_j, M_j, H_j correspond to $\mu_{low(F_j)}$, $\mu_{medium(F_j)}$, $\mu_{high(F_j)}$ respectively. For the first phase of the GA three different pools are formed, using one crude subnetwork for class 1 and two crude subnetworks for class 2 respectively. Three partially trained subnetworks result from each of these pools. They are then concatenated to form $(1 \times 2) = 2$ networks. The population for the final phase of the GA is formed with

these networks and perturbations about them. The steps followed in obtaining the final network are illustrated in Figure 6.3.

Remarks:

(i) The use of rough sets for knowledge encoding provides an established mathematical framework for network decomposition. Knowledge encoding not only produces an initial network close to the optimal one, it also reduces the search space. The initial network topology is automatically determined and provides good *building blocks* for the GA.

(ii) In earlier concurrent algorithms for neural network learning, there exist no guidelines for the decomposition of network modules [172]. Arbitrary subnetworks are assigned to each of the classes. Use of networks with the same number of hidden nodes for all classes leads to overlearning in the case of simple classes and poor learning in complex classes. Use of rough set theory circumvents the above problem.

(iii) Sufficient reduction in training time is obtained, as the above approach parallelizes the GA to an extent. The search string of the GA for subnetworks being smaller, more than linear decrease in searching time is obtained. Also very small number of training cycles are required in the refinement phase, as the network is already very close to the solution. Note that the modular aspect of our algorithm is similar to the co-evolutionary algorithm (CEA) used for solving large scale problems with EAs [172].

(iv) The splitting of an M-class problem into M two-class problems bears an analogy to the well known *divide and conquer* strategy and speeds up the search procedure significantly. Here one can use a smaller chromosome and/or population size, thereby alleviating to some extent the space-time complexity problem.

(v) The algorithm indirectly constrains the solution in such a manner that a structure is imposed on the connection weights. This is helpful for subsequent rule-extraction from the weights, as the resultant network obtained has sparse but strong interconnection among the nodes. Although in the above process some amount of optimality is sacrificed, and often for many-class problems the number of nodes required may be higher than optimal, yet the network is less redundant. However the nature of the objective function considered and the modular knowledge based methodology used enables sufficient amount of link pruning, and the total number of links are found to be significantly less. The use of *restricted* mutation (as defined in Section 6.3.2) minimizes

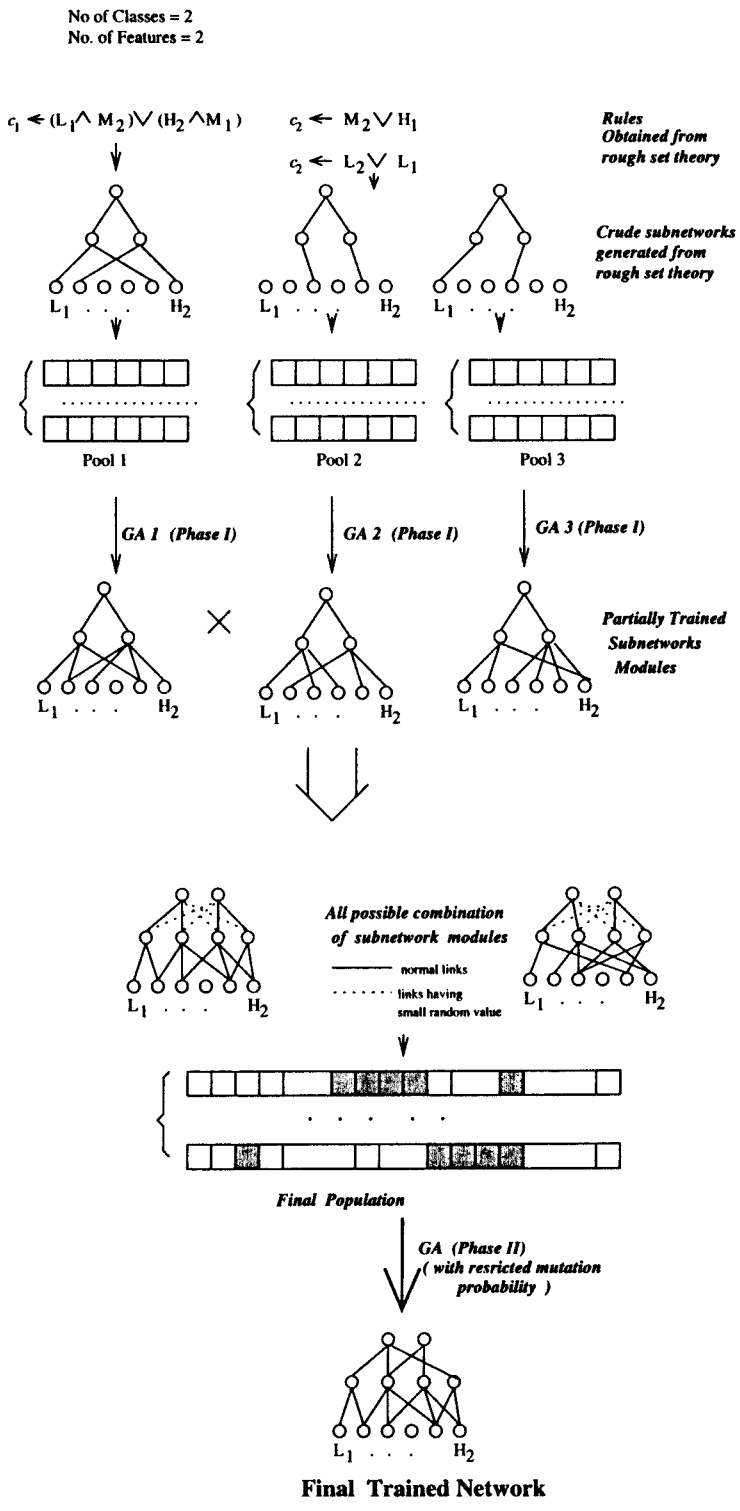


Figure 6.3: Steps for designing a sample modular rough-fuzzy MLP

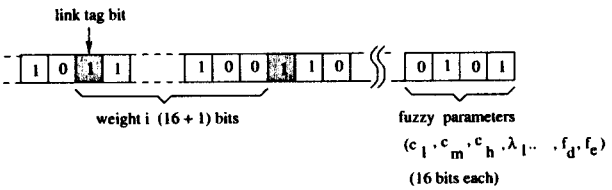


Figure 6.4: Chromosome representation

the destruction of encoded rule structures in the knowledge based networks.

(vi) For each two-class (sub)problem a set of subnetworks encoding separate decision rules is available. Since all possible combinations of these subnetworks are considered for the final evolutionary training, greater diversity within the population is possible. This results in faster convergence of the GA which utilizes multiple theories about a domain. This also ensures that all the clusters in the feature space are adequately represented in the final solution.

6.3.2 Evolutionary design

Here we discuss different features of genetic algorithms [46] with relevance to our algorithm.

Chromosomal representation

The problem variables consist of the weight values and the input/output fuzzification parameters. Each of the weights is encoded into a binary word of 16 bit length, where [000...0] decodes to -128 and [111...1] decodes to 128. An additional bit is assigned to each weight to indicate the presence or absence of the link. The fuzzification parameters tuned are the center (c) and radius (λ) for each of the linguistic attributes *low*, *medium* and *high* of each feature, and the output fuzzifiers f_d and f_e [122]. These are also coded as 16 bit strings in the range $[0, 2]$. For the input parameters, [000...0] decodes to 0 and [111...1] decodes to 1.2 times the maximum value attained by the corresponding feature in the training set. The chromosome is obtained by concatenating all the above strings (Figure 6.4). Sample values of the string length are around 2000 bits for reasonably sized networks.

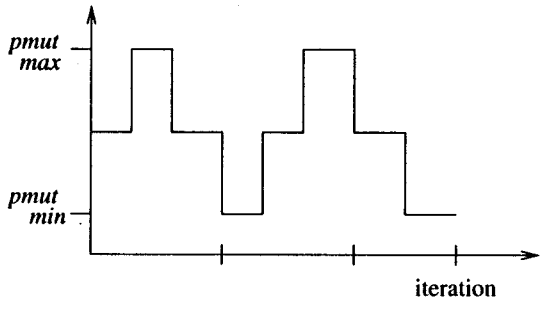


Figure 6.5: Variation of mutation probability with iteration

Initial population is generated by coding the networks obtained by rough set based knowledge encoding, and by random perturbations about them. A population size of 64 was considered.

Crossover

It is obvious that due to the large string length, single point crossover would have little effectiveness. Multiple point crossover is adopted, with the distance between two crossover points being a random variable between 8 and 24 bits. This is done to ensure a high probability for only one crossover point occurring within a word encoding a single weight. The crossover probability is fixed at 0.7.

Mutation

The search string being very large, the influence of mutation is more on the search compared to crossover. Each of the bits in the string is chosen to have some mutation probability (*pmut*). The mutation probability has a spatio-temporal variation. The variation of *pmut* with iteration is shown in Figure 6.5. The maximum value of *pmut* is chosen to be 0.4 and the minimum value as 0.01. The mutation probabilities also vary along the encoded string, the bits corresponding to inter-module links being assigned a probability *pmut* (*i.e.,* the value of *pmut* at that iteration) and intra-module links assigned a probability *pmut*/10. This is done to ensure least alterations in the structure of the individual modules already evolved. Hence, the mutation operator indirectly incorporates the domain knowledge extracted through rough set theory.

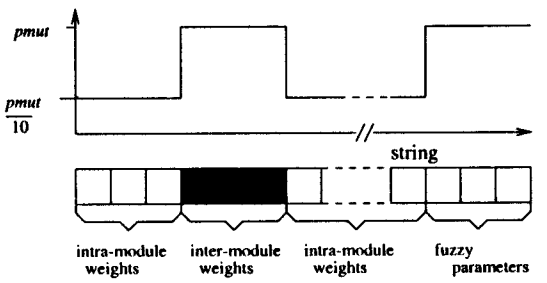


Figure 6.6: Variation of mutation probability along the encoded string (chromosome)

Choice of fitness function

An objective function of the form described below is chosen.

$$F_{\text{obj}} = \alpha_1 f_1 + \alpha_2 f_2 \ , \tag{6.6}$$

where

$$f_1 = \frac{\textit{No. of Correctly Classified Sample in Training Set}}{\textit{Total No. of Samples in Training Set}}$$

$$f_2 = 1 - \frac{\textit{No. of links present}}{\textit{Total No. of links possible}}.$$

Here α_1 and α_2 determine the relative weight of each of the factors. α_1 is taken to be 0.9 and α_2 is taken as 0.1, to give more importance to the classification score compared to the network size in terms of number of links. Note that we optimize the network connectivity, weights and input/output fuzzification parameters simultaneously.

Selection

Selection is done by the *roulette wheel* method. The probabilities are calculated on the basis of ranking of the individuals in terms of the objective function, instead of the objective function itself. *Elitism* is incorporated in the selection process to prevent oscillation of the fitness function with generation. The fitness of the best individual of a new generation is compared with that of the current generation. If the latter has a higher value the corresponding individual replaces a randomly selected individual in the new population.

6.4 Rule Generation and Quantitative Evaluation [124]

6.4.1 Rule extraction methodology

Algorithms for rule generation from neural networks mainly fall in two categories - pedagogical and decompositional [160]. Our algorithm can be categorized as decompositional. It is described below.

1. Compute the following quantities:
   $PMean$= Mean of all positive weights, $PThres_1$= Mean of all positive weights less than $PMean$, $PThres_2$= Mean of all weights greater than $PMean$. Similarly calculate $NThres_1$ and $NThres_2$ for negative weights.

2. For each hidden and output unit

   (a) for all weights greater than $PThres_1$ search for positive rules only, and for all weights less than $NThres_1$ search for negated rules only by *Subset* method.

   (b) search for combinations of positive weights above $Pthres_2$ and negative weights greater than $NThres_1$ that exceed the bias. Similarly search for negative weights less than $NThres_2$ and positive weights below $PThres_1$ to find out rules.

3. Associate with each rule j a confidence factor

$$cf_j = \inf_{j:\ all\ nodes\ in\ the\ path} \frac{(\Sigma_i w_{ji} - \theta_j)}{\Sigma_i w_{ji}}, \tag{6.7}$$

   where w_{ji} is the ith incoming link weight to node j.

Since our training algorithm imposes a structure on the network, resulting in a sparse network having few strong links, the $PThres$ and $NThres$ values are well separated. Hence the above rule extraction algorithm generates most of the embedded rules over a small number of computational steps.

The computational complexity of our algorithm is as follows. Let the network have i, h, o numbers of input, hidden and output nodes respectively. Let us make the assumption that $i = h = o = k$. Let the fraction of weights having value in $[0, PThres_1)$,

$[PThres_1, PThres_2)$, $[PThres_2, \infty)$, be p_1, p_2, p_3 respectively. Similarly let the corresponding fractions for negative weights be n_1, n_2, n_3. Then the computational complexity ($\mathcal{C}$) becomes

$\mathcal{C} = k.(\ 2^{(p_2+p_3)k+1} + 2^{(n_2+n_3)k+1} + 2^{(p_3+n_1)k+1} + 2^{(p_1+n_3)k+1}\ )$.

If $n_1,\ n_2,\ p_1,\ p_2 \ll p_3,\ n_3$,

$\mathcal{C} \approx 4k.\ (2^{p_3 k} + 2^{n_3 k}) = 4k.\ (e^{\ln 2.p_3 k} + e^{\ln 2.n_3 k})$.

Also if $p_3,\ n_3 \ll 1$,

$\mathcal{C} \approx 4k.(1 + \ln 2.(p_3 + n_3)k + 0.5.(\ln 2.(p_3 + n_3))^2 k^2$, *i.e.*, $\mathcal{C} \approx \mathcal{O}(k^3)$.

An important consideration is the order of application of rules in a rule base. Since most of the real life patterns are noisy and overlapping, rule bases obtained are often not totally consistent. Hence multiple rules may fire for a single example. Several existing approaches apply the rules sequentially, often leading to degraded performance. The rules extracted by our method have confidence factors associated with them. Therefore if multiple rules are fired, we use the strongest rule having the highest confidence.

Two existing rule extraction algorithms, similar in spirit to the proposed algorithm, are the *Subset* method [42] and *M of N* method [162]. The major problem with the *Subset* algorithm is that the cost of finding all subsets grows as the size of the power set of the links to each unit. It requires lengthy, exhaustive searches of size $\mathcal{O}(2^k)$ for a hidden/output node with a fan-in of k and extracts a large set of rules, upto $\beta_p * (1+\beta_n)$, where β_p and β_n are the number of subsets of positively and negatively weighted links respectively. Some of the generated rules may be repetitive, as permutations of rule antecedents are not taken care of automatically. Moreover, there is no guarantee that all useful knowledge embedded in the trained network will be extracted. Computational complexity of the *M of N* algorithm is $\mathcal{O}(k^3 + (k^2.j))$, where j is the number of examples. Additionally, the rule extraction procedure involves a backpropagation step requiring significant computation time. The algorithm has good generalization (accuracy), but can have degraded comprehensibility [160]. Note that one considers groups of links as equivalence classes, thereby generating a bound on the number of rules rather than establishing a ceiling on the number of antecedents.

6.4.2 Quantitative measures

Here we provide some measures in order to evaluate the performance of the rules. Among them, *Certainty* and *Confusion*, reflecting the confidence and ambiguity in a decision, are newly defined. Note that these aspects had not been considered earlier.

Let N be an $M \times M$ matrix whose (i,j)th element n_{ij} indicate the number of patterns actually belonging to class i, but classified as class j.

i) *Accuracy:* It is the correct classification percentage, provided by the rules on a test set defined as $\frac{n_{ic}}{n_i}.100$, where n_i is equal to the number of points in class i and n_{ic} of these points are correctly classified.

ii) *User's Accuracy* [151]: If n'_i points are found to be classified into class i, then the user's accuracy (U) is defined as $U = n_{ic}/n'_i$. This gives a measure of the confidence that a classifier attributes to a region as belonging to a class. In other words, it denotes the level of purity associated with a region.

iii) *Kappa* [151]: The coefficient of agreement called 'kappa' measures the relationship of beyond chance agreement to expected disagreement. It uses all the cells in the confusion matrix, not just the diagonal elements. The estimate of kappa (K) is the proportion of agreement after chance agreement is removed from consideration. The kappa value for class i (K_i) is defined as

$$K_i = \frac{n.n_{ic} - n_i.n'_i}{n.n'_i - n_i.n'_i}. \tag{6.8}$$

The numerator and denominator of overall kappa are obtained by summing the respective numerators and denominators of K_i separately over all classes.

iv) *Fidelity* [160]: This represents how closely the rule base approximates the parent neural network model [160]. We measure this as the percentage of the test set for which network and the rule base output agree. Note that fidelity may or may not be greater than accuracy.

v) *Confusion:* This measure quantifies the goal that the "*Confusion should be restricted within minimum number of classes*". This property is helpful in higher level decision making. Let $\hat{n}_{ij}$ be the mean of all n_{ij} for $i \neq j$. Then we define

$$Conf = \frac{Card\{n_{ij} : n_{ij} \geq \hat{n}_{ij}, i \neq j\}}{M} \tag{6.9}$$

for an M class problem. The lower the value of $Conf$, lesser is the number of classes between which confusion is occurs.

vi) *Cover:* Ideally the rules extracted should cover all the cluster regions of the pattern space. We use the percentage of examples from a test set for which no rules are fired as a measure of the uncovered region. A rule base having a smaller uncovered region is superior.

vii) *Rule base size:* It is measured in terms of the number of rules. Lower the value is, more compact is the rule base.

viii) *Computational complexity:* Here we present the CPU time required.

ix) *Certainty:* By certainty of a rule base we quantify the confidence of the rules as defined by the certainty factor cf (Equation 6.7).

6.5 Results and Comparison [124]

The modular rough-fuzzy MLP, described in Sections 6.3 and 6.4, has been implemented on both real life (Vowel, Hepatobiliary and Cervical cancer) and artificially generated (Pat) data. These data sets have overlapping and nonlinear class boundaries. The details of the data are provided in Appendix A.

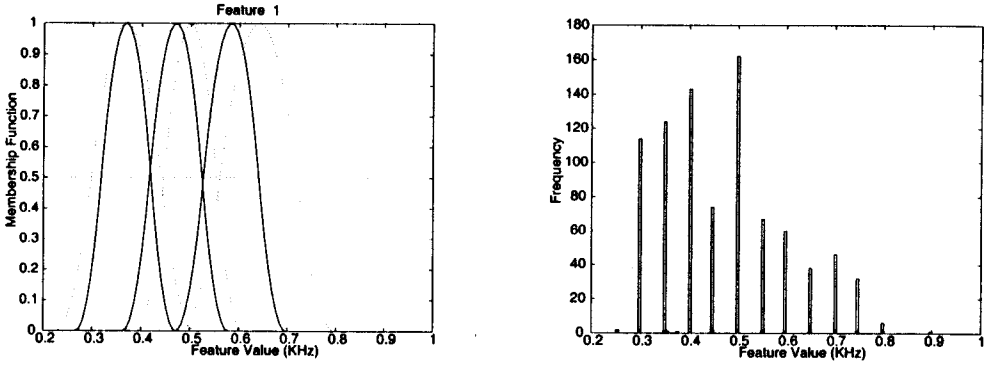
Let the proposed methodology be termed Model S. Other models compared include:

Model O: An ordinary MLP trained using backpropagation (BP) with weight decay.

Model F: A fuzzy MLP trained using BP [122] (with weight decay).

Model R: A fuzzy MLP trained using BP (with weight decay), with initial knowledge encoding using rough sets [10].

Model FM: A modular fuzzy MLP trained with GAs along with tuning of the fuzzification parameters. Here the term modular refers to the use of subnetworks corresponding to each class, that are later concatenated using GAs.



(a) (b)

Figure 6.7: (a) Input π-functions and (b) data distribution along F_1 axis for the Vowel data. Solid lines represent the initial functions and dashed lines represent the functions obtained finally after tuning with GAs. The horizontal dotted lines represents the threshold level

6.5.1 Classification

Recognition scores obtained for Vowel, Hepatobiliary and Pat data by the proposed soft modular network (Model S) are presented in Table 6.2. It also shows a comparison with other related MLP-based classification methods (Models O, F, R and FM). In all cases, 10% of the samples are used as training set, and the remaining samples are used as test set. Ten such independent runs are performed and the mean value and standard deviation of the classification accuracy, computed over them, are presented in Table 6.2.

The dependency rules, as generated via rough set theory and used in the encoding scheme, are shown in Table 6.1 only for Vowel data, as an example. The values of input fuzzification parameters used are also presented in Table 6.1. The corresponding π-functions are shown in Figure 6.7 only for feature F_1, as an illustration. In Table 6.1, F_i, where F stands for *low*, *medium* or *high*, denotes a property F of the ith feature [122]. The integrated networks contain 18, 15 and 10 hidden nodes in a single layer for Vowel, Pat, and Hepatobiliary data respectively. After combination 96, 61 and 16 networks were obtained respectively. The initial population of the GA was formed using 64 networks in each of these cases. In the first phase of the GA (for models FM and S), each of the subnetworks are partially trained for 10 sweeps.

Table 6.1: Rough set dependency rules for Vowel data along with the input fuzzification parameter values

$$
\begin{aligned}
c_1 &\leftarrow M_1 \vee L_3 \\
c_1 &\leftarrow M_1 \vee M_2 \\
c_2 &\leftarrow M_2 \vee M_3 \vee (H_1 \wedge M_2) \\
c_2 &\leftarrow M_2 \vee H_3 \\
c_3 &\leftarrow (L_1 \wedge H_2) \vee (M_1 \wedge H_2) \\
c_3 &\leftarrow (L_1 \wedge H_2) \vee (L_1 \wedge M_3) \\
c_4 &\leftarrow (L_1 \wedge L_2) \vee (L_1 \wedge L_3) \vee (L_2 \wedge M_3) \vee (L_1 \wedge M_3) \\
c_5 &\leftarrow (H_1 \wedge M_2) \vee (M_1 \wedge M_3) \vee (M_1 \wedge M_2) \vee (M_2 \wedge L_1) \\
c_5 &\leftarrow (H_1 \wedge M_2) \vee (M_1 \wedge M_2) \vee (H_1 \wedge H_3) \vee (H_2 \wedge L_1) \\
c_5 &\leftarrow (L_2 \wedge L_1) \vee (H_3 \wedge M_3) \vee M_1 \\
c_6 &\leftarrow L_1 \vee M_3 \vee L_2 \\
c_6 &\leftarrow M_1 \vee H_3 \\
c_6 &\leftarrow L_1 \vee H_3 \\
c_6 &\leftarrow M_1 \vee M_3 \vee L_2.
\end{aligned}
$$

Fuzzification Parameters:

Feature 1: $c_L = 0.348$, $c_M = 0.463$, $c_H = 0.613$, $\lambda_L = 0.115$, $\lambda_M = 0.150$, $\lambda_H = 0.134$
Feature 2: $c_L = 0.219$, $c_M = 0.437$, $c_H = 0.725$, $\lambda_L = 0.218$, $\lambda_M = 0.253$, $\lambda_H = 0.288$
Feature 3: $c_L = 0.396$, $c_M = 0.542$, $c_H = 0.678$, $\lambda_L = 0.146$, $\lambda_M = 0.140$, $\lambda_H = 0.135$

The classification accuracies obtained by the models are analyzed for statistical significance. Tests of significance (as described in Section 2.5.1) are performed for the inequality of means (of accuracies) obtained using the proposed algorithm and the other methods compared. In Table 6.2, we present the mean and standard deviation (SD) of the accuracies. Using the means and SDs, the value of the test statistics is computed. If the value exceeds the corresponding tabled value, the means are unequal with statistical significance (algorithm having higher mean accuracy being significantly superior to the one having lower value).

It is observed from Table 6.2 that Model S performs the best (except for Model R on Vowel data and Model F on Hepatobiliary data) with the least network size as well as least number of sweeps. For Model R with Vowel data and Model F with Hepatobiliary data, the classification performance on test set is marginally better than that of Model S, but with significantly higher number of links and training sweeps required. Comparing models F and R, we observe that the incorporation of domain knowledge in the latter through rough sets boosts its performance. Similarly, using the modular approach with GA (Model FM) improves the efficiency of Model F. Since

Model S encompasses the principle of both models R and FM, it results in the least redundant yet most effective model. The variation of the classification accuracy of the models with iteration is also studied. As expected, Model S is found to have high recognition score at the very beginning of evolutionary training, the next values are attained by models R and FM, and the lowest being attained by models O and F using backpropagation. For example, in the case of Vowel data, these figures are 64% for S, 52% for R, 44% for FM, and 0% for F and O. Model S converges after about 90 iterations of the GA, providing the highest accuracy compared to all the other models. The backpropagation based models require about 2000-5000 iterations for convergence.

It may be noted that the training algorithm suggested is successful in imposing a structure among the connection weights. As seen from Figure 6.8, for Vowel data, the weight values for a fuzzy MLP trained with BP (Model F) is more or less uniformly distributed between the maximum and minimum values. On the other hand, the modular rough-fuzzy MLP (Model S) has most of its weight values zero while majority of its non-zero weights have a high value. Hence it can be inferred that the former model results in a dense network with weak links, while the incorporation of rough sets, modular concepts and GAs produces a sparse network with strong links. The latter is suitable for rule extraction. The connectivity (positive weights) of the trained network is shown in Figure 6.9.

6.5.2 Rule extraction

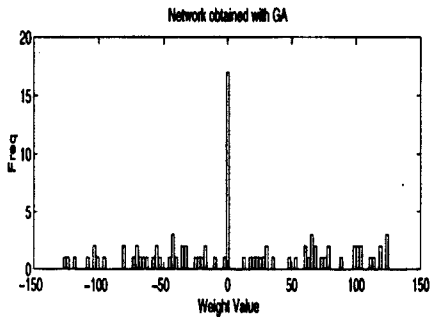
We use the algorithm explained in Section 6.4.1 to extract rules from the trained network (Model S). These rules are compared with those obtained by the *Subset* method [42], *M of N* method [162], a pedagogical method X2R [85] and a decision tree-based method C4.5 [145] in terms of the performance measures (Section 6.4.2). The set of rules extracted from the proposed network (Model S) is presented in Table 6.4 along with their certainty factors (*cf*) for Vowel, Hepatobiliary and Pat data. The values of the fuzzification parameters of the membership functions L, M and H are also mentioned. For the Hepatobiliary data we present the fuzzification parameters only for those features that appear in the extracted rules.

A comparison of the performance indices of the extracted rules is presented in Table 6.3. Since the network obtained using Model S contains fewer links, the generated rules

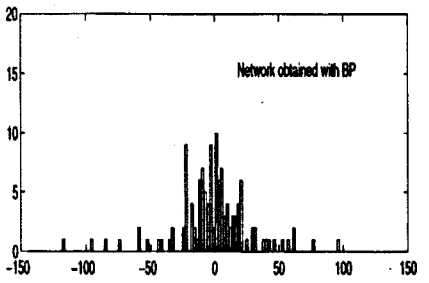
Table 6.2: Comparative performance of different models

Models	Model O		Model F		Model R		Model FM		Model S	
	Train	Test	Train	Test	Train	Test	Train	Test	Train	Test
Vowel data										
Accuracy(%) (Mean SD)	65.4 0.5	64.1 0.5	84.1 0.4	81.8 0.5	86.7 0.3	86.0 0.2	85.3 0.4	82.3 0.5	87.1 0.2	85.8 0.2
# links	131		210		152		124		84	
Sweeps	5600		5600		2000		200		90	
Pat data										
Accuracy(%) (Mean SD)	55.1 0.4	54.8 0.3	68.7 0.5	68.1 0.5	73.1 0.4	71.1 0.4	70.2 0.5	69.8 0.4	75.7 0.5	74.7 0.4
# links	62		105		82		84		72	
Sweeps	2000		2000		1500		150		90	
Hepatobiliary data										
Accuracy(%) (Mean SD)	70.1 0.4	60.0 0.3	66.1 0.4	69.8 0.5	76.9 0.4	68.0 0.5	76.8 0.4	67.4 0.5	78.4 0.4	68.9 0.5
# links	143		310		190		230		108	
Iterations	2500		2500		1500		200		110	

SD: Standard Deviation



(a)



(b)

Figure 6.8: Histogram plot of the distribution of weight values with (a) Model S and (b) Model F for Vowel data

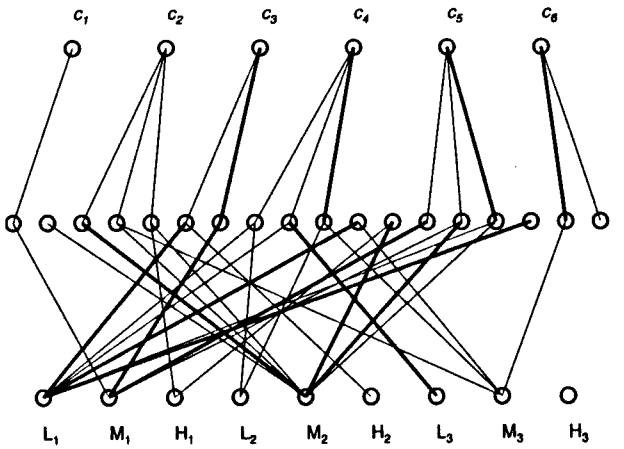


Figure 6.9: Positive connectivity of the network obtained for the Vowel data, using Model S. (Bold lines indicate weights greater than $PThres_2$, while others indicate values between $PThres_1$ and $PThres_2$)

Table 6.3: Comparison of the performance of the rules extracted by various methods for Vowel, Pat and Hepatobiliary data

	Algorithm	Accuracy (%)	Users' Accuracy (%)	Kappa (%)	Uncovered Region (%)	No. of Rules	CPU time (Sec)	*Conf*
V	Model S	81.02	83.31	78.17	3.10	10	1.1	1.4
O	Subset	82.01	82.72	77.29	2.89	16	1.4	1.9
W	M of N	79.00	80.01	74.55	2.10	14	1.2	1.9
E	X2R	76.00	75.81	72.34	2.72	14	0.9	1.7
L	C4.5	79.00	79.17	77.21	3.10	16	1.0	1.5
	Model S	70.31	74.44	71.80	2.02	8	1.0	1.1
P	Subset	71.02	73.01	70.09	1.91	16	1.1	1.5
A	M of N	70.09	71.12	70.02	2.02	11	1.1	1.5
T	X2R	67.82	68.23	67.91	1.91	10	0.9	1.4
	C4.5	71.02	73.44	72.00	2.02	11	1.1	1.2
H	Model S	64.90	64.70	64.10	8.02	7	0.9	1.4
E	Subset	65.00	65.41	64.44	7.52	11	1.0	1.8
P	M of N	63.91	64.00	63.02	8.02	10	1.0	1.8
A	X2R	61.02	60.90	60.90	7.91	9	0.9	1.7
TO	C4.5	64.01	64.23	64.90	7.91	10	0.9	1.4

are less in number and they have high *certainty factor*. Accordingly, it possesses relatively higher percentage of uncovered region, though the accuracy did not suffer much. Although the *Subset* algorithm achieves the highest *accuracy*, it requires the largest number of rules and computation time. In fact, the accuracy/computation time of Subset method is marginally better/worse than Model S, while the size of the rule base is significantly less for Model S.

The accuracy achieved by Model S is better than that of *M of N*, X2R and C4.5, except for the *Pat* data with C4.5. Also considering *user's accuracy* and *kappa*, the best performance is obtained by Model S. The X2R algorithm requires least computation time but achieves least accuracy with more rules. The *Conf* index is the minimum for rules extracted by Model S; it also has high *fidelity* (e.g., 94.22%, 89.17% and 74.88% for Vowel, Pat and Hepatobiliary data respectively).

In a part of the experiment, we also conducted a comparison with Models F, R and FM for rule extraction. It was observed that the performance degrades substantially for them because these networks are less structured and hence less suitable, as compared to Model S, for rule extraction.

Table 6.4: Rules extracted from trained networks (Model S) for Vowel, Pat and Hepatobiliary data along with the input fuzzification parameter values

Vowel data

$c_1 \leftarrow M_1 \vee L_3 \vee M_2 \quad cf = 0.851$
$c_1 \leftarrow H_1 \vee M_2 \quad cf = 0.755$
$c_2 \leftarrow M_2 \vee M_3 \quad cf = 0.811$
$c_2 \leftarrow \neg M_1 \wedge \neg H_1 \wedge L_2 \wedge M_2 \quad cf = 0.846$
$c_3 \leftarrow L_1 \vee H_2 \quad cf = 0.778$
$c_4 \leftarrow L_1 \wedge L_2 \wedge \neg L_3 \quad cf = 0.719$
$c_5 \leftarrow M_1 \wedge H_2 \quad cf = 0.881$
$c_5 \leftarrow M_1 \wedge M_2 \quad cf = 0.782$
$c_5 \leftarrow H_1 \wedge M_2 \quad cf = 0.721$
$c_6 \leftarrow \neg H_2 \quad cf = 0.717$

FuzzificationParameters :

Feature 1 : $c_L = 0.34$, $c_M = 0.502$, $c_H = 0.681$
Feature 1 : $\lambda_L = 0.122$, $\lambda_M = 0.154$, $\lambda_H = 0.177$
Feature 2 : $c_L = 0.217$, $c_M = 0.431$, $c_H = 0.725$
Feature 2 : $\lambda_L = 0.211$, $\lambda_M = 0.250$, $\lambda_H = 0.288$
Feature 3 : $c_L = 0.380$, $c_M = 0.540$, $c_H = 0.675$
Feature 3 : $\lambda_L = 0.244$, $\lambda_M = 0.212$, $\lambda_H = 0.224$

Pat data

$c_1 \leftarrow M_1 \wedge M_2 \quad cf = 0.674$
$c_1 \leftarrow M_1 \wedge H_1 \wedge \neg L_2 \quad cf = 0.875$
$c_2 \leftarrow L_2 \wedge H_1 \quad cf = 0.80$
$c_2 \leftarrow L_2 \wedge M_1 \quad cf = 0.778$
$c_3 \leftarrow L_1 \wedge L_2 \quad cf = 0.636$
$c_3 \leftarrow H_1 \wedge H_2 \quad cf = 0.674$
$c_3 \leftarrow M_1 \wedge M_2 \wedge \neg L_2 \quad cf = 0.636$
$c_3 \leftarrow M_1 \wedge M_2 \wedge \neg L_2 \quad cf = 0.636$

FuzzificationParameters :

Feature 1 : $c_L = 0.216$ $c_M = 0.499$ $c_H = 0.751$
Feature 1 : $\lambda_L = 0.282$ $\lambda_M = 0.265$ $\lambda_H = 0.252$
Feature 2 : $c_L = 1.266$ $c_M = 1.737$ $c_H = 2.511$
Feature 2 : $\lambda_L = 0.244$ $\lambda_M = 0.235$ $\lambda_H = 0.226$

Hepatobiliary data

$c_1 \leftarrow L_3 \wedge M_6 \wedge \neg L_1 \quad cf = 0.857$
$c_1 \leftarrow L_3 \wedge \neg L_6 \wedge L_1 \quad cf = 0.800$
$c_2 \leftarrow L_2 \wedge M_2 \wedge M_3 \quad cf = 0.846$
$c_2 \leftarrow M_6 \quad cf = 0.571$
$c_3 \leftarrow L_3 \wedge L_2 \wedge M_3 \quad cf = 0.800$
$c_4 \leftarrow L_3 \wedge L_6 \wedge \neg L_1 \quad cf = 0.833$
$c_4 \leftarrow M_2 \wedge L_2 \wedge \neg M_3 \quad cf = 0.833$

FuzzificationParameters :

Feature 1 : $c_L = 52.47$ $c_M = 112.88$ $c_H = 289.17$
Feature 1 : $\lambda_L = 62.44$ $\lambda_M = 118.35$ $\lambda_H = 176.40$
Feature 2 : $c_L = 24.04$ $c_M = 53.41$ $c_H = 125.35$
Feature 2 : $\lambda_L = 29.15$ $\lambda_M = 55.14$ $\lambda_H = 72.08$
Feature 3 : $c_L = 336.15$ $c_M = 477.95$ $c_H = 844.00$
Feature 3 : $\lambda_L = 140.00$ $\lambda_M = 254.44$ $\lambda_H = 367.01$
Feature 6 : $c_L = 12.15$ $c_M = 17.27$ $c_H = 25.52$
Feature 6 : $\lambda_L = 5.11$ $\lambda_M = 7.18$ $\lambda_H = 9.25$

Rules for staging of cervical cancer with binary feature inputs [97]:

Investigation is also made to demonstrate the effectiveness of the aforesaid concept of modular rule evolution to the problem of staging of cervical cancer where the rules corresponding to four stages are validated by oncologists. Here the symptoms (features) are binary valued. Therefore conventional MLP is used, instead of fuzzy MLP. Knowledge encoding is done using rough set theoretic rules which are generated directly from the feature values (without fuzzification). One thus obtains a modular rough MLP (denoted by Model RM, say), instead of the modular rough-fuzzy MLP (Model S) studied in earlier experiments. Before we present the experimental results, we describe, in brief, the problem of cancer staging, details of the features (clinical measurements) involved and the patient data used for building the modular rough MLP model.

Staging is a process that uses information learnt about cancer through diagnostic processes, such as the size of the tumor, how deeply the tumor has invaded tissues at the site of the origin, the extent of any invasion into surrounding organs, and the extent of metastasis (spread) to lymph nodes or distant organs. This is a very important process because proper staging is the most important factor in selecting the right treatment plan. Cervical cancer is most frequently staged using the FIGO (International Federation of Gynaecology and Obstetrics) System of Staging. This system classifies the disease in Stages I through IV.

The data used consists of a set of 221 cervical cancer patient cases obtained from the database of the Chittaranjan National Cancer Institute (CNCI), Calcutta. There are four classes corresponding to Stages I, II, III and IV of the cancer, containing 19, 41, 139, and 19 patient cases respectively. The features of the proposed model represent the presence or absence of the symptoms, and the signs observed upon physical examination. The 21 boolean input features refer to *Vulva: healthy (Vu(h)), Vulva: lesioned (Vu(l)), Vagina: healthy (Va(h)), Vagina: spread to upper part (Va(u)), Vagina: spread to middle part (Va(m)), Vagina: spread to lower part (Va(l)), Cervix: healthy (Cx(h)), Cervix: eroded (Cx(e)), Cervix: small ulcer (Cx(su)), Cervix: ulcerative growth (Cx(u)), Cervix: proliferative growth (Cx(p)), Cervix: ulcero-proliferative growth (Cx(l)), Paracervix: free (PCx(f)), Paracervix: infiltrated (PCx(i)), Urinary bladder base: soft (BB(s)), Urinary bladder base: hard (BB(h)), Rectrovaginal septum: free (RVS(f)), Rectrovaginal septum: infiltrated (RVS(i)), Parametrium: free*

Table 6.5: Crude rules obtained via rough set theory for staging of cervical cancer

I	Cx(su) ∨ Para(f), Cx(p) ∨ Para(f), Cx(su) ∨ Para(nu)
II	Va(h) ∨ Cx(u), Va(h) ∨ Cx(l), Va(u) ∨ Cx(u), Para(nu), Pcx(f)
III	Para(nu), Para(u), Va(u) (Va(u) ∧ Cx(u)) ∨ Cx(l) ∨ Va(m) (Va(h) ∧ Cx(u)) ∨ (Va(u) ∧ Cx(u)) ∨ Cx(l) (Va(u) ∧ Cx(p)) ∨ Va(m) ∨ Cx(l)
IV	(Va(l) ∧ Cx(u)) ∨ (Cx(u) ∧ Va(u)) ∨ (Va(l) ∧ Para(u)) (Va(l) ∧ Cx(p)) ∨ Va(m).

Table 6.6: Rules extracted from the modular rough MLP for staging of cervical cancer

$$
\begin{aligned}
I &\leftarrow (Va(h) \wedge Para(f)) \vee (Cx(h) \wedge Cx(u) \wedge BB(s)) \\
II &\leftarrow (PCx(f) \wedge PCx(i)) \vee Para(f) \vee Para(nu) \\
III &\leftarrow Va(h) \wedge Cx(u) \wedge Cx(l) \wedge Para(u) \\
IV &\leftarrow Va(m) \vee (Cx(u) \wedge Cx(p)) \vee (Para(nu) \wedge Para(u)).
\end{aligned}
$$

(Para(f)), Parametrium: spread, but not upto (Para(nu)) and *Parametrium: spread upto (Para(u))* respectively.

The dependency rules generated via rough set theory and used in the encoding scheme are provided in Table 6.5. The evolved network is found to have (for recognition score around 80%) 118 links in 50 iterations, *vis-a-vis* 175 links in 90 iteration for the conventional MLP (Model O). A sample set of refined rules extracted from the network is presented in Table 6.6.

The expertise obtained from oncologists regarding different stages is provided below. In Stage I the cancer has spread from the lining of the cervix into the deeper connective tissue of the cervix. But it is still confined within the cervix. Stage II signifies the spread of cancer beyond the cervix to nearby areas like parametrial tissue, that are still inside the pelvic area. In Stage III the cancer has spread to the lower part of the vagina or the pelvic wall. It may be blocking the ureters (tubes that carry urine from the kidneys to the bladder). Stage IV is the most advanced stage of cervical cancer. Now the cancer has spread to other parts of the body, like rectum, bladder or lungs. It may be mentioned here that the rules generated by the proposed algorithm (Table 6.6)

conform to the experts' opinion.

The performance of the popular C4.5 machine learning system [145] on the data set was also studied as a benchmark. Sample rules generated by C4.5 are:

I $\leftarrow$ Va(h) $\wedge$ PCx(f) $\wedge$ Para(f)
II $\leftarrow$ Para(f)
II $\leftarrow$ BB(s)
III $\leftarrow$ BB(s) $\wedge$ Para(u)

Note that, the rules obtained using C4.5 are significantly poorer than those obtained by the proposed methodology. This is due to the fact that only statistically significant instances of the stages are represented in the rules by C4.5. On the other hand, in the proposed model the rare patient cases are also preserved and incorporated into the network in the process of knowledge encoding and structured training. This leads to a more complete rule base.

6.6 Conclusions and Discussion

A methodology for modular evolution of a rough-fuzzy MLP using genetic algorithms for designing a knowledge-based network for pattern classification and rule generation is presented. The proposed algorithm involves synthesis of several MLP modules, each encoding the rough set rules for a particular class. These knowledge-based modules are refined using a GA. The genetic operators are implemented in such a way that they help preserve the modular structure already evolved. It is seen that this methodology along with modular network decomposition results in accelerated training and more sparse (compact) network with comparable classification accuracy, as compared to earlier hybridizations.

The aforesaid model is used to develop a new rule extraction algorithm. The extracted rules are compared with the ones generated from some of the related rule extraction techniques on the basis of some quantitative performance indices. These indices reflect the knowledge discovery aspect. Two new measures, introduced in this regard to evaluate the confidence and ambiguity in a decision, are found to be satisfactory. It

is observed that the proposed methodology extracts rules which are less in number, yet accurate, and have high certainty factor and low confusion with less computation time. The investigation, besides having significance in soft computing research, has potential for application to large scale problems involving knowledge discovery tasks [104], particularly related to mining of linguistic classification rules.

Chapter 7

Conclusions and Scope for Further Research

7.1 Conclusions

In every chapter we have presented conclusions drawn from the respective methodologies developed and the experimental results therein. Here we consolidate them to provide an overall picture of the contributions of the thesis.

The thesis dealt with certain pattern recognition tasks essential for data mining. Tasks considered include data condensation, feature selection, case generation, clustering, classification and rule generation/evaluation. Various methodologies have been developed using both classical and soft computing approaches (integrating fuzzy logic, artificial neural networks, rough sets, genetic algorithms). The emphasis of the proposed methodologies is given on handling data sets which are large (both in size and dimension) and involve classes that are overlapping, intractable and/or having nonlinear boundaries. Several strategies based on data reduction, dimensionality reduction, active learning, granular computing and efficient search heuristics are employed for dealing with the issue of 'scaling up' in learning problem. The problems of handling linguistic input and ambiguous output decision, learning of overlapping/intractable class structures, selection of optimal parameters, and discovering human comprehensible knowledge (in the form of linguistic rules) are addressed in soft computing framework. Different features of the methodologies, along with comparisons with those of the related ones, are demonstrated extensively on different real life data sets. These data have number of dimensions ranging from 2 to 649 and samples ranging from 150 to 581012, taken from varied domains e.g., geographical information systems, remote sensing imagery, population census, speech recognition and cancer management. Superiority of the proposed models over several related ones is found to be statistically significant.

The data condensation algorithm of Chapter 2 performs non-parametric data reduction in a multiresolution manner based on the density underlying the data. The method can obtain reduced sets to represent the data at different degrees of detail (scales). The representation gives adequate importance to different regions of the feature space based on the respective probability densities. The said scale structure is efficient in terms of density estimation error and provides a natural representation of the data distribution. The algorithm obtains a generic representative condensed set, independent of the task performed with it later, and suitable for a number of data mining applications e.g.,

classification, clustering and rule generation.

The unsupervised feature selection algorithm (described in Chapter 3) is based on pairwise feature similarity measures. The novelty of the method, as compared to other conventional feature selection algorithms, is the absence of search process which contributes to the high computational time requirement of those feature selection algorithms. Unlike other approaches which are based on optimizing either classification or clustering performance explicitly, here we determine a set of maximally independent features by discarding the redundant ones. This enhances the applicability of the resulting features to compression and other tasks like forecasting, summarization, association mining in addition to classification/clustering. Another characteristic of the algorithm is its capability of multiscale representation of data sets. The scale parameter k used for feature clustering efficiently parametrizes the trade-off between representation accuracy and feature subset size. All these make it suitable for a wide variety of mining tasks.

The first algorithm, described in Chapter 4, for active support vector learning demonstrates the advantages of active resampling over random sample selection. The second one, based on the statistical query model of learning, involves a query strategy which uses an adaptive confidence factor to handle the trade-off between selecting interior points and points close to the current separating hyperplane. In the initial phase of learning it explores more number of interior points, while in the final phase it focuses only on the points close to the separating hyperplane and ignores the redundant interior points. This helps the algorithm to achieve fast and smooth (oscillation free) convergence as compared to the preceding two methods.

The methodologies for case generation and clustering presented in Chapter 5 exploit the merits of rough-fuzzy hybridization for granular computing. Fuzzy set theory is used to represent a pattern in terms of its membership to some linguistic sets; thereby producing a fuzzy granulated feature space. Rough set theory is used to obtain cases (class prototypes) through crude rules from the fuzzy granulated feature space. Since the algorithm deals with information granules, and not the original data, case generation time is reduced. Also, since only the informative regions and the relevant characterizing subset of features are stored (i.e., the generated cases are represented by different reduced number of features), case retrieval time decreases significantly. Therefore, this case generation algorithm is suitable for mining data sets, large both in

dimension and size. Note that, while the methods in Chapters 2 and 3 perform data condensation and dimensionality reduction separately, the cases generated in Chapter 5 represent a condensed version of the data set with reduced dimension.

Rough-fuzzy granulation is also found to be successful not only in circumventing the initialization and local minima problems of iterative refinement clustering algorithms (like, EM and k-means), but also in improving their clustering performance. Besides these, the contribution of the chapter lies in the development of a methodology integrating the merits of graph-theoretic clustering (e.g., capability of generating non-convex clusters) and iterative refinement clustering (such as low computational time requirement) for efficient detection of non-convex clusters.

A rough-fuzzy MLP is used in Chapter 6 for designing a modular knowledge-based network for pattern classification and linguistic rule generation. A new concept of variable mutation operator is introduced. This helps in preserving the individual clusters in the final solution. It is seen that the modular network decomposition results in accelerated training and more sparse (compact) network with comparable classification accuracy, as compared to earlier related hybridizations.

The aforesaid model is used to develop a rule extraction algorithm. Two measures are newly introduced to evaluate quantitatively the confidence and ambiguity in a decision caused by the rules. These indices along with other measures, like accuracy, kappa value, fidelity, and coverage, reflect the knowledge discovery aspect and are used to compare the performance of the rule extraction algorithm.

The algorithm for multiscale data condensation (Chapter 2) is found to have superior performance as compared to the methods based on random sampling [22], self organizing map [72], and uniform scale method [9] in terms of error in density estimate. The MLP and k-NN classifiers, when designed using the condensed set obtained by our algorithm, provide higher accuracy rate compared to the cases when these classifiers are designed using the condensed sets obtained by other algorithms based on stratified sampling [22], condensed nearest neighbor [54], learning vector quantization [72] and locally adaptive asymmetrically weighted metric [150]. If the points in the condensed set, obtained by our multiscale method, are used as the prototypes for clustering, then the resulting clusters have β value higher than that generated by the k-means algorithm [30]. Also, the rules extracted from the multiscale condensed set (using the C4.5

algorithm [145]) are compact, yet having higher accuracy rate and cover value as compared to those obtained by the algorithms based on random sampling [22], stratified sampling [22], condensed nearest neighbor [54] and uniform scale method [9]. Besides these, the proposed data condensation algorithm is found to be scalable and efficient in terms of sample complexity, in the sense that the (density estimation) error level decreases quickly with the increase in size of the condensed set.

The unsupervised feature selection algorithm in Chapter 3 is seen to be superior (in terms of clustering/ classification performance and redundancy reduction) to four related methods *viz*, branch and bound algorithm [30], sequential floating forward search [144], sequential forward search [30] and stepwise clustering [69], when real life data sets with dimension ranging from 4 to 649 are considered. It requires several orders less CPU time compared to search based methods like branch and bound algorithm [30], sequential floating forward search [144], and sequential forward search [30]. The maximal information compression index, used as feature similarity measure, is seen to be more effective for redundancy reduction as compared to other such similarity measures e.g., correlation and least square regression error.

The method of support vector learning based on active resampling (Chapter 4) has higher classification score, lower $\mathcal{D}$ value and faster convergence compared to random SVM [153]. However, the method for active SV learning, based on statistical query, performs the best in terms of speed and robustness when compared with the two preceding algorithms and the query SVM [21].

Cases generated using the rough-fuzzy scheme in Chapter 5 are found to be better in terms of 1-NN classification accuracy, average number of features per case, case generation time and average case retrieval time, when compared with the conventional IB3 and IB4 algorithms [5], and the random case selection method [164].

Rough set with fuzzy discretization enhances the performance of EM algorithm both in terms of β-value (cluster quality) and computation time. Integration of minimal spanning tree with rough-fuzzy initialized EM, results in further improvement of performance with a slight increase in computational time. This hybridization provides, in addition, the capability of detecting non-convex clusters efficiently. These conclusions also hold good for the problem of segmentation of multispectral satellite images into different landcover types.

Superiority of the modular rough-fuzzy MLP model (Chapter 6) to conventional MLP, fuzzy MLP and rough-fuzzy MLP is experimentally demonstrated in terms of classification accuracy, network size and training time when both real life (speech and medical) and artificially generated data sets, with class boundaries overlapping as well as non-linear, are considered as input. The linguistic rules extracted from the modular rough-fuzzy MLP are less in number, yet accurate, and have high certainty factor and low confusion with less computation time as compared to those extracted using *Subset* [42], *M of N* [162] and X2R [85]. This investigation, besides having significance in soft computing research, has potential for application to large scale problems involving knowledge discovery tasks [104], particularly related to mining of linguistic classification rules.

7.2 Scope for Further Research

The data condensation methodology, described in Chapter 2, involves non-parametric density estimation and data reduction. A mathematical framework of the notion of data condensation is required to be developed for more comprehensive study of the problem. The asymptotic convergence of the condensation procedure and its finite sample error rate need to be analyzed. It may be noted that k-nearest neighbor density estimate (used in the methodology) from finite and non-i.i.d. samples is an open research area which has drawn recently the attention of researchers from different fields.

A way of reducing the time complexity of the aforesaid algorithm is to use approximate nearest neighbor (ANN) computations using specialized data structures like k-d trees [7]. Probabilistic nearest neighbor search methods [36], having expected $\mathcal{O}(1)$ time complexity and $\mathcal{O}(N)$ storage complexity, may also be used for this purpose.

The feature selection algorithm (Chapter 3) is more related to feature selection for information compression rather than for classification/clustering. Recently, several information theoretic criteria are being used for incremental feature selection. Relationship of our method with these algorithms needs to be studied.

In Chapter 4, we have presented a statistical query based algorithm for active support vector learning. The nature of the query probability varies adaptively over iteration.

A decision theoretic generalization of the above scheme may provide better active learning strategies. Also, the relationship of the proposed active learning strategy with the mistake bound model of online learning may be investigated.

Chapter 5 demonstrates the power of granular computing by developing a rough-fuzzy scheme for case (class prototypes) generation and clustering in large data sets. In this regard a simple rough set rule generation strategy is adopted along with fuzzy granulation. However, more general rough set models like tolerance relations and rough mereology may yield better performance. Also, the capability of rough mereology for handling heterogeneous, symbolic and relational data may be utilized for problems like multimedia mining and genomic data analysis.

The modular rough-fuzzy MLP (Chapter 6) generates a structured network providing high classification accuracy. This is achieved by constrained evolution of the network, implemented by a modified genetic algorithm. In other words, the search is performed over a restricted hypothesis space. It is observed that the weight values of the solution network obtained using the above approach are not uniformly distributed, there is presence of a few strong links, others being mostly non-existent. Such networks are known to have better generalization capability. Its VC-dimension is likely to be lower than that of the ordinary MLP. Establishing this theoretically may constitute an interesting future research problem. Again, one may investigate the sensitivity of the rule evaluation indices with respect to network weights.

We have used various indices for quantitative evaluation of the linguistic rules. Some of these indices (e.g., fidelity, coverage, confusion, certainty) may be used in a suitable combination to act as the objective function of the network, instead of classification accuracy, for generating a knowledge based connectionist system. This formulation is geared towards maximizing the utility of the network with respect to knowledge discovery tasks.

Over the last decade, we have witnessed an explosive growth in the information available on the World Wide Web (WWW). Web mining, though considered to be a particular application of data mining, warrants a separate field of research mainly because of the typical characteristics of web data and human interface related issues. The pattern recognition and soft computing algorithms studied in the thesis have potential of being used in web mining applications [128].

Appendix A

Data Sets Used in Experiments

We present below the details of the data sets used in empirical evaluation and comparison of the algorithms developed. They are listed in the order of their size (number of samples and dimensions).

1. *Forest cover type*: The data represents forest cover types of 30m × 30m cells obtained from US Forest Service (USFS) Region 2 Resource Information System (RIS). There are 581012 instances, with 54 attributes representing cartographic variables (hillshade, distance to hydrology, elevation, soil type etc), of which 10 are quantitative and 44 binary. The task is to classify the observations into seven categories representing the forest cover types, namely – Spruce/Fir, Lodgepole Pine, Ponderosa Pine, Cottonwood/Willow, Aspen, Douglas-fir, Krummholz. Source: UCI KDD Archive [57].

2. *PUMS census*: Population census data for the Los Angeles and Long Beach area. The data contains 320,000 samples and 133 attributes (mostly categorical or integer valued). The task is to identify two groups of population namely those who have undergone/not undergone 'higher education', measured in terms of number of years in college. Source: UCI KDD Archive [57].

3. *Satellite image*: Gray level images of four different spectral bands obtained by the Indian Remote Sensing satellite of the city of Calcutta in India. Each image is 512 × 512 pixel in size. Source: NRSA data center, India.

4. *Isolet*: The data consists of several spectral coefficients of utterances of English alphabets by 150 subjects. There are 617 features all real in the range $[0, 1]$, 7797 instances and 26 classes. Source: UCI Machine Learning Repository [15].

5. *Multiple features*: This data set consists of features of handwritten numerals ('0'-'9') extracted from a collection of Dutch utility maps. There are total 2000 patterns, 649 features and 10 classes. Source: UCI Machine Learning Repository [15].

6. *Twonorm*: Artificial data [18] having 20000 samples, 20 features and 2 classes. Each class follows multivariate normal distribution with covariance matrix as the identity matrix. Class 1 has mean $(a, a, \ldots, a)$ and class 2 has mean $(-a, -a, \ldots, -a)$. $a = \frac{2}{\sqrt{20}}$. Source: UCI Machine Learning Repository [15].

7. *Ringnorm*: Artificial data [18] having 20000 samples, 20 features and 2 classes. Each class is multivariate normal. Class 1 has mean $(0, 0, \ldots, 0)$ and covariance matrix as 4 time the identity matrix, class 2 has mean $(a, a, \ldots, a)$ and covariance matrix as the identity matrix. $a = \frac{2}{20^{\frac{1}{2}}}$. Source: UCI Machine Learning Repository [15].

8. *Waveform*: Noisy artificial data [18]. It consists of 5000 instances having 40 attributes each. The attributes are continuous valued, and some of them are noise. The task is to classify an instance into one of the 3 categories of waves. Source: UCI Machine Learning Repository [15].

9. *Spambase*: Word frequencies of email, used to classify an email into spam or non-spam category. There are 4601 instances, 57 continuous valued attributes denoting word frequencies, and 2 classes. Source: UCI Machine Learning Repository [15].

10. *Arrhythmia*: Parameters of ECG measurements used to classify a patient into classes of cardiac arrhythmia. It contains 452 samples each having 279 attributes. Among the attributes 195 are real valued, and are used for our experiments. Source: UCI Machine Learning Repository [15].

11. *Heart*: Diagnostic measurements of Cleveland heart disease. It contains 1535 data points belonging to 2 classes. Number of features is 16. Source: UCI Machine Learning Repository [15].

12. *Vowel*: Formant frequencies of Indian Telugu vowels [117] uttered in consonant-vowel-consonent context by 3 male speakers in the age group of 30-35 years. It contains 871 samples, 3 features and 6 classes. Source: Machine Intelligence Unit, Indian Statistical Institute, Calcutta.

13. *Pat*: Artificial linearly nonseparable data as shown in Figure 5.8 [123]. There are 880 samples, 2 features and 2 classes. Source: Machine Intelligence Unit, Indian Statistical Institute, Calcutta.

14. *Pima*: Clinical measurements to detect diabetes disease of Pima Indian tribe. There are 768 samples, 8 features and 2 classes. Source: UCI Machine Learning Repository [15].

15. *Wisconsin cancer*: Clinical measurements to detect breast cancer. It contains 9 features, 684 instances and 2 classes. Source: UCI Machine Learning Repository [15].

16. *Hepatobiliary*: Results of biochemical tests (e.g., Glutamic Oxalacetic Transaminate, Glutamic Pyruvic Transaminase, Lactate Dehydrase, Gamma Glutamyl Transpeptidase, Blood Urea Nitrogen) used to detect Hepatobiliary disorders like Alcoholic Liver Damage, Primary Hepatoma, Liver Cirrhosis and Cholelithiasis [56]. There are 536 samples, 9 features and 4 classes.

17. *Monks-2*: AI game playing moves data having 432 samples, 6 features and 2 classes. Source: UCI Machine Learning Repository [15].

18. *Ionosphere*: The data represents autocorrelation functions of radar measurements. The task is to classify them into 2 classes denoting passage or obstruction in ionosphere. There are 351 instances and 34 attributes, all continuous. Source: UCI Machine Learning Repository [15].

19. Cervical cancer: Clinical measurements for staging of cervical cancer [97]. There are 221 samples, 21 features and 4 classes. Source: Machine Intelligence Unit, Indian Statistical Institute, Calcutta.

20. *Iris*: Measurements of Iris flowers. There are 150 samples, 4 features and 3 classes. Source: UCI Machine Learning Repository [15].

21. *Norm*: Artificial bivariate normal data with zero mean and covariance matrix as the identity matrix [100]. It contains 500 samples and 2 features.

Bibliography

[1] R. Agrawal, H. Mannila, R. Srikant, H. Toivonen, and I. Verkamo. Fast discovery of association rules. In U. M. Fayyad, G. Piatetsky-Shapiro, P. Smyth, and R. Uthuruswamy, editors, *Advances in Knowledge Discovery and Data Mining*, pages 307–328. MIT Press, Cambridge, MA, 1996.

[2] D. W. Aha. Tolerating noisy, irrelevant and novel attributes in instance based learning algorithms. *International Journal of Man Machine Studies*, 36:266–287, 1992.

[3] D. W. Aha. Editorial on lazy learning. *AI Review, Spl. issue on lazy learning*, 11(1-5):7–10, 1997.

[4] D. W. Aha and R. L. Bankert. A comparative evaluation of sequential feature selection algorithms. In D. Fisher and J.-H. Lenz, editors, *Artificial Intelligence and Statistics V*. Springer Verlag, New York, 1996.

[5] D. W. Aha, D. Kibler, and M. K. Albert. Instance-based learning algorithms. *Machine Learning*, 6:37–66, 1991.

[6] D. Angluin. Queries and concept learning. *Machine Learning*, 2:319–342, 1988.

[7] S. Arya, D. M. Mount, N. S. Netanyahu, R. Silverman, and A. Y. Wu. An optimal algorithm for approximate nearest neighbor searching. *Journal of the ACM*, 45:891–923, 1998.

[8] A. Aspin. Tables for use in comparisons whose accuracy involves two variances. *Biometrika*, 36:245–271, 1949.

[9] M. M. Astrahan. Speech analysis by clustering, or the hyperphoneme method. In *Stanford A.I. Project Memo.* Stanford University, CA, 1970.

[10] M. Banerjee, S. Mitra, and S. K. Pal. Rough fuzzy MLP: Knowledge encoding and classification. *IEEE Trans. Neural Networks*, 9(6):1203–1216, 1998.

[11] D. Barbará, W. DuMouchel, C. Faloutsos, P. J. Haas, J. M. Hellerstein, Y. E. Ioannidis, H. V. Jagadish, T. Johnson, R. T. Ng, V. Poosala, K. A. Ross, and K. C. Sevcik. The New Jersey data reduction report. *IEEE Data Engineering Bulletin*, 20(4):3–45, 1997.

[12] E. B. Baum and D. Haussler. What size nets give valid generalization? *Neural Computation*, 1:151–160, 1989.

[13] J. L. Bentley. Multidimensional divide and conquer. *Comm. ACM*, 23(4):214–219, 1980.

[14] J. C. Bezdek and S. K. Pal, editors. *Fuzzy Models for Pattern Recognition: Methods that Search for Structures in Data.* IEEE Press, New York, 1992.

[15] C. L. Blake and C. J. Merz. *UCI Repository of machine learning databases.* University of California, Irvine, Dept. of Information and Computer Sciences, http://www.ics.uci.edu/~mlearn/MLRepository.html, 1998.

[16] P. Bradley, U. M. Fayyad, and C. Reina. Scaling clustering algorithms to large databases. In *Proc. 4th Intl. Conf. Knowledge Discovery and Data Mining*, pages 9–15, NY, 1998. AAAI Press, CA.

[17] P. S. Bradley and O. L. Mangasarian. Massive data discrimination via linear support vector machines. *Optimization Methods and Software*, 13(1):1–10, 2000.

[18] L. Breiman, J. H. Friedman, R. A. Olshen, and C. J. Stone. *Classification and Regression Trees.* Wadsworth and Brooks/Cole, Monterey, CA, 1984.

[19] H. Bunke and A. Kandel, editors. *Neuro-Fuzzy Pattern Recognition.* World Scientific, Singapore, 2001.

[20] C. J. C. Burges. A tutorial on support vector machines for pattern recognition. *Data Mining and Knowledge Discovery*, 2(2):1–47, 1998.

[21] C. Campbell, N. Cristianini, and A. Smola. Query learning with large margin classifiers. In *Proc. 17th Intl. Conf. Machine Learning*, pages 111–118, Stanford, CA, 2000. Morgan Kaufmann, CA.

[22] J. Catlett. *Megainduction: Machine learning on very large databases.* PhD thesis, Department of Computer Science, University of Sydney, Australia, 1991.

[23] D. Chaudhuri, C. A. Murthy, and B. B. Chaudhuri. Finding a subset of representative points in a dataset. *IEEE Trans. Syst. Man. Cybern.*, 24:1416–1424, 1994.

[24] K. Cios, W. Pedrycz, and R. Swiniarski. *Data Mining Methods for Knowledge Discovery.* Kluwer Academic Publishers, Boston, MA, 1998.

[25] D. Cohn, L. Atlas, and R. Ladner. Improving generalization with active learning. *Machine Learning*, 15:201–221, 1994.

[26] S. K. Das. Feature selection with a linear dependence measure. *IEEE Trans. Computers*, 20:1106–1109, 1971.

[27] B. V. Dasarathy. *Nearest Neighbor (NN) Norms: NN Patterns Classification Techniques.* IEEE Computer Society Press, Los Alamitos, 1991.

[28] A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the EM algorithm. *Journal of the Royal Statistical Society, Series B*, 39:1–38, 1977.

[29] K. Deng and A. W. Moore. Multiresolution instance-based learning. In *Proc. Intl. Joint Conf. Artificial Intelligence (IJCAI-95)*, pages 1233–1242, Montreal, Canada, 1995. Morgan Kaufmann, CA.

[30] P. A. Devijver and J. Kittler. *Pattern Recognition: A Statistical Approach.* Prentice Hall, Englewood Cliffs, 1982.

[31] C. Domeniconi and D. Gunopulos. Adaptive nearest neighbor classification using support vector machines. In *Advances in Neural Information Processing System 14 (NIPS'2001)*, Vancouver, Canada, 2001. MIT Press, MA.

[32] R. O. Duda, P. E. Hart, and D. G. Stork. *Pattern Classification (2nd Edition).* Wiley-Interscience, New York, 2000.

[33] W. DuMouchel, C. Volinsky, T. Johnson, C. Cortes, and D. Pregibon. Squashing flat files flatter. In *Proc. 5th ACM Conf. Knowledge Discovery and Data Mining,* pages 6–15, San Diego, CA, 1999. ACM Press, NY.

[34] J. Dy and C. Brodley. Feature subset selection and order identification for unsupervised learning. In *Proc. 17th Intl. Conf. Machine Learning,* pages 247–254, Stanford, CA, 2000. Morgan Kaufmann, CA.

[35] J. Ester, H.-P. Kriegel, J. Sander, and X. Xu. A density-based algorithm for discovering clusters in large spatial databases with noise. In *Proc. 2nd Intl. Conf. Knowledge Discovery and Data Mining (KDD'96),* pages 226–231, Portland, OR, 1996. AAAI Press, CA.

[36] A. Faragó, T. Linder, and G. Lugosi. Nearest neighbor search and classification in $\mathcal{O}(1)$ time. *Problems of Control and Information Theory,* 20(6):383–395, 1991.

[37] U. M. Fayyad, G. Piatetsky-Shapiro, P. Smyth, and R. Uthurusamy, editors. *Advances in Knowledge Discovery and Data Mining.* MIT Press, Menlo Park, CA, 1996.

[38] U. M. Fayyad and R. Uthurusamy. Data mining and knowledge discovery in databases. *Comm. ACM,* 39(11):24–27, 1996.

[39] Y. Freund and R. E. Schapire. Large margin classification using the perceptron algorithm. *Machine Learning,* 37(3):277–296, 1999.

[40] T. Friess, N. Cristianini, and C. Campbell. The kernel adatron algorithm: a fast and simple learning procedure for support vector machine. In *Proc. 15th Intl. Conf. Machine Learning,* pages 188–196, Madison, WI, 1998. Morgan Kaufmann, CA.

[41] K. S. Fu. *Syntactic Pattern Recognition and Applications.* Academic Press, London, 1982.

[42] L. M. Fu. Knowledge-based connectionism for revising domain theories. *IEEE Trans. Systems, Man, and Cybernetics,* 23:173–182, 1993.

[43] K. Fukunaga and J. M. Mantock. Nonparametric data reduction. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 6:115–118, 1984.

[44] J. Ghosh. Multiclassifier systems: Back to the future. In J. Kittler and F. Roli, editors, *Multiple Classifier Systems*, volume 2364 of *Lecture Notes in Computer Science*, pages 1–15. Springer Verlag, London, 2002.

[45] C. Glymour, D. Madigan, D. Pregibon, and P. Smyth. Statistical inference and data mining. *Comm. ACM*, 39:35–41, 1996.

[46] D. E. Goldberg. *Genetic Algorithms in Search, Optimization and Machine Learning.* Addison-Wesley, Reading, MA, 1989.

[47] J. Gray, S. Chaudhuri, A. Bosworth, A. Layman, D. Reichart, M. Venkatrao, F. Pellow, and H. Pirahesh. Data cube: A relational aggregation operator generalizing group-by, cross-tab, and sub-totals. *Data Mining and Knowledge Discovery*, 1(1):29–53, 1997.

[48] R. M. Gray. Vector quantization. *IEEE ASSP Mag.*, 1:4–29, 1984.

[49] S. Guha, R. Rastogi, and K. Shim. CURE: An efficient clustering algorithm for large databases. In *Proc. ACM SIGMOD Intl. Conf. Management of Data*, pages 73–84, New York, 1998. ACM Press, NY.

[50] M. A. Hall. Correlation based feature selection for discrete and numeric class machine learning. In *Proc. 17th Intl. Conf. Machine Learning*, Stanford, CA, 2000. Morgan Kaufmann, CA, http://citeseer.nj.nec.com/hall99correlationbased.htm.

[51] J. Han and M. Kamber. *Data Mining: Concepts and Techniques.* Morgan Kaufmann, San Mateo, CA, 2000.

[52] D. Hand, H. Mannila, and P. Smyth. *Principles of Data Mining.* MIT Press, Menlo Park, CA, 2001.

[53] B. M. Happel and J. J. Murre. Design and Evolution of Modular Neural Network Architectures. *Neural Networks*, 7:985–1004, 1994.

[54] P. E. Hart. The condensed nearest neigbor rule. *IEEE Trans. Information Theory*, 14:515–516, 1968.

[55] T. Hastie, R. Tibshirani, and J. Friedman. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction.* Springer Verlag, NY, 2001.

[56] Y. Hayashi. A neural expert system with automated extraction of fuzzy if-then rules and its application to medical diagnosis. In R. P. Lippmann, J. E. Moody, and D. S. Touretzky, editors, *Advances in Neural Information Processing Systems*, pages 578–584. Morgan Kaufmann, Los Altos, CA, 1991.

[57] S. Hettich and S. D. Bay. *The UCI KDD Archive.* University of California, Irvine, Dept. of Information and Computer Sciences, http://kdd.ics.uci.edu, 1999.

[58] R. P. Heydorn. Redundancy in feature extraction. *IEEE Trans. Computers*, pages 1051–1054, 1971.

[59] T. Imeliensky and H. Mannila. A database perspective on knowledge discovery. *Comm. ACM*, 39:58–64, 1996.

[60] A. K. Jain, R. P. W. Duin, and J. Mao. Statistical pattern recognition: A review. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 22:4–37, 2000.

[61] L. Kanal. Patterns in pattern recognition. *IEEE Trans. Information Theory*, 20:697–722, 1974.

[62] A. Kandel. *Fuzzy Techniques in Pattern Recognition.* Wiley Interscience, New York, 1982.

[63] A. Kandel, M. Last, and H. Bunke, editors. *Data Mining and Computational Intelligence.* Physica Verlag, Heidelberg, 2001.

[64] H. Kargupta and P. Chan, editors. *Advances in Distributed and Parallel Knowledge Discovery.* MIT/AAAI Press, Menlo Park, CA, 2001.

[65] L. Kaufmann. Solving the quadratic programming problem arising in support vector classification. In B. Scholkopf, C. J. C. Burges, and A. J. Smola, editors, *Advances in Kernel Methods - Support Vector Learning*, pages 147–168. MIT Press, MA, 1998.

[66] M. J. Kearns. Efficient noise-tolerant learning from statistical queries. In *Proc. 25th ACM Symposium on Theory of Computing*, pages 392–401, San Diego, CA, 1993. ACM Press, NY.

[67] R. L. Kennedy, Y. Lee, B. van Roy, C. D. Reed, and R. P. Lippman. *Solving Data Mining Problems Through Pattern Recognition.* Prentice Hall, NJ, 1998.

[68] R. Khosla and T. S. Dillon. Welding symbolic AI systems with neural networks and their applications. In *Proc. IEEE Int. Joint Conf. Neural Networks (IJCNN'98)*, pages 29–34, Anchorage, AL, 1998. IEEE Press, NJ.

[69] B. King. Step-wise clustering procedures. *Journal of American Statistical Association*, pages 86–101, 1967.

[70] K. Kira and L. Rendell. A practical approach to feature selection. In *Proc. 9th Intl. Workshop on Machine Learning*, pages 249–256, San Mateo, CA, 1992. Morgan Kaufmann, CA.

[71] J. Kivinen and H. Mannila. The power of sampling in knowledge discovery. In *Proc. 1994 ACM SIGACT-SIGMOD Symposium on Principles of Database Theory (PODS'94)*, pages 77–85, Minneapolis, MN, 1994. ACM Press, NY.

[72] T. Kohonen. The Self-Organizing Map. *Proc. IEEE*, 78:1464–1480, 1990.

[73] D. Koller and M. Sahami. Towards optimal feature selection. In *Proc. 13th Intl. Conf. Machine Learning*, pages 284–292, San Fransico, CA, 1996. Morgan Kaufmann, CA.

[74] J. L. Kolodner. *Case-Based Reasoning.* Morgan Kaufmann, San Mateo, 1993.

[75] J. Komorowski, Z. Pawlak, L. Polkowski, and A. Skowron. A rough set perspective on data and knowledge. In W. Klosgen and J. Zytkow, editors, *The Handbook of Data Mining and Knowledge Discovery.* Oxford University Press, Oxford, UK, 1999.

[76] I. Kononenko. Estimating attributes: Analysis and extension of Relief. In *Proc. 7th European Machine Learning Conference*, pages 171–182, Berlin, 1994. Springer Verlag.

[77] M. Kudo and J. Sklansky. Comparison of algorithms that selects features for pattern classifiers. *Pattern Recognition*, 33:25–41, 2000.

[78] M. Last, A. Kandel, and O. Maimon. Information-theoretic algorithm for feature selection. *Pattern Recognition Letters*, 22(6/7):799–811, 2001.

[79] M. Last, Y. Klein, and A. Kandel. Knowledge discovery in time series databases. *IEEE Trans. Systems, Man, and Cybernetics*, 31(1):160–169, 2001.

[80] Y. Leung, J.-S. Zhang, and Z.-B. Xu. Clustering by scale-space filtering. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 22:1396–1410, 2000.

[81] D. D. Lewis and J. Catlett. Heterogeneous uncertainty sampling for supervised learning. In *Proc. 11th Intl. Conf. Machine Learning (ICML-1994)*, pages 148–156, San Francisco, CA, 1994. Morgan Kaufmann, CA.

[82] T. Y. Lin, Y. Y. Yao, and L. Zadeh, editors. *Data Mining, Rough Sets and Granular Computing.* Physica Verlag, Berlin, 2002.

[83] H. Liu and H. Motoda. *Feature Selection for Knowledge Discovery and Data Mining.* Kluwer Academic Publication, Boston, 1998.

[84] H. Liu and H. Motoda. On issues of instance selection. *Data Mining and Knowledge Discovery, Spl. issue on instance selection*, 6(2):115–130, 2002.

[85] H. Liu and S. T. Tan. X2R: A fast rule generator. In *Proc. IEEE Intl. Conf. System Man Cybernetics*, pages 215–220, Vancouver, 1995.

[86] J. N. K. Liu, B. N. L. Li, and T. S. Dillon. An improved naive Bayesian classifier technique coupled with a novel input solution method. *IEEE Trans. Systems, Man and Cybernetics*, 31(2):249–256, 2001.

[87] D. O. Loftsgaarden and C. P. Quesenberry. A nonparametric estimate of a multivariate density function. *Annals of Math. Statistics*, 36:1049–1051, 1965.

[88] H. Lu, R. Setiono, and H. Liu. Effective data mining using neural networks. *IEEE Trans. Knowledge and Data Engineering*, 8(6):957–961, 1996.

[89] O. Maimon, A. Kandel, and M. Last. Information theoretic fuzzy approach to data reliability and data mining. *Fuzzy Sets and Systems*, 117(2):183–194, 2001.

[90] J. Main, T. S. Dillon, and R. Khosla. Use of fuzzy feature vectors and neural networks for case retrieval in case based systems. In *Proc. Biennial Conf. North American Fuzzy Information Processing Society (NAFIPS'96)*, pages 438–443, Berkeley, CA, 1996. IEEE Press, NJ.

[91] D. P. Mandal, C. A. Murthy, and S. K. Pal. Determining the shape of a pattern class from sampled points in R^2. *International Journal of General Systems*, 20(4):307–339, 1992.

[92] H. Mannila. Theoretical frameworks for data mining. *SIGKDD Explorations*, 1(2):30–32, 2000.

[93] P. Masson and W. Pieczynski. SEM algorithm and unsupervised statistical segmentation of satellite images. *IEEE Trans. Geoscience and Remote Sensing*, 31:618–633, 1993.

[94] M. Meila and D. Heckerman. An experimental comparison of several clustering and initialization methods. *Microsoft Research Technical Report*, MSR-TR-98-06, ftp://ftp.research.microsoft.com/pub/tr/TR-98-06.PS, 1998.

[95] T. Mitchell. Machine learning and data mining. *Comm. ACM*, 42(11):30–36, 1999.

[96] P. Mitra, S. Mitra, and S. K. Pal. Rough fuzzy MLP: Evolutionary design. In *Recent Advances in Rough Sets, Fuzzy Sets, Data Mining and Granular Computing*, volume 1711 of *Lecture Notes in Artificial Intelligence*, pages 128–136. Springer Verlag, Singapore, 1999.

[97] P. Mitra, S. Mitra, and S. K. Pal. Staging of cervical cancer with soft computing. *IEEE Trans. Biomedical Engineering*, 47(7):934–940, 2000.

[98] P. Mitra, S. Mitra, and S. K. Pal. Evolutionary modular MLP with rough sets and ID3 algorithm for staging of cervical cancer. *Neural Computing and Applications*, 10:67–76, 2001.

[99] P. Mitra, C. A. Murthy, and S. K. Pal. Data condensation in large databases by incremental learning with support vector machines. In *Proc. Intl. Conf. Pattern Recognition (ICPR2000)*, pages 712–715, Barcelona, Spain, 2000.

[100] P. Mitra, C. A. Murthy, and S. K. Pal. Density based multiscale data condensation. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 24(6):734–747, 2002.

[101] P. Mitra, C. A. Murthy, and S. K. Pal. Unsupervised feature selection using feature similarity. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 24(3):301–312, 2002.

[102] P. Mitra, C. A. Murthy, and S. K. Pal. Active support vector learning with statistical queries. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 2002 (communicated).

[103] S. Mitra, P. Mitra, and S. K. Pal. Evolutionary modular design of rough knowledge-based network using fuzzy attributes. *Neurocomputing*, 36:45–66, 2001.

[104] S. Mitra, S. K. Pal, and P. Mitra. Data mining in soft computing framework: A survey. *IEEE Trans. Neural Networks*, 13(1):3–14, 2002.

[105] T. Mollestad and A. Skowron. A rough set framework for data mining of propositional default rules. In Z. W. Ras and M. Michalewicz, editors, *Foundations of Intelligent Systems*, volume 1079 of *Lecture Notes in Computer Science*, pages 448–457. Springer Verlag, Berlin, 1996.

[106] A. W. Moore and M. S. Lee. Cached sufficient statistics for efficient machine learning with large datasets. *Journal of Artificial Intelligence Research*, 8:67–91, 1998.

[107] A. W. Moore, J. Schneider, and K. Deng. Efficient locally weighted polynomial regression predictions. In *Proc. 14th Int. Conf. Machine Learning*, pages 236–244, Nashville, TN, 1997. Morgan Kaufmann, CA.

[108] Spl. issue on neural networks for data mining and knowledge discovery. *IEEE Trans. Neural Networks*, 11(3), 2000.

[109] Spl. issue on rough-neuro computing. *Neurocomputing*, 36(1-4), 2001.

[110] E. Osuna, R. Freund, and F. Girosi. An improved training algorithm for support vector machines. In *Proc. IEEE Workshop on Neural Networks for Signal Processing*, pages 276–285, Brisbane, Australia, 1997. IEEE Press, NJ.

[111] A. Pal and S. K. Pal. Pattern recognition: Evolution of methodologies and data mining. In S. K. Pal and A. Pal, editors, *Pattern Recognition: From Classical to Modern Approaches*, pages 1–23. World Scientific, Singapore, 2001.

[112] S. K. Pal and D. Bhandari. Selection of optimum set of weights in a layered network using genetic algorithms. *Information Sciences*, 80:213–234, 1994.

[113] S. K. Pal, R. K. De, and J. Basak. Unsupervised feature evaluation: A neuro-fuzzy approach. *IEEE Trans. Neural Network*, 11:366–376, 2000.

[114] S. K. Pal, T.S. Dillon, and D.S. Yeung. *Soft Computing in Case Based Reasoning.* Springer Verlag, London, 2000.

[115] S. K. Pal and A. Ghosh. Image segmentation using fuzzy correlation. *Information Sciences*, 62:223–250, 1992.

[116] S. K. Pal, A. Ghosh, and B. Uma Shankar. Segmentation of remotely sensed images with fuzzy thresholding, and quantitative evaluation. *International Journal of Remote Sensing*, 21(11):2269–2300, 2000.

[117] S. K. Pal and D. Dutta Majumder. Fuzzy sets and decision making approaches in vowel and speaker recognition. *IEEE Trans. Systems, Man, and Cybernetics*, 7:625–629, 1977.

[118] S. K. Pal and D. Dutta Majumder. *Fuzzy Mathematical Approach to Pattern Recognition.* John Wiley (Halsted Press), New York, 1986.

[119] S. K. Pal and P. Mitra. Case generation: A rough fuzzy approach. In *Proc. Intl. Conf. Case Based Reasoning (ICCBR2001)*, pages 236–242, Vancouver, Canada, 2001.

[120] S. K. Pal and P. Mitra. Case generation using rough sets with fuzzy representation. *IEEE Trans. Knowledge and Data Engineering*, 2002 (communicated).

[121] S. K. Pal and P. Mitra. Multispectral image segmentation using rough set initialized EM algorithm. *IEEE Trans. Geoscience and Remote Sensing*, 2002 (to appear).

[122] S. K. Pal and S. Mitra. Multi-layer perceptron, fuzzy sets and classification. *IEEE Trans. Neural Networks*, 3:683–697, 1992.

[123] S. K. Pal and S. Mitra. *Neuro-fuzzy Pattern Recognition: Methods in Soft Computing.* John Wiley, New York, 1999.

[124] S. K. Pal, S. Mitra, and P. Mitra. Rough fuzzy MLP: Modular evolution, rule generation and evaluation. *IEEE Trans. Knowledge and Data Engineering*, 15(1), 2003.

[125] S. K. Pal and A. Pal, editors. *Pattern Recognition: From Classical to Modern Approaches.* World Scientific, Singapore, 2001.

[126] S. K. Pal, L. Polkowski, and A. Skowron, editors. *Rough-Neuro Approach: A Way to Computing with Words.* Springer, Heidelberg, 2002 (to appear).

[127] S. K. Pal and A. Skowron, editors. *Rough-Fuzzy Hybridization: New Trends in Decision Making.* Springer Verlag, Singapore, 1999.

[128] S. K. Pal, V. Talwar, and P. Mitra. Web mining in soft computing framework: Relevance, state of the art and future directions. *IEEE Trans. Neural Networks*, 13(5):1163–1177, 2002.

[129] S. K. Pal and P. P. Wang, editors. *Genetic Algorithms for Pattern Recognition.* CRC Press, Boca Raton, 1996.

[130] D. Pavlov, J. Mao, and B. Dom. Scaling-up support vector machines using boosting algorithm. In *Proc. 15th Intl. Conf. Pattern Recognition*, pages 219–222, Barcelona, Spain, 2000.

[131] Z. Pawlak. Rough sets. *International Journal on Computer and Information Sciences*, 11:341–356, 1982.

[132] Z. Pawlak. *Rough Sets, Theoretical Aspects of Reasoning About Data.* Kluwer Academic, Dordrecht, 1991.

[133] Z. Pawlak. Rough sets and decision algorithms. In *Proc. Intl. Conf. Rough Sets and Current Trends in Computing (RSTC'2000)*, pages 1–16, Banff. Canada, 2000.

[134] W. Pedrycz. Fuzzy set technology in knowledge discovery. *Fuzzy Sets and Systems*, 98:279–290, 1998.

[135] W. Pedrycz. Shadowed sets: Representing and processing fuzzy sets. *IEEE Trans. Systems, Man and Cybernetics B*, 28:103–109, 1998.

[136] W. Pedrycz. Granular computing in data mining. In M. Last and A. Kandel, editors, *Data Mining and Computational Intelligence*. Springer Verlag, Singapore, 2001.

[137] W. Pedrycz and A. Bargiela. Granular clustering: A granular signature of data. *IEEE Trans. Systems, Man and Cybernetics*, 32(2):212–224, 2002.

[138] W. Pedrycz and G. Vukovich. Abstraction and specialization of information granules. *IEEE Trans. Systems, Man and Cybernetics*, 31(1):106–111, 2001.

[139] J. F. Peters, A. Skowron, L. Han, and S. Ramanna. Towards rough neural computing based on rough neural networks. In *Proc. Intl. Conf. Rough Sets and Current Trends in Computing (RSTC'2000)*, pages 572–579, Banff. Canada, 2000.

[140] J. C. Platt. Fast training of support vector machines using sequential minimal optimisation. In B. Scholkopf, C. J. C. Burges, and A. J. Smola, editors, *Advances in Kernel Methods - Support Vector Learning*, pages 185–208. MIT Press, Cambridge, MA, 1998.

[141] M. Plutowski and H. White. Selecting concise training sets from clean data. *IEEE Trans. Neural Networks*, 4(2)(2):305–318, 1993.

[142] L. Polkowski, A. Skowron, and J. Komorowski. Approximate case-based reasoning: A rough mereological approach. In H.D. Burkhard and M. Lenz, editors, *Proc. 4th German Workshop on Case-Based Reasoning, System Deveolpment and Evaluation*, pages 144–151, Humboldt University, Berlin, 1996.

[143] F. Provost and V. Kolluri. A survey of methods for scaling up inductive algorithms. *Data Mining and Knowledge Discovery*, 2:131–169, 1999.

[144] P. Pudil, J. Novovicova, and J. Kittler. Floating search methods in feature selection. *Pattern Recognition Letters*, 15:1119–1125, 1994.

[145] J. R. Quinlan. *C4.5, Programs for Machine Learning.* Morgan Kaufmann, CA, 1993.

[146] N. Ramakrishnan and A. Y. Grama. Data mining: From serendipity to science. *IEEE Computer*, 34(8):34–37, 1999.

[147] V. Ramamurti and J. Ghosh. Structurally adaptive modular networks for non-stationary environments. *IEEE Trans. Neural Networks*, 10(1):152–160, 1999.

[148] C. R. Rao. *Linear Statistical Inference and its Applications.* John Wiley, 1973.

[149] M. L. Raymer, W. F. Punch, E. D. Goodman, L. A. Kuhn, and A. K. Jain. Dimensionality reduction using genetic algorithm. *IEEE Trans. Evolutinary Computation*, 4:164–172, 2000.

[150] F. Ricci and P. Avesani. Data compression and local metrics for nearest neighbor classification. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 21:380–384, 1999.

[151] G. H. Rosenfeld and K. Fitzpatrick-Lins. Coefficient of agreement as a measure of thematic classification accuracy. *Photogrammetric Engineering and Remote Sensing*, 52:223–227, 1986.

[152] N. Roy and A. McCallum. Towards optimal active learning through sampling estimation of error reduction. In *Proc. 18th Intl. Conf. Machine Learning (ICML-2001)*, pages 441–448, Williams College, MA, 2001. Morgan Kaufmann, CA.

[153] N. A. Sayeed, H. Liu, and K. K. Sung. A sudy of support vectors on model independent example selection. In *Proc. 1st Intl. Conf. Knowledge Discovery and Data Mining*, pages 272–276, San Diego, CA, 1999. AAAI Press, CA.

[154] G. Schohn and D. Cohn. Less is more: Active learning with support vector machines. In *Proc. 17th Intl. Conf. Machine Learning*, pages 839–846, Stanford, CA, 2000..Morgan Kaufmann, CA.

[155] D. Skalak. Prototype and feature selection by sampling and random mutation hill climbing algorithms. In *Proc. 11th Intl. Conf. Machine Learning*, pages 293–301, New Brunswick, NJ, 1994. Morgan Kaufmann, CA.

[156] A. Skowron and L. Polkowski, editors. *Rough Sets in Knowledge Discovery.* Physica-Verlag, Heidelberg, 1998.

[157] A. Skowron and C. Rauszer. The discernibility matrices and functions in information systems. In R. Slowiński, editor, *Intelligent Decision Support, Handbook of Applications and Advances of the Rough Sets Theory*, pages 331–362. Kluwer Academic, Dordrecht, 1992.

[158] A. Skowron and R. Swiniarski. Rough sets in pattern recognition. In S. K. Pal and A. Pal, editors, *Pattern Recognition: From Classical to Modern Approaches*, pages 385–428. World Scientific, Singapore, 2001.

[159] I. A. Taha and J. Ghosh. Symbolic interpretation of artificial neural networks. *IEEE Trans. Knowledge and Data Engineering*, 11(3):448–463, 1999.

[160] A. B. Tickle, R. Andrews, M. Golea, and J. Diederich. The truth will come to light: Directions and challenges in extracting the knowledge embedded within trained artificial neural networks. *IEEE Trans. Neural Networks*, 9:1057–1068, 1998.

[161] S. Tong and D. Koller. Support vector machine active learning with application to text classification. *Journal of Machine Learning Research*, 2:45–66, 2001.

[162] G. G. Towell and J. W. Shavlik. Extracting refined rules from knowledge-based neural networks. *Machine Learning*, 13:71–101, 1993.

[163] V. Vapnik. *Statistical Learning Theory.* Wiley, New York, 1998.

[164] D. R. Wilson and T. R. Martinez. Reduction techniques for instance-based learning algorithms. *Machine Learning*, 38(3):257–286, 2000.

[165] L. A. Zadeh. Fuzzy sets. *Information and Control*, 8:338–353, 1965.

[166] L. A. Zadeh. Outline of a new approach to the analysis of complex systems and decision processes. *IEEE Trans. Systems, Man, and Cybernetics*, 3:28–44, 1973.

[167] L. A. Zadeh. Fuzzy logic, neural networks, and soft computing. *Comm. ACM*, 37:77–84, 1994.

[168] L. A. Zadeh. Toward a theory of fuzzy information granulation and its centrality in human reasoning and fuzzy logic. *Fuzzy Sets and Systems*, 90:111–127, 1997.

[169] L. A. Zadeh. A new direction in AI: toward a computational theory of perceptions. *AI Magazine*, 22:73–84, 2001.

[170] C. T. Zahn. Graph-theoretical methods for detecting and describing gestalt clusters. *IEEE Trans. on Computer*, 20:68–86, 1971.

[171] T. Zhang, R. Ramakrishnan, and M. Livny. BIRCH: An efficient data clustering method for large databases. In *Proc. ACM SIGMOD Intl. Conf. Management of Data*, pages 103–114, New York, 1996. ACM Press, NY.

[172] Q. Zhao. A Co-Evolutionary Algorithm for Neural Network Learning. In *Proc. IEEE Intl. Conf. Neural Networks*, pages 432–437, Houston, TX, 1997. IEEE Press, NJ.

List of Publications of the Author Related to the Thesis

1. P. Mitra, C. A. Murthy, and S. K. Pal. Density based multiscale data condensation. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 24(6):734–747, 2002.

2. P. Mitra, C. A. Murthy, and S. K. Pal. Unsupervised feature selection using feature similarity. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 24(3):301–312, 2002.

3. S. Mitra, S. K. Pal, and P. Mitra. Data mining in soft computing framework: A survey. *IEEE Trans. Neural Networks*, 13(1):3–14, 2002.

4. S. K. Pal, V. Talwar, and P. Mitra. Web mining in soft computing framework: Relevance, state of the art and future directions. *IEEE Trans. Neural Networks*, 13(5):1163–1177, 2002.

5. S. K. Pal and P. Mitra. Case generation: A rough fuzzy approach. In *Proc. Intl. Conf. Case Based Reasoning (ICCBR2001)*, pages 236–242, Vancouver, Canada, 2001.

6. S. Mitra, P. Mitra, and S. K. Pal. Evolutionary modular design of rough knowledge-based network using fuzzy attributes. *Neurocomputing*, 36:45–66, 2001.

7. P. Mitra, S. Mitra, and S. K. Pal. Evolutionary modular MLP with rough sets and ID3 algorithm for staging of cervical cancer. *Neural Computing and Applications*, 10:67–76, 2001.

8. P. Mitra, S. Mitra, and S. K. Pal. Staging of cervical cancer with soft computing. *IEEE Trans. Biomedical Engineering*, 47(7):934–940, 2000.

9. P. Mitra, C. A. Murthy, and S. K. Pal. Data condensation in large databases by incremental learning with support vector machines. In *Proc. Intl. Conf. Pattern Recognition (ICPR2000)*, pages 712–715, Barcelona, Spain, 2000.

10. P. Mitra, S. Mitra, and S. K. Pal. Rough fuzzy MLP: Evolutionary design. In *Recent Advances in Rough Sets, Fuzzy Sets, Data Mining and Granular Com-*

puting, volume 1711 of *Lecture Notes in Artificial Intelligence*, pages 128–136. Springer Verlag, Singapore, 1999.

11. S. K. Pal and P. Mitra. Multispectral image segmentation using rough set initialized EM algorithm. *IEEE Trans. Geoscience and Remote Sensing*, 2002 (accepted).

12. S. K. Pal, S. Mitra, and P. Mitra. Rough fuzzy MLP: Modular evolution, rule generation and evaluation. *IEEE Trans. Knowledge and Data Engineering*, 15(1), 2003.

13. S. K. Pal and P. Mitra. Case generation using rough sets with fuzzy representation. *IEEE Trans. Knowledge and Data Engineering*, 2002 (under review).

14. P. Mitra, C. A. Murthy, and S. K. Pal. Active support vector learning with statistical queries. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 2002 (communicated).