A CLASSIFICATION ALGORITHM USING MAHALANOBIS DISTANCE CLUSTERING OF DATA WITH APPLICATIONS ON BIOMEDICAL DATA SETS

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Bahadır DURAK

ABSTRACT

A CLASSIFICATION ALGORITHM USING MAHALANOBIS DISTANCE CLUSTERING OF DATA WITH APPLICATIONS ON BIOMEDICAL DATA SETS

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The concept of classification is used and examined by the scientific community for hundreds of years. In this historical process, different methods and algorithms have been developed and used.

Today, although the classification algorithms in literature use different methods, they are acting on a similar basis. This basis is setting the desired data into classes by using defined properties, with a different discourse; an effort to establish a relationship between known features with unknown result. This study was intended to bring a different perspective to this common basis.

In this study, not only the basic features of data are used, the class of the data is also included as a parameter. The aim of this method is also using the information in the algorithm that come from a known value. In other words, the class, in which the data is included, is evaluated as an input and the data set is transferred to a higher dimensional space which is a new working environment. In this new environment it is not a classification problem anymore, but a clustering problem. Although this logic is similar with Kernel Methods, the methodologies are different from the way that how they transform the working space. In the projected new space, the clusters based on calculations performed with the Mahalanobis Distance are evaluated in original space with two different heuristics which are center-based and KNN-based algorithm. In both heuristics, increase in classification success rates achieved by this methodology. For center based algorithm, which is more sensitive to new input parameter, up to 8% of enhancement is observed.

Keywords: Data Mining, Classification, Clustering, Mahalanobis Distance, Kernel Function.

ÖZ

BİOMEDİKAL VERİ KÜMELERİ ÜZERİNDE MAHALANOBIS UZAKLIĞI VERİ KÜMELENMESİ İLE SINIFLANDIRMA ALGORİTMASI

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Sınıflandırma kavramı bilimsel çevrelerce yüzlerce yıldır kullanılmakta ve incelenmektedir. Bu tarihsel süreç içerisinde farklı yöntemler ve algoritmalar geliştirilmiş ve kullanılmıştır.

Bugün literature geçmiş olan sınıflandırma algoritmaları, farklı yöntemler kullanmakta olsalar da benzer bir temel üzerinde hareket etmektedirler. Bu temel, tanımlı özellikleri kullanarak, istenen verileri belirlenmiş sınıflarda toplama, farklı bir söylemle, tanımlanmış nedenler ile sonuç arasında bir ilişki kurabilme çabasıdır. Bu çalışma, bugüne kadar kullanılmakta olan bu temele farklı bir bakış açısı getirmeyi amaçlamıştır.

Bu çalışmada, verilerin sadece temel özellikleri değil, sınıfları da bir parametre olarak kullanılmıştır. Söz konusu yöntemdeki amaç, bilinen bir değerden gelecek olan bilgiyi de algoritmada kullanma çabasıdır. Diğer bir ifadeyle, verinin dahil olduğu sınıf, bir girdi olarak değerlendirilmiş ve veri kümesi üst bir uzaya transfer edilerek yeni bir çalışma ortamı yaratılmıştır. Aynı zamanda bu yeni ortamda artık problem bir sınıflandırma problemi değil, kümeleme problemidir. Her ne kadar bu mantık Kernel Yöntemini çağrıştırsa da, yöntemin kullanılış biçimi tamamen farklıdır. Oluşturulan yeni uzayda Mahalanobis Uzaklığı ile yapılan hesaplamalar ve oluşturulan kümeler, orijinal uzayda merkez temelli ve KNN temelli 2 farklı sınıflandırma algoritması ile değerlendirilmiştir. Bu yeni yöntem ile her iki algoritmada da ulaşılan başarı oranlarında artış yakalanmıştır. Yeni yönteme daha duyarlı olan merkez temelli algoritma ile başarı oranındaki artışın %8 seviyelerine kadar çıktığı gözlenmiştir.

Anahtar Kelimeler: Veri Madenciliği, Sınıflandırma, Kümeleme, Mahalanobis, Kernel.

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I would like to thank my supervisor Assist. Prof. Cem Iyigün who guided and motivated me in this study.

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TABLE OF CONTENTS

CHAPTERS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1

INTRODUCTION

Various classification approaches try to find a function that estimates the class labels from the feature-space in a data set. In these methodologies, named *"supervised learning"*, the features are accepted as input while the class labels are accepted as output. On the other hand, in the clustering approaches (*unsupervised learning*) there are no class labels. Instead, they try to create groups according to similarities of the data points. In this approach there is no class information and only feature space is used in clustering process.

Both classification and clustering approaches do not use the information from class labels as a parameter in the process. This study searches a methodology which takes this information into consideration. There are two new heuristics developed in which the information from the class is integrated: *Center based algorithm* and *KNN based algorithm.*

In *center based heuristic*, information from the class labels is included to feature space in training stage. By this, the dimension of feature space increases by one and the problem becomes a clustering problem. There are two important processes which are hidden in this methodology. First, data points are mapped to a high dimensional space, so that kernel logic is used in this methodology. Second the classification problem turns into a clustering problem, such that the original problem is transformed into a new clustering problem.

In *KNN based heuristic* the class information is included in feature space similar with center based heuristic. The difference is the algorithm keeps this information as class information, too. There is also kernel logic since the original problem mapped to a high dimensional space, but the original problem is still a classification problem.

This new methodology arises new questions. One of these questions is how to weight the information from the class labels, which is a new parameter, to produce better classification results. The label information can have equal effect or the feature can have higher effect with different weights. In order to find the effects of new parameter, a compound distance is generated unifying the distance in the feature space and class labels. This approach is explained and studied in this thesis.

Other question is which distance measure should be used as a basis of this new distance function. The distance measure may differ in various classification problems, the content and the application area mostly determine~~s~~ the selection of the distance function used. The data types and the relationships between them determine the type of the distance measure. For example, in biomedical data sets there are some correlations within the features (variables). In this study the data sets are numerical and to take into account the correlations, **Mahalanobis Distance** is chosen. In order to measure the effect of this choice, Euclidean distance is also used to compare the results. If the variables are not numeric (which is common in biological and biomedical data sets), then a suitable distance, i.e. hamming distance, need to be used.

Another question is how the other parameters affect the classification success rate. The effect of number of clusters in center based algorithm and number of neighbours in KNN based algorithm are investigated. The effects of these parameters are explained and illustrated in the study.

CHAPTER 2

GENERAL BACKGROUND

2.1. Data

Observations (data points) are the objects of data mining. Data points are consist of different attributes which are in an order. A data point **x** with m attributes is an m-dimensional vector, **x** = $(x_1, x_2, \dots, x_m)$. N data points $\mathbf{x_i}$ form a set

$$D = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_\mathrm{N}) \subset \mathbb{R}^m \qquad \textbf{(1.1)}$$

Called the **data set.** D can be represented by an $N \times m$ matrix

$$D = (x_{ij}) \qquad \textbf{(1.2)}$$

where x_{ij} is the j^{th} component of the data point $\mathbf{x_i}$.

2.2.Data mining

Generally speaking, data mining is the process of extracting or 'mining' implicit and relevant information from large sets of data. A more precise definition of the term would be "*the non trivial extraction of implicit, previously unknown, and potentially useful knowledge from large volumes of actual data*" (Piateski & Frawley, 1991, cited by Lee & Kim, 2002, pp. 42) Data mining is also known by several other terms depending on the situation and context, such as knowledge mining from data, knowledge extraction, data/pattern analysis, data archaeology, and data dredging. The primary aim of data mining is to gather sense, or extract predictive information, from large amounts of mostly unsupervised data, in a particular domain. The largest group of data mining users is businesses, since collecting large amount of data and making sense out of it happens to be one of their routine activities. (Cios et. al., 2007, pp. 3-4)

2.3.Estimation

Estimating outputs based on input variables is one of the most important problems in empirical research. The meaning of estimation is the calculated approximation of a result when there is an uncertainty in finding the output or the inputs are not known exactly. In a wide range of engineering areas, estimation techniques are used. Aerospace systems, communications, manufacturing and biomedical engineering are the areas that estimation techniques are mostly used. The estimation of the health of a person's hearth based on an electrocardiogram (ECG) is a specific example of usage in biomedical engineering (Kamen & Su, 1999, pp. 1).

2.4.Distances

There are several techniques used for data mining. Several such techniques, for instance nearest neighbor classification methods, cluster analysis, and multidimensional scaling methods, are based on the measures of similarity between objects. Instead of measuring similarity, dissimilarity between the objects too will give the same results. For measuring dissimilarity one of the parameters that can be used is distance. This category of measures is also known as separability, divergence or discrimination measures. (Hand, Mannila, & Smyth, 2001, pp. 31) A distance metric is a real-valued function *d*, such that for any points **x, y**, and **z**:

$$d(\mathbf{x},\mathbf{y}) \geq 0 \text{ , and } (\mathbf{x},\mathbf{y}) = 0 \text{ , if and only if } \mathbf{x} = \mathbf{y} \qquad \textbf{(2.1)}$$

$$d(\mathbf{x},\mathbf{y}) = d(\mathbf{y},\mathbf{x}) \qquad \textbf{(2.2)}$$

$$d(\mathbf{x},\mathbf{z}) \leq d(\mathbf{x},\mathbf{y}) + d(\mathbf{y},\mathbf{z}) \qquad \textbf{(2.3)}$$

The first property, **positive definiteness**, assures that distance is always a non-negative quantity, so the only way distance can be zero is for the points to be the same. The second property indicates the symmetry nature of distance. The third property is the triangle inequality, according to which introducing a third point can never shorten the distance between two points. (Larose, 2005, pp. 99) There are several measures of distance which satisfy the metric properties, some of which are discussed below:

2.4.1. Euclidean distance

The Euclidean distance is the most common distance metric used in low dimensional data sets. It is also known as the **L_2 norm**. The Euclidean distance is the usual manner in which distance is measured in real world. In this sense, Manhattan distance tends to be more robust to noisy data.

$$d_{euclidean}(\mathbf{x},\mathbf{y}) = \sqrt{\sum_i (x_i - y_i)^2} \qquad \textbf{(2.4)}$$

where **x** and **y** are m-dimensional vectors and denoted by **x** = $(x_1, x_2, x_3 \ldots x_m)$ and **y** = $(y_1, y_2, y_3 \ldots y_m)$ represent the m attribute values of two records. (Larose, 2005, pp. 99) While Euclidean metric is useful in low dimensions, it doesn't work well in high dimensions and for categorical variables. The drawback of Euclidean distance is that it ignores the similarity between attributes. Each attribute is treated as totally different from all of the attributes. (Ertöz, Steinbach & Kumar, 2003, pp. 49)

2.4.2. Manhattan distance

This metric is also known as the **L_1 norm** or **the rectilinear distance**. This is also a common distance metric and gets its name from the rectangular grid patterns of streets in midtown Manhattan. Hence, another name for the distance metric is also **city block distance**. It is defined as the sum of distances travelled along each axis. The Manhattan distance looks at the absolute differences between coordinates. In some situations, this metric is more preferable to Euclidean distance, because the distance along each axis is not squared so a large difference in one dimension will not dominate the total distance. (Berry & Linoff, 2009: 363)

$$d_{Manhattan}(\mathbf{x},\mathbf{y}) = \sum_{i=1}^{m} |x_i - y_i| \qquad \textbf{(2.5)}$$

2.4.3. L_∞ norm

The **L_∞ norm** is the maximum of the absolute differences in any single dimension. It is also known as **sup norm** or the **maximum norm**. Another name for L_∞ norm is **Chebyshev norm**. **Chebyshev norm** is also called as chessboard distance; since it is equal to the number of moves it takes a chess king to occupy any other point on the chessboard. This distance metric looks only at the measurement on which attributes deviates the most. Chebyshev distances are piecewise linear. In fact, like the Manhattan distance, the Chebyshev distance examines the absolute magnitude of the element-wise differences between the attributes. (Bock & Krischer, 1998, pp. 13)

$$d_{\mathrm{L}\infty}(\mathbf{x},\mathbf{y}) = \max_{i=1,2,\ldots,m}|x_i - y_i| \tag{2.6}$$

2.4.4. Mahalanobis Distance

Mahalanobis distance is a well known statistical distance function. Here, a measure of variability can be incorporated into the distance metric directly. Mahalanobis distance is a distance measure between two points in the space defined by two or more correlated variables. That is to say, Mahalanobis distance takes the correlations within a data set between the variable into consideration. If there are two non-correlated variables, the Mahalanobis distance between the points of the variable in a 2D scatter plot is same as Euclidean distance. In mathematical terms, the Mahalanobis distance is equal to the Euclidean distance when the covariance matrix is the unit matrix. This is exactly the case then if the two columns of the standardized data matrix are orthogonal. The Mahalanobis distance depends on the covariance matrix of the attribute and adequately accounts for the correlations. Here, the covariance matrix is utilized to correct the effects of cross-covariance between two components of random variable. (Hill & Lewicki, 2006, pp. 164)

The Mahalanobis distance is the distance between an observation and the center for each group in m-dimensional space defined by m variables and their covariance. Thus, a small value of Mahalanobis distance increases the chance of an observation to be closer to the group's center and the more likely it is to be assigned to that group. Mahalanobis distance between two samples (**x**, **y**) of a random variable is defined as (McLachlan, 1999, pp. 21):

$$d_{Mahalanobis}(\mathbf{x},\mathbf{y}) = \sqrt{(\mathbf{x}-\mathbf{y})^T\, \Sigma^{-1}(\mathbf{x}-\mathbf{y})} \qquad \textbf{(2.7)}$$

Here, Σ^{-1} is the inverse of covariance matrix. The Mahalanobis metric is defined in independence of the data matrix. Unlike most other distance measures, this method is not dependent upon the scale on which the variables are measured. Mahalanobis distance is a distance in geometrical sense because the covariance matrix and its inverse are positive definite matrices. The metric defined by the covariance matrix provides a normalization of the data relative to their spread. The Mahalanobis distance or its square can be used to measure how close an object is from another, when these objects can be characterized by a series of numerical measurements. An important property of the Mahalanobis distance is that it is normalized. Thus, it is not necessary to normalize the data, provided rounding errors in inverting the covariance matrix are kept under control (Besset, 2001, pp. 618; Eyob, 2009, pp. 272)

In the case of $\Sigma = \mathrm{I}$, Mahalanobis distance is the same with Euclidean distance:

$$d_{Mahalanobis}(\mathbf{x},\mathbf{y}) = \sqrt{(\mathbf{x}-\mathbf{y})^T\, \mathrm{I}^{-1}(\mathbf{x}-\mathbf{y})} = \sqrt{(\mathbf{x}-\mathbf{y})^2} = d_{euclidean}(\mathbf{x},\mathbf{y}) \qquad \textbf{(2.8)}$$

In a data set, usage of Euclidean Distance or Mahalanobis Distance affects the expected results. The following example illustrates this idea:

Example 2.1:

A data set in $\mathbb{R}^2$ with N = 200 data points shown in Figure 2.1. The data was simulated from normal distributions $N\ (\mu_i\ , \sigma_i)$ with:

$$\mu_1 = (0,0), \quad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

$$\mu_2 = (3,0), \quad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

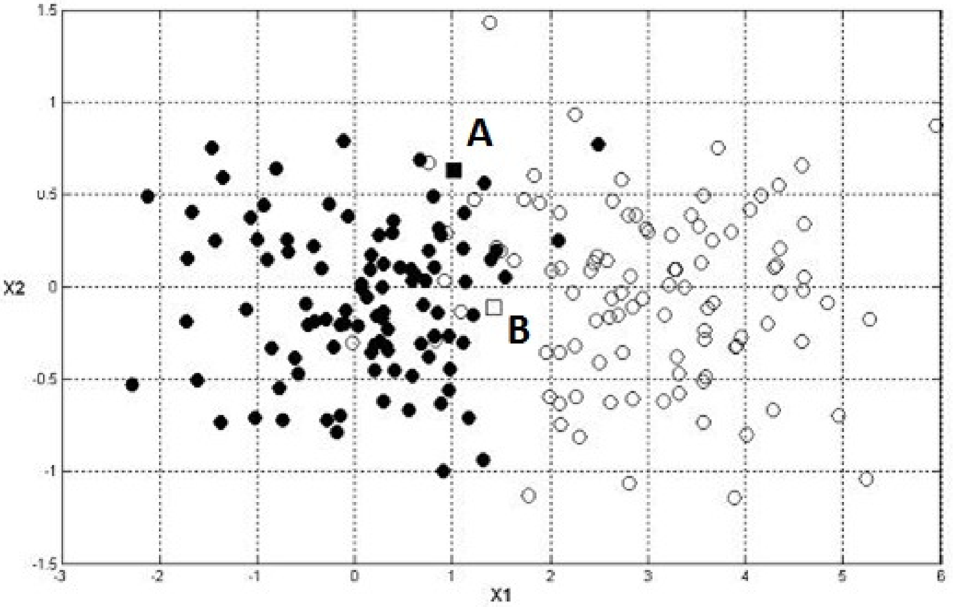


Figure 2-1 – Generated data and selected points A, B

In *Figure 2-1* A and B are the points which selected randomly in the data set. Two different distance measures, Euclidean distance and Mahalanobis distance, are calculated between these points after normalizing data set. The value of $d_{Euclidean}(A,B)=1.8211$ is slightly greater than the value $d_{Mahalanobis}(A,B)=1.8197$.

Example 2.2:

A data set in $\mathbb{R}^2$with N = 200 data points shown in *Figure 2-1*. The data was simulated from normal distributions $N\ (\mu_i\ ,\sigma_i)$ with:

$$\mu_1 = (0,0), \quad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

$$\mu_2 = (6,0), \quad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

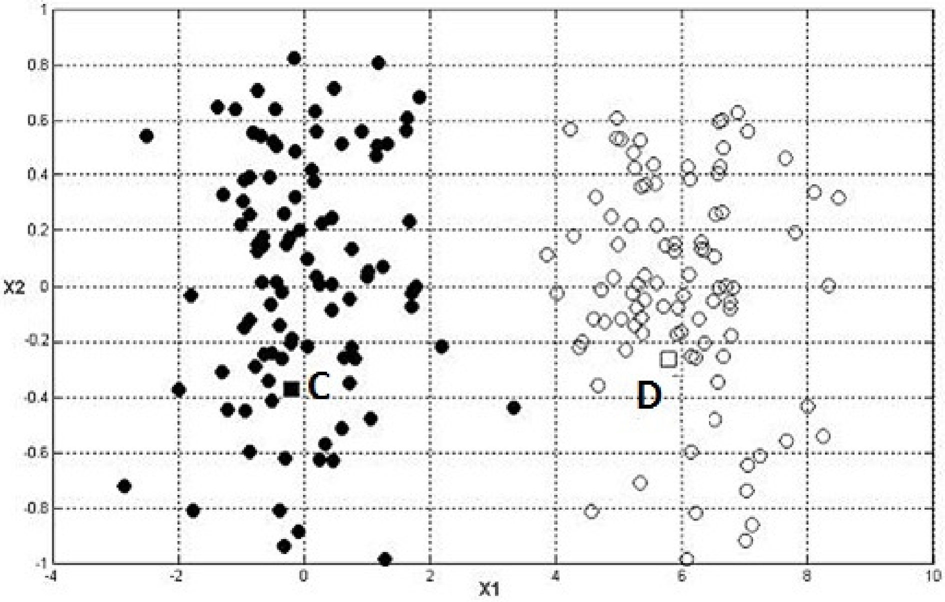


Figure 2-2 – Generated data and selected points C, D

In *Figure 2-2* C and D are the points which selected randomly in the data set. Same with *example 2.1*, two different distance measures, Euclidean distance and Mahalanobis distance, are calculated between these points after normalizing data set. Contrary to *example 2.1*, the value of $d_{Euclidean}(C,\mathrm{D}) = 1.9099$ is now smaller than the value $d_{Mahalanobis}(\mathrm{C},\mathrm{D}) = 7.7996$.

So, it can be seen from the results of examples 2.1 and 2.2 that:

$$d_{Euclidean}(\mathrm{A}, \mathrm{B}) > d_{Mahalanobis}(\mathrm{A}, \mathrm{B}) \quad \textbf{(2.9)}$$

But on the contrary,

$$d_{Euclidean}(\mathrm{C}, \mathrm{D}) < d_{Mahalanobis}(\mathrm{C}, \mathrm{D}) \quad \textbf{(2.10)}$$

It illustrates the effect of covariance matrix Σ on the distance. Depending on the structure of the data, Σ can produce a shorter distance or longer distance than Euclidean Distance.

2.5. Learning

The term learning refers acquiring knowledge from a set of data or briefly understanding the data. The learning process is executed in a partition of the original set which is called training set. Since training sets are finite and the future is not certain, the performance of the learning process should be measured. This can be done by using test set, another partition of original data set. In the area of data mining, learning techniques are classified in two classes:

2.5.1. Supervised Learning

This is also known as **directed data mining**. In supervised learning the variables that are under investigation are first separated into two groups: input variables, and one output variable or more than one output variables (labels). (Taylor & Agah, 2008, pp. 50) Pre-classification is a prerequisite for supervised learning. That is to say, the variables in the data set need to be already placed in groups or assigned some value or result. (Shmueli et. al., 2008, pp. 11) Supervised learning is predictive in nature i.e. data is learnt with an answer. The aim of the data mining exercise is to find a relationship between these two types of variables. An important requirement for supervised learning is that the values of the output variable (label) must be known for a sufficiently large part of the data set. (Wübben, 2008, pp. 137)

2.5.2. Unsupervised Learning

Unlike for supervised learning, unsupervised learning does not require the target variable to be well defined and that a sufficiently large number of values are known. In case of unsupervised learning, the target variable is unknown. (Taylor & Agah, 2008, pp. 50) Unsupervised learning occurs when the data is not previously classified. Here, the data mining process cannot take value decisions. The data mining process can find correlations within data, but cannot make any inferences on what the patterns mean. (Shmueli et. al., 2008, pp. 11)

2.5.3. Supervised Learning vs. Unsupervised Learning

Supervised learning tries to discover a relationship between the input and the output by using a set of data (training data) which contains the knowledge of both input and output. This relationship can be used as a function to predict the output value when the input variables are known. On the contrary, in unsupervised learning there is no output to find this kind of function. Unsupervised learning tries to discover how the data are organized, so it is descriptive in nature. It is not predictive i.e. the data is learnt without any knowledge of the outcome. Compared to supervised learning, unsupervised learning is much more exploratory in nature and all variable are treated in the same way i.e. there is no distinction between explanatory and dependent variables. (Wübben, 2008, pp. 137)

Table 2.1. - Supervised Learning vs. Unsupervised Learning

Supervised Learning	Unsupervised Learning
• Use training data to find a relationship and test it with test data • Data labels are known • Use the relationship between the input and the output variables of data points • Predictive in nature	• No training data, use one kind of data to discover the organization • Data labels are unknown • Use the similarities/differences between the input variables of different data points • Descriptive in nature

2.6. Classification Methods

One of the most commonly applied data mining methods is classification. It is a form of predictive modeling and defines groups within the population. The process of classification aims to find a model or function describing and distinguishing data classes or concepts. The aim of classification is to use the derived function to predict label of data points with unknown class labels. Using classification method, one can learn functions or rules that form categories of data. (Han & Kamber, 2006, pp. 24) The functions or rules are derived by an analysis of a set of data objects with known labels which can be called as training data. The process of classification has several applications in varied fields such as medicine, credit card portfolio and credit ranking, customer purchase behavior, and strategic management. (Li and Shi, 2005, pp. 758)

For classification task, input data is a collection of observations. Each observation, also known as example or instance, is denoted by (**x,** *y*), where **x** is the vector of attributes and *y* is the class label or category of the observation. Classification is the process of learning a function *f* that matches each attribute vector **x** with one of previously defined class labels *y*. This process is shown simply in the *Figure 2-3*.

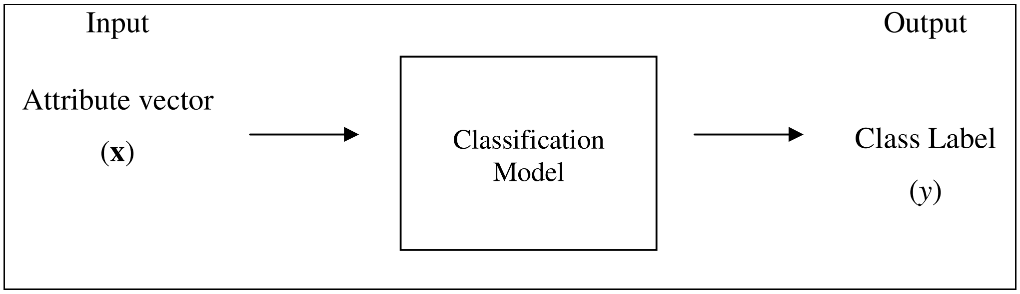


Figure 2-3 – Classification Process

The probability of a class membership can be predicted by classification models which use the information gathered from input variables. The process of classification is done in two steps. First, a model is built which describes a previously determined set of data classes or concepts; second, the model is used for classification. The first step is known as training phase, where algorithms are used to learn models to fit training data. The second step is known as testing phase where testing data is used on obtained models to measure learning success by predicting class labels of this data set. (Leondes, 2005, pp. 117) From the description of the process above, two main goals of the classification process can be gleaned: an accurate model, which can be used in the prediction; and an explanation of the models itself i.e. a comprehensible explanation for human experts. Classification focuses primarily on inclusion or exclusion in small set of specific categories. In case of classification in data mining, the focus is less on model assumptions and more on the model's ability to actually predict outcomes. The classification methods used in data mining are similar, if not identical, to those used for statistical inference. These methods are explained in the following sections in an order of increasing complexity. (Cerrito, 2007, pp. 242-243)

2.6.1. K-nearest neighbor algorithm

The K-nearest neighbor algorithm (KNN) is one of the basic and common classification algorithms. No pre-processing of labeled data samples is needed before using this algorithm. A dominated class label in K-nearest neighbors of a data point is assigned as class label to that data point. A tie occurs when neighborhood has same amount of labels from multiple classes. To break the tie, the distances of neighbors can be summed up in each class that is tied and vector **f** is assigned to the class with minimal distance. Or, the class can be chosen with the nearest neighbor. Clearly, tie is still possible here, in which case an arbitrary assignment is taken.

The KNN algorithm is very easy to implement. It performs well in practice provided that the different attributes or dimensions are normalized, and that the attributes are independent of one another and relevant to the prediction task at hand. The main drawback of the KNN algorithm is that each of the K-nearest neighbors is equally important. However, it is obvious that the closer a neighbor is, the more is the possibility of having the vector **f** in the class of this neighbor. Hence, it is better to assign the neighbors with different voting weights based on their distance with the vector **f**. (Thuraisingham, et. al., 2009, pp. 196)

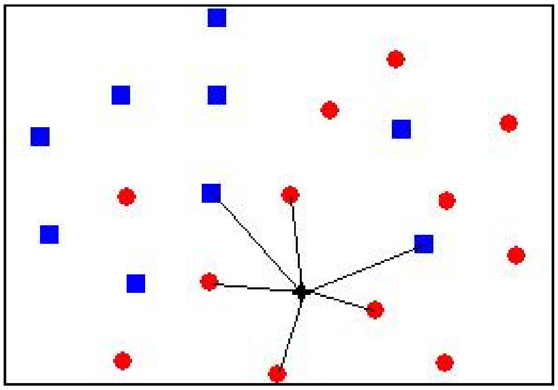


Figure 2-4- Geometrical representation of k-nearest neighbor algorithm

2.6.2. Neural Networks

A neural network, when used for classification, is typically a collection of neuron-like processing units with weighted connections between the units. Artificial neural networks (ANN) are simple computer programs which can automatically find relationships in data without any predefined model. ANNs are highly parameterized nonlinear statistical models. An ANN transforms a real-valued vector in the input space to a real-valued vector in some output space. They can be used to predict new characteristics e.g. class membership of points in the input space. ANNs first linearly transform the input vector by multiplying it with a weight matrix (Weight matrix = $[w_{ij}]$ in *Figure 2-4*). Then, a nonlinear function is applied to each coordinate of the resulting vector to produce a value. An activation function (g in *Figure 2-4*) produces the output by comparing this value with threshold (t in *Figure 2-4*). This is an example of a single layer network. A multilayer network can be constructed by subsequent application to another weight matrix and a nonlinear transformation. Training an ANN involves determining the weight matrix that minimizes the prediction error for a set of training data for which there is knowledge of what the output vector should be. (Han and Kamber, 2006, pp. 327; Maimon and Rokach, 2005, pp. 488)

The most common application of neural network is to train it on historical data and then use this model to predict the outcome for new combinations of inputs. The network possibly extracts a general relationship which holds for all combination of inputs. In classification problems, the output will have one of two values, representing belongs to the set and does not belong to the set, whereas in regression problems the output is a continuous variable. Neural networks do not give an exact physical model but learn to represent the relationship in terms of the activation functions of the neurons. (Maimon and Rokach, 2005, pp. 488)

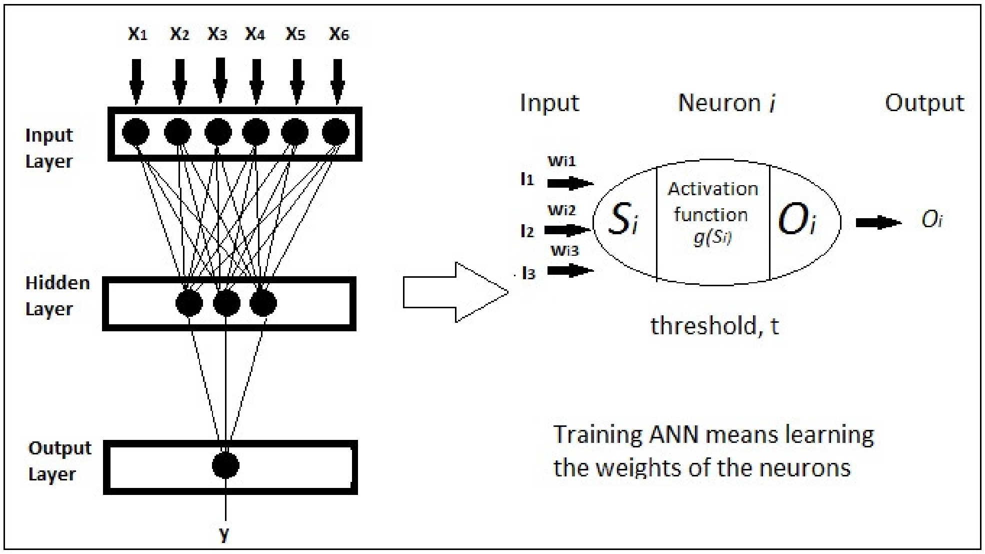


Figure 2-5 - The basic architecture of the feed forward neural network

2.3.3. Support Vector Machine

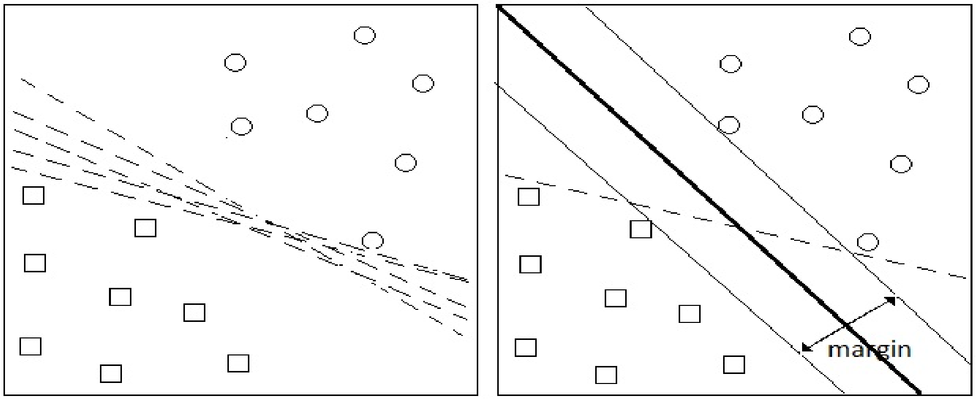
Support Vector Machines (SVMs) are one of the most recent additions to machine learning algorithms. Basically, the SVM is binary learning with some highly elegant property. They calculate a hyperplane between that separates two different classes in the training set. Each object can be transformed as another point in a high-dimensional space. Sometimes it is not possible to separate the points of two different classes by a hyperplane in the original space. That is why a transformation may be needed. Transformed points may be separated by a hyperplane in a high-dimensional space. These kind of transformations may not be so easy. In SVM, the kernel is introduced so that computing the hyperplane becomes very fast. (Hearst, 1998, pp. 19)

Support vectors are the data vectors with shortest distance to the separating hyperplane. Vectors are simply those data points (for the linearly separable case) that are the most difficult to classify and optimally separated from each other. That's why the hyperplane which has maximum margin is the best separator. In a support vector machine, the selection of basis function is required to satisfy Mercer's theorem; that is, each basis function is in the form of a positive definite inner-product kernel:

$$K(\mathbf{x_i}, \mathbf{x_j}) = \phi(\mathbf{x_i}) \cdot \phi(\mathbf{x_j}) \qquad \textbf{(2.11)}$$

Here, $\mathbf{x_i}$, $\mathbf{x_j}$ are input vectors examples i and j, and φ is the vector of hidden-unit outputs for inputs $\mathbf{x_j}$. The hidden (feature) space is chosen as a high dimensional space, since transformation of the problem from a nonlinear separable classification to a linear separable classification becomes possible. The above condition is also known as the kernel trick. When there are K>2 classes, SVMs can be used to build K hyperplanes each separating one class from the union of all other classes. Classification of a test data point starts with computing its distance to each of the K hyperplanes. The data point is assigned to the class for which this distance is maximal. (Zhang et. al., 2005, pp. 62)

SVM is currently the best of all classification techniques available. SVMs are usually considered to be non-parametric models, not because they do not have any parameters, but because these parameters are not previously defined and their number depends on the training data used. The only drawback of SVM is the complexity of training. The SVM also faces problems due to optimization, but this is solved in a dual formulation which makes its size dependent on the number of the support vectors and not on the dimensionality of the input space. This allows the use of kernel functions in the linearly separable case without increasing the algorithmic complexity of the method. These advantages coupled with the sound and well developed theoretical foundations in mathematical optimizations make SVM one of the most widely implemented classification methods. (Gallus, et. al. 2008, pp. 62)



- Possible hyperplanes that separate data

The hyperplane that has maximum margin is the best separator

Figure 2-6 - Principle of Support Vector Machine

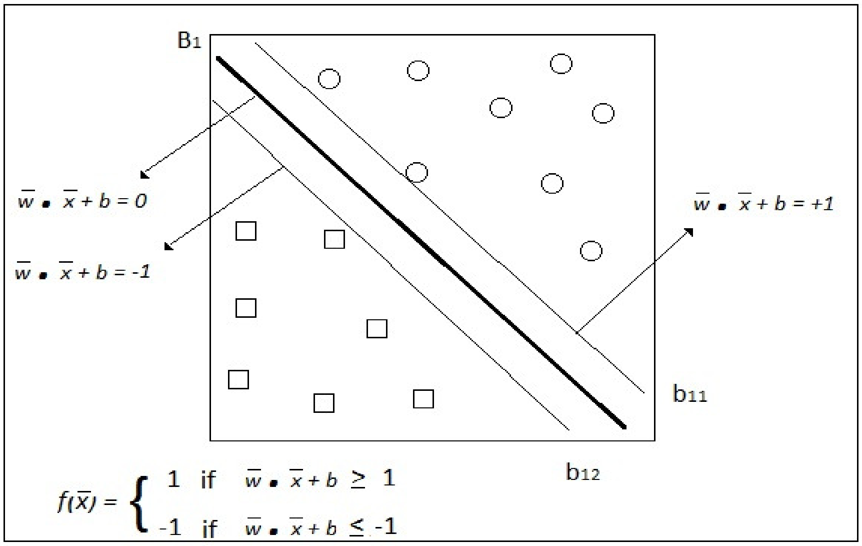


Figure 2-7 - Mathematical Expressions of Support Vector Machine

2.3.4. Kernel Methods

Most of the methods usually consider classification as a linear function of the training data or a hyperplane that can be defined by a set of linear equations on the training data. However, it is also possible that there exists no hyperplane to separate the data. As an alternative, a way to build a nonlinear decision surface can also be a solution. An extremely useful generalization that can give nonlinear surfaces and improved separation of data are possible. The solution given was by means of a Kernel Transformation. The Kernel method is to note that there are classes of function Φ that satisfy the special property of a kernel function K where,

$$K(\mathbf{x_i}, \mathbf{x_j}) = \phi(\mathbf{x_i}) \cdot \phi(\mathbf{x_j}) \qquad \textbf{(2.11)}$$

Then everywhere that $\mathbf{x_i} \cdot \mathbf{x_j}$ occurs, it is replaced by $K(\mathbf{x_i}, \mathbf{x_j})$. It is not necessary to compute $\phi(\mathbf{x})$ explicitly. Only Kernel functions need to be computed. In fact, an explicit representation of ϕ is not necessary at all, only K is required. A function can be defined as a Kernel function if it satisfies Mercer's condition. (Camps-Valls and Bruzzone, 2009, pp. 66-67)

Kernel methods are a popular class of algorithms for data mining forming the most successfully applied classes of learning algorithms. These methods are a special class of instance-based classifiers that allow an instance-based solution for the problem of estimating the best separating hyperplane required to train a classifier. Instance-based learning algorithms using kernel algorithms are known as kernel methods. Mapping the original data into a beneficial space K by using a mapping function $: X \rightarrow K$ is the basic idea of kernel methods. In this new space it is possible to discover a linear algorithm to cover nonlinear patterns in original space. Kernel methods consist of two parts: a kernel function and a kernel-based learning algorithm. The kernel function is a positive definite function on the instances which isolates the learning algorithm from the instances. The learning algorithm does not need to access any particular aspect of an instance – it relies on kernels between instances only. Hence, kernel methods can be applied on any data structure by defining a suitable kernel function. (Wrobel et. al., 2005, pp. 76-77)

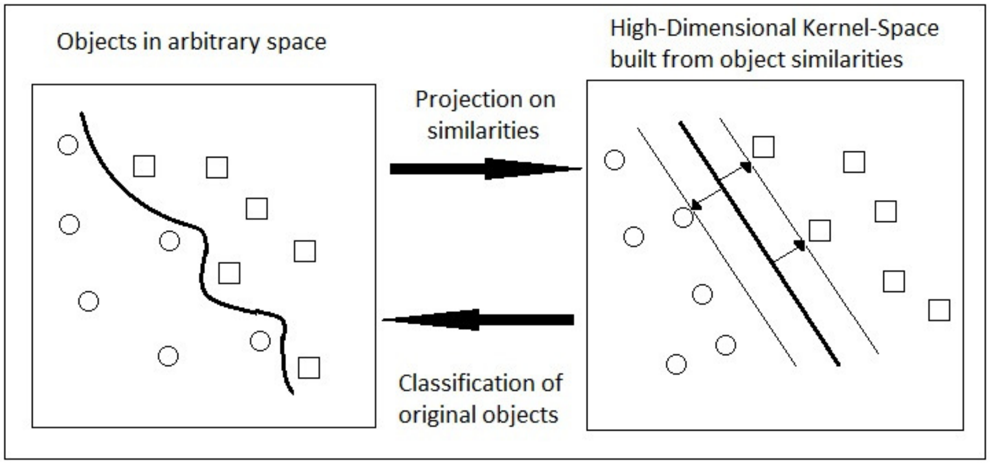


Figure 2-8- Principle of Kernel Methods

2.4. Clustering Methods

Clustering arises as an algorithmic framework for data mining. It is an important task in several data mining applications including document retrieval and image segmentation. The word clustering is a kind of decomposition of a set of data points into natural groups. In other words, it is process of finding and describing cluster i.e. homogenous groups of entities, in data sets. There are two aspects to this task: the first involves algorithmic issues on how to find such decompositions i.e. tractability, while the second concerns quality assignment, i.e. how good is the computer decomposition. Clustering was originally introduced to the data mining research as the unsupervised classification of patterns into groups. Clustering techniques help us to form groups that are internally dense and that are similar with each other. (Rastegar et. al., 2005, pp. 144)

Clustering needs two basic processes. First one is the creation of a similarity matrix or distance matrix. A number of techniques can be used to calculate the distance metric such as Euclidean distance or the use of a standard correlation coefficient.

2.4.1. Hierarchical Clustering

Hierarchical clustering is a methodology to form good clusters in the data set using a computationally efficient technique. This type of method allows a user to ascertain for a comprehensible solution without having to investigate all possible arrangements. Hierarchical clustering algorithms include a consecutive process and are a type of unsupervised learning. Algorithms are found to figure out how to cluster an unordered set of input data without ever being given any training data with the correct answer. As the name implies, the output of a hierarchical clustering algorithm is a bunch of fully nested sets. The smallest sets are the individual sets while the largest is the whole data set. (Minh, et. al, 2006, pp. 160)

After hierarchical clustering is completed, the results are usually viewed in a type of graph called dendogram, which displays the nodes arranged into their hierarchy. A dendogram not only uses connections to show which items ended up in each cluster, it also shows how far apart the items were. *Figure 2-9* below shows a sample dendogram. From the figure, it is clear that the EF cluster is a lot closer to the individual E and F items than the BC cluster is to the individual B and C items. Rendering the graph this way can help to determine how similar the items within a cluster are, which could be interpreted as the tightness of the cluster.

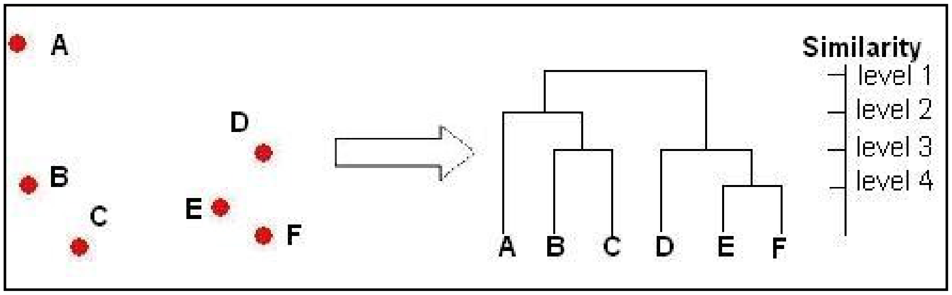


Figure 2-9- Sample Dendogram

Hierarchical clustering techniques can be classified into the following two types (In practice, both approaches often result in similar trees):

2.4.1.1. Agglomerative Hierarchical Approach

This approach is bottom-up and consists of clumping. In each step of the agglomerative hierarchical approach, a new cluster is formed by merging an observation into a previously defined cluster. This process is irreversible; in other words, any two items merged into a cluster cannot be separated in any following steps. The relationship between the two items joined is defined by a metric such as the Euclidean distance. In this process, the clusters grow larger while the number of cluster shrinks. If one starts with n clusters i.e. individual items, they end with one single cluster containing the entire data set. A clustering tree is defined by the path taken to achieve the structure. Agglomerative techniques conduce to give more precision at the bottom of a tree. Agglomerative approach is the more preferred choice. As the process of hierarchical method is irreversible, an optional approach is to carry a hierarchical procedure followed by a partitioning procedure in which items can be moved from one cluster to another. (Pedrycz, 2005, pp. 6) The number of ways of partitioning a set of n items into k clusters is given by

$$N(n,k) = \frac{1}{k!}\sum_{i=1}^{k}(ki)(-1)^{k-i}i^{n} \qquad \textbf{(2.12)}$$

Algorithms that are representative of the agglomerative clustering approach include the ones given below. The algorithms differ from each other in terms of their definition of the distances between two clusters. The closest clusters or the clusters with the smallest distance between them are merged (Seber, 2004, pp. 359).

Algorithm 2.1 - Agglomerative Hierarchical Approach Algorithm

```
Step 0. Begin with the disjoint clustering having level L(0) = 0 and
        sequence number m = 0

Step 1. Find the least dissimilar pair of clusters, say pair (r), (s):
        d[(r),(s)] = min d[(i),(j)]        for all pairs i ,j where i ≠ j.

Step 2. Update m :=m +1. Merge clusters (r) and (s) into a single
        cluster, Set the level of this clustering to L(m) = d[(r),(s)]

Step 3. Update the proximity matrix by deleting the rows and columns
        corresponding to clusters (r) and (s) and adding a row and
        column corresponding to the newly formed cluster.

Step 4. If all objects are in one cluster, stop. Else, go to step 1.
```

i. Single Linkage

This is also known as the **nearest neighbor algorithm**. Here, the distance between the closest pair of data points define the distance between the clusters. Pairs consisting of one case from each group are used in the calculation. The first cluster is formed by merging the two closest groups. The process continues in this manner until there is one group. In some cases, single linkage can lead to chaining of observations, where those on the ends of the chain might be very dissimilar. For two clusters C_A and C_B, the minimum distance is give by d(C_A, C_B) = min {d(x_i, x_j), for x_i in C_A and x_j in C_B}. Here, d(x_i, x_j) is the Euclidean distance or some other distance between the vectors x_i & x_j (Seber, 2004, pp. 360).

ii. Complete Linkage

This is also known as the **furthest neighbor algorithm**. The process for this algorithm is similar to single linkage but the clustering criterion is different. Instead of the closet pair, the distance between the groups is the most distant pair of observations. The logic behind using this type of similarity criterion is that the maximum distance represents the smallest sphere that can enclose all of the objects in both clusters. Thus, the closest of these cluster pairs should be grouped together. The complete linkage method does not have the chaining problem that single linkage has. (Seber, 2004, pp. 361)

iii. Average Linkage

This method is also similar to the above two algorithms and the cluster distance is the average distance between all pairs. In this method, all pairwise distances between observations in each cluster are found and average is taken. This linkage method tends to combine clusters with small variances and to produce clusters with approximately equal variance. Average distance between C_A and C_B is calculated by:

$$d(C_A, C_B) = \frac{1}{n_A n_B} \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} d(\mathbf{x_i}, \mathbf{x_j}) \qquad \textbf{(2.13)}$$

where n_A and n_B refers to number of data points in C_A and C_B, respectively. (Seber, 2004, pp. 363)

iv. Centroid Linkage

In this method, the distance between the centers is the distance between the two clusters (the m-dimensional sample mean for those observations that belong to the different cluster). Whenever clusters are merged together or an observation is added to a cluster, the center is recalculated. Distance between two clusters A and B is

$$\mathrm{d}(C_A, C_B) = d(\overline{x_A}, \overline{x_B}) \qquad \textbf{(2.14)}$$

Here, $\overline{x_A}, \overline{x_B}$ are the mean vectors for the observation vectors in C_A and observation vectors in C_B respectively. After the two clusters C_A and C_B are joined, the center of the new cluster C_{AB} is given by the weighted average (Seber, 2004, pp. 362):

$$\overline{x_{AB}} = \frac{n_A\,\overline{x_A} + n_B\overline{x_B}}{n_A + n_B} \qquad \textbf{(2.15)}$$

v. Wald's Algorithm

The distance between two clusters is defined as the incremental sum of the squares between the two clusters. To merge clusters, the within-group sum-of-squares (sum of squared distances between all observations in a cluster and its center) is minimized over all partitions obtained by combining two clusters. This method produces clusters with about the same number of observations in each one. (Seber, 2004, pp. 363)

2.4.1.2. Divisive Hierarchical Approach

This approach is top-down and consists of splitting. In the initial phase of this approach, all items are in one cluster. At each step, one cluster is divided into two clusters. The items cannot be moved to another cluster, after the splitting is done.

At the end of this approach, there are n clusters and each cluster contains only one data point in it. A clustering tree is defined by the path taken to achieve the structure. Divisive approach is the less preferred choice. Several analysts however consider divisive method to be superior because: the approach begins with the maximum information content; divisions till n clusters of one object are available is not needed; also if the number of variables/ characteristics is less than the objects, the computation needed is less. In case of large n and moderate m, the divisive methods are the only realistic option. Divisive techniques offer more precision at the top of a tree; better suited for finding few, large cluster. (Pedrycz, 2005, pp. 6)

Divisive algorithms are generally of two classes: monothetic and polythetic. Division into two groups is based on presence or absence of an attribute. The variable is chosen that maximizes a chi-square statistic or an information statistic. In a monothetic approach, the division of a group into two subgroups is based on a single variable, whereas, the polythetic approach uses all m variables to make the split. If the variables are binary, the monothetic approach can easily be applied. With divisive methods, dividing the n objects into two groups is the first step. There is 2^{n-1}-1 different ways to complete this step, so that it is hard to examine every such division even with a large computer. Because of that, most of the early techniques were monothetic. However, this method was sensitive to errors in recording or coding the variable used for the division so that the outliers can lead to progression down a wrong branch of the hierarchy. By contrast, agglomerative methods are polythetic by nature as the fusion process is based on all the variables. A monothetic system can be made polythetic using iterative relocation of all objects at each division. According to many researchers, monothetic divisive programs are still the only realistic approach to cluster analysis when n is very large and m is moderate. However, monothetic divisive programs are not favored in taxonomic studies, as they frequently lead to misclassifications. (Seber, 2004, pp. 377-378)

2.4.2. Center-Based Clustering Algorithms

Center-based clustering algorithms use the distances between the data points and centers of the clusters while forming the clusters. The objective of these algorithms is minimizing the total distance between the points and their clusters. The best-known and most commonly used center-based clustering algorithm, k-means algorithm, is explained in the following part. (Iyigun, 2010, pp.4-5)

2.4.2.1. K-means algorithm

It is also known as the centroid-based technique. The K-means approach is a much faster clustering method that is more suitable for large-scale applications. K-means is a partitioning method where there are "K" randomly generated seed clusters. Each data points associated with each of the clusters based on similarity and the mean of each cluster is generated. K-means is a common clustering algorithm. Its purpose is to divide n data points ($\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n$) into K clusters. The initial clusters centers ($\mathbf{c}_1, \mathbf{c}_2, ..., \mathbf{c}_k$) are assigned randomly and are updated by a concordant method. The main characteristic of the clustering method is that the resulting similarity within a cluster is high but the similarity between different clusters is low. (Han and Kamber, 2006, pp. 402) The algorithm works as follows:

Algorithm 2.2. - K-means clustering algorithm

```
Step 0. Initialization: Given Data Set $\mathcal{D}$, Decide the number of clusters K and
        assign values to centers ($\mathbf{c}_1, \mathbf{c}_2, ...., \mathbf{c}_k$)
Step 1. Calculate the distances $d(\mathbf{x}_i, \mathbf{c}_k)$ for all i and k.
Step 2. Assign every data point to the closest cluster
Step 3. Re-calculate the distances $d(\mathbf{x}_i, \mathbf{c}_k)$ for all i and k.
Step 4. Re-assign every data point to the closest cluster. If the centers have not
        change stop, otherwise go to Step 3.
```

K-means is advantageous for clustering large data sets due to its faster running time O(KnrD), where K is the number of clusters and n is the total number of inputs. (Thuraisingham, et. al., 2009, pp. 159)

K-means is an iterative clustering algorithm that searches from the best splitting of the data into a predetermined number of clusters (k). K random points are chosen to be the centers of the k clusters at the first iteration and each instance is assigned to the closest cluster centre. The next step is to recalculate the centers of each cluster to be the centroid i.e. mean of the instances belonging to the cluster. All instances are reassigned again to the closest cluster center. This step is repeated until no more reassigning occurs and the cluster centers are established.

As with all clustering algorithms, a distance function needs to be chosen to measure the closeness of the instances to the cluster centers. Here, also Euclidean distance is the most commonly used metric; however, the choice of the function depends primarily on the problem being solved. For a given value of the parameter k, the k-means algorithm with always find k clusters, regardless of the quality of clustering. This makes the choice of parameter k very important. In the cases when there is no prior knowledge of k, the algorithm might start with a minimum two clusters and then the value of k can increase until a certain limit of the distance between the centre of a cluster and instances assigned to it is reached. The k-means clustering algorithm is very sensitive to choice of the initial cluster centers. Since, the sum of distances from each instance to its respective cluster center is minimized, only a local minimum can be found. To attempt to find the global minimum, the algorithm might have to be run several times for choosing the best clustering.

There are some points that should be decided carefully for the K-means algorithm. First, the reassigned K could not be optimal. Even if K is optimal, because the initial K centers are selected randomly, it cannot be ensured that the clustering result is optimal. In addition, because K-means is essentially a hill-climbing algorithm, it is guaranteed to converge on a local optimum, but there is no guarantee for reaching a global optimum. In other words, the quality of the results is sensitive to the choices of the initial centers. (Thuraisingham, et. al., 2009, pp. 159)

2.4.2.2. Fuzzy k-means

Fuzzy k-means algorithm is the adapted k-means algorithm to soft clustering. The algorithm has an objective function to be minimized:

$$f = \sum_{i=1}^{n} \sum_{k=1}^{K} u_{ik}^{m} d_{ik}^{2} \qquad \textbf{(2.16)}$$

Where u_{ik} are the probabilities that $\mathbf{x_i}$ belongs to $\boldsymbol{C_k}$, d_{ik} are the distance between data point $\mathbf{x_i}$ and center of $\boldsymbol{C_k}$ and m is the fuzzifier that satisfy the conditions below (Iyigun, 2010, pp.4-5):

$$\sum_{i=1}^{n} \sum_{k=1}^{K} u_{ik} = 1 \qquad \textbf{(2.17)}$$

$$u_{ik} \geq 0 \text{ , for all } i \text{ and } k \qquad \textbf{(2.18)}$$

$$m \geq 1 \qquad \textbf{(2.19)}$$

The centers of the cluster are calculated by:

$$c_k = \frac{\sum_{i=1}^{n} u_{ik}^{m} x_i}{\sum_{i=1}^{n} u_{ik}^{m}} \quad \text{, k = 1, … , K.} \qquad \textbf{(2.20)}$$

2.5. Validation

The meaning of term “Validation” is to test to find if the desired specifications are met. The specifications are defined before the validation process. During the validation, one controls the data according to these specifications. Cases which are not consistent with the specifications are accepted as error. If the model is unable to satisfy the expected requirements or the error rate is too high to confirmation, one should redesign the model. One of the most common validation method, and the validation method used in this study, is k fold cross validation. The details of this method are explained in the next section.

2.5.1. K fold cross validation

The cross-validation method is one of the most common complexity regulation methods for estimating the empirical out-of-sample error. Ideally, if enough data was available, a validation set would be set aside and used for asses the performance of the prediction mode. (Principe, et. al., 2010, pp. 36)

However, as data are often scarce, this is usually not possible. K-fold cross-validation is adopted when the number of instances is small to finesse the problem. K-fold cross validation is actually a powerful and common model validation procedure in its own right, regardless of the size of the data set. It is an extension of the holdout method in that the data set is split for model training and testing. Here, part of the available data is used to fit the model, and a different part of the data is used to test it. Ten-fold cross-validation is often used i.e. model is divided into 10 parts. Model is then trained on nine-tenths of the data before calculating the error rate. Once this is complete, the next tenth of the data is held back while the model is continued to be trained on the remaining none-tenths. Again the error rate is calculated. This process is repeated until all 10 parts have been held out and the resultant model will have been trained and evaluated on ten different individual data sets. each case will have been included nine times in the overall training process and once in the evaluation process. The mean of the 10 error rates is then calculated to provide an overall estimate of the error. (Priddy and Keller, 2005, pp. 102)

K-fold cross-validation is a common approach to estimating prediction accuracy. K-fold cross-validation means that k is left out off the cross validation. Here, the data set which comprises on n instances is randomly partitioned into k disjoint subsets. k is typically a small number such as 5 or 10. Each of the k parts have equal number of observations if n is exactly divisible by k; otherwise the final partition will have less observation than the other k-1 parts. At each of these k iterations or fold of cross-validation process, k-1 data subsets are used for classifier and remaining subset is used for testing, which becomes the test set.

That is to say, a total of k runs is carried out in which each of the k parts in turn is used as a test set and the other k-1 parts are used as a training set. (Principe, et. al., 2010, pp. 36) The process is illustrated in the figure below.

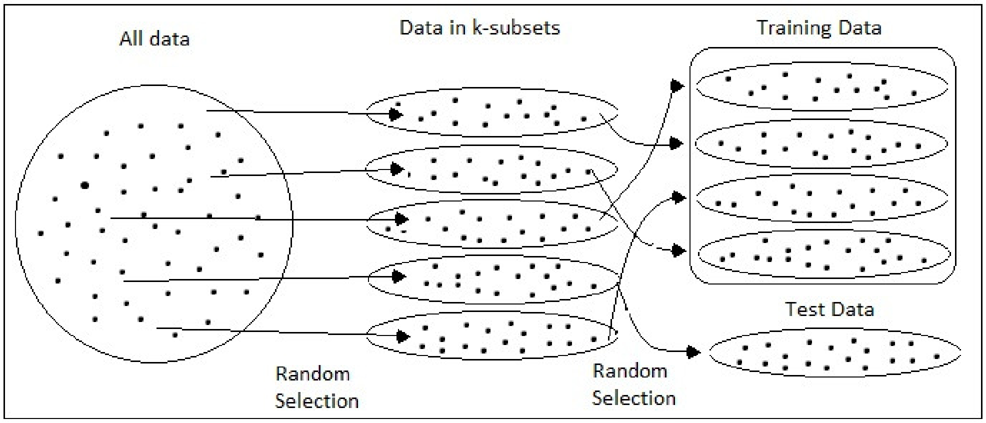


Figure 2-10 - K-fold Cross Validation Process

While the k test sets in k-fold cross-validation are disjoint, the learning sets may overlap. The use of a testing i.e. validation set is necessary to avoid over-learning the training data, especially when no statistical significance test is included in the learning algorithm. k-fold cross-validation is a costly way to estimate the true predictive accuracy of data mining method: It requires building k different models, each using a different part of the training set. Due to the high variance of cross-validation results, there is a need for running k-fold cross-validation on the same data set many and then averaging the obtained validation accuracy. For k-fold cross validation, it is always recommended to retain a third fraction of the complete data set for testing. In other words, some data needs to be held back so that the model can be applied to the data that is not a part of the training or the testing process. (Principe, et. al., 2010, pp. 36)

2.5.2. Type-I and Type-II Error

The case that an individual is accepted as free of disease when he has the disease is different from the case that the individual accepted that has the disease when he is free of disease. Because of this difference two types of incorrect results can be concluded:

Type-I Error

It is also known as **"error of the first kind".** In this case the test gives a positive result, when actually the truth is not the same. An example of this would be if a test shows that a woman is unproductive when in reality she is not. That is why type-I error is accepted as **"false positive".**

Type-II Error

It is also known as **"error of the second kind".** In this case the test gives a negative result, when actually there is a positive situation. An example of this would be if a test shows that a woman is not pregnant when in reality she is. That is why type-II error is accepted as **"false negative".**

CHAPTER 3

METHODOLOGY

3.1. Terminology

Every data point, in m dimensional space, is shown as a vector **x** which has parameters ($x_1, x_2, x_3, \ldots , x_m$). This m dimensional space is denoted as **x-space**. Similarly every data point has a class or label, shown as y_i. This 1 dimensional space is denoted as y-space.

Table 3.1 - The meanings of x-space and y-space

x-space (variables)	**y-space (labels)**
x_{11} x_{12} x_{13} … x_{1m}	y_1
x_{21} x_{22} x_{23} … x_{2m}	y_2
…	…
x_{n1} x_{n2} x_{n3} … x_{nm}	y_n

The distances, explained in section 2.1. , are shown as d($\mathbf{x_1}$,$\mathbf{x_2}$) in the following parts. Here, $\mathbf{x_1}$ is the **x-space** parameters of point 1 and $\mathbf{x_2}$ is the **x-space** parameters of point 2. So the distance d($\mathbf{x_1}$,$\mathbf{x_2}$) is the **x-space distance** between these two points. Similarly we name the distance d(y_1,y_2) as the **y-space distance** between the labels y_1 and y_2 . As a result, the term **distance,** in this paper, is used as a combination of these two distances:

$$\mathcal{D}(\mathbf{x_1},\mathbf{x_2}) = \mathrm{d}(\mathbf{x_1},\mathbf{x_2}) + \alpha\,.\,\mathrm{d}(y_1,y_2) \tag{3.1}$$

$$\alpha \geq 0 \tag{3.2}$$

Here, α is the coefficient of **y-space distance.** In the case of $\alpha = 0$ the **distance** is equal to **x-space distance**. In the case of very large α values the effect of **x-space distance** become negligible. But the other cases the **distance** is affected by both **x-space distance** and **y-space distance.** The value of α changes the weights of the effects of **x-space distance** and **y-space distance** on the **distance function.**

Three types of data set can be observed and expressed as follows:

- Separable Case: Different classes of data set can be separated easily. At least one hyperplane (a line in two dimensions) can separate the data into classes. *Figure 3-1.* is the geometrical representation of the following example which is a separable case.

Example 3.1: A data set in $\mathbb{R}^2$with N = 200 data points shown in *Figure 3-1*. The data was simulated from normal distributions $N\ (\mu_i\ , \sigma_i)$ with:

$$\mu_1 = (0,0), \quad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

$$\mu_2 = (8,0), \quad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

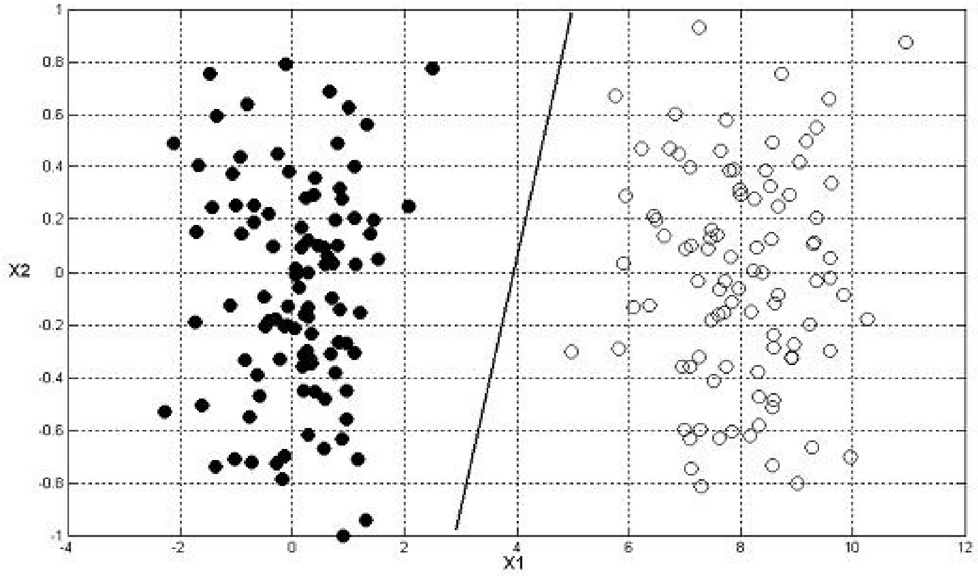


Figure 3-1 - Separable Case

- *Half-Separable Case:* Different classes of data set can be separated with small errors. At least one hyperplane (a line in two dimensions) can separate the data with a low misclassification rate. *Figure 3-2* is the geometrical representation of the following example which is a half - separable case.

Example 3.2: A data set in $\mathbb{R}^2$ with N = 200 data points shown in *Figure 3-2*. The data was simulated from normal distributions $N\ (\mu_i\,, \sigma_i)$ with:

$$\mu_1 = (0,0), \quad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

$$\mu_2 = (4,0), \quad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

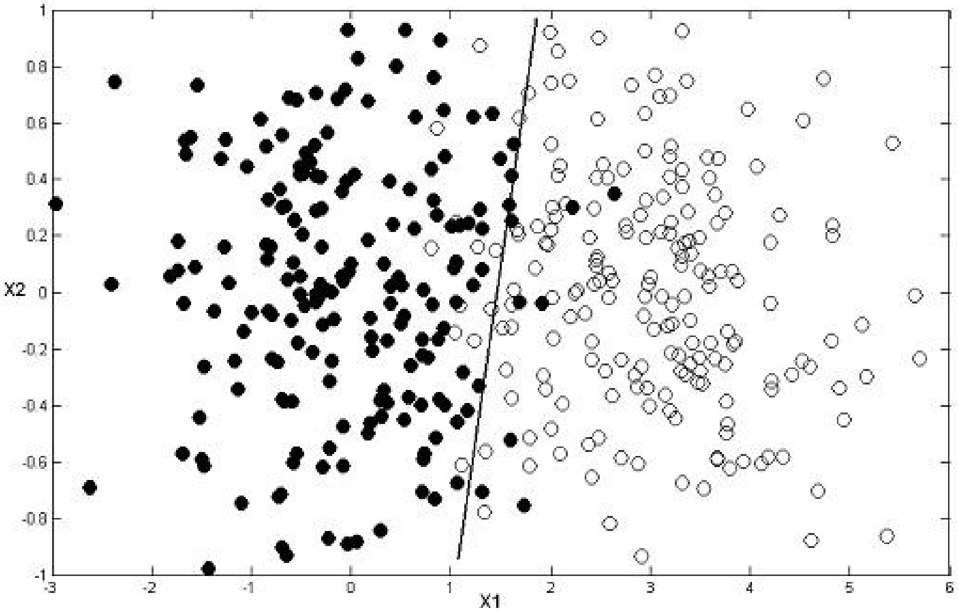


Figure 3-2 – Half - Separable Case

- *Not-Separable Case:* Different classes of data set cannot be separated. *Figure 3-3* is the geometrical representation of an example of not-separable case.

Example 3.3: A data set in $\mathbb{R}^2$ with N = 200 data points shown in *Figure 3-3*. The data was simulated from normal distributions $N\ (\mu_i\ ,\sigma_i)$ with:

$$\mu_1 = (0,0), \quad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

$$\mu_2 = (1,0), \quad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}, \quad \text{(100 points)}$$

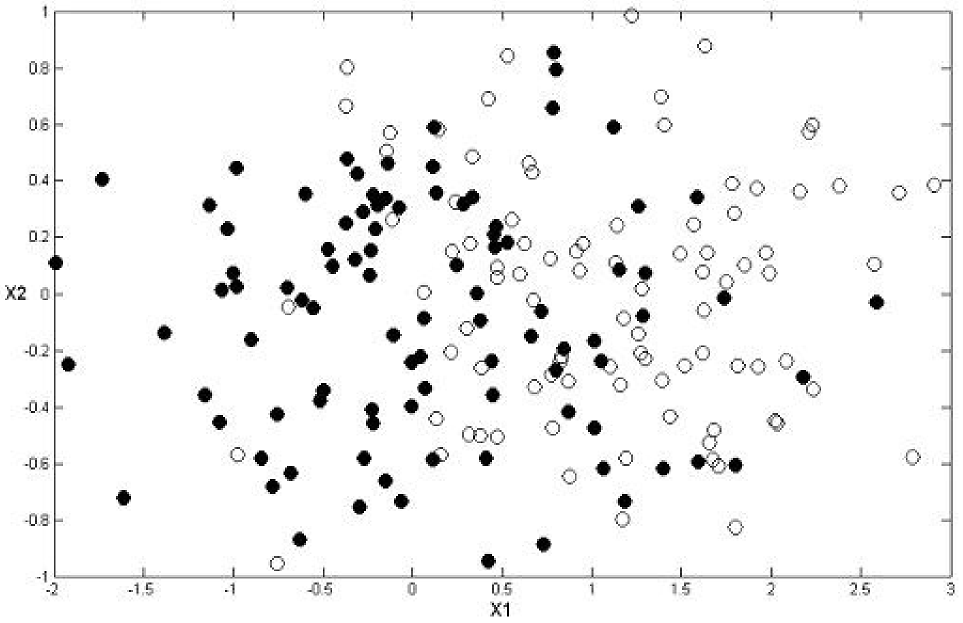
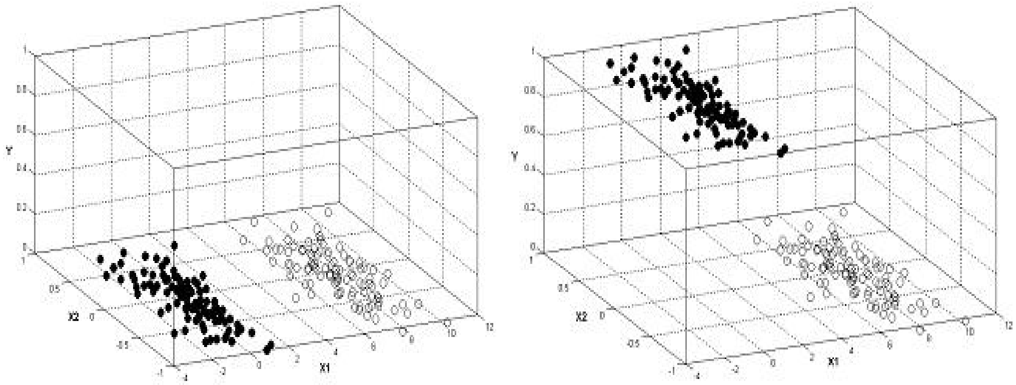


Figure 3-3 – Not-Separable Case

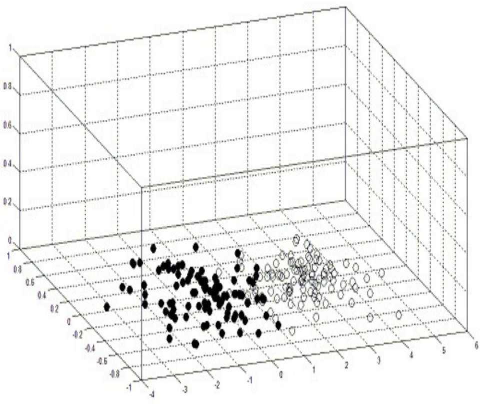
3.2. Effect of α and Geometrical Interpretation

In kernel methods, the not-separable data can be transformed to separable data by mapping the data points into a high-dimensional space. The α value has a similar effect. By the value α, a new dimension is included to the x-space, so the point is mapped to a high-dimensional space. The difference is that there is no transformation in the data values, but addition of a new dimension is in question. The *Figure 3-4, Figure 3-5* and *Figure 3-6* are the figures which are demonstrate the geometrical effect of value α. Although in the separable case the effect of α is relatively small, in the other two cases it is not the same. α transforms the half-separable and not-separable data to separable data by using another dimension.



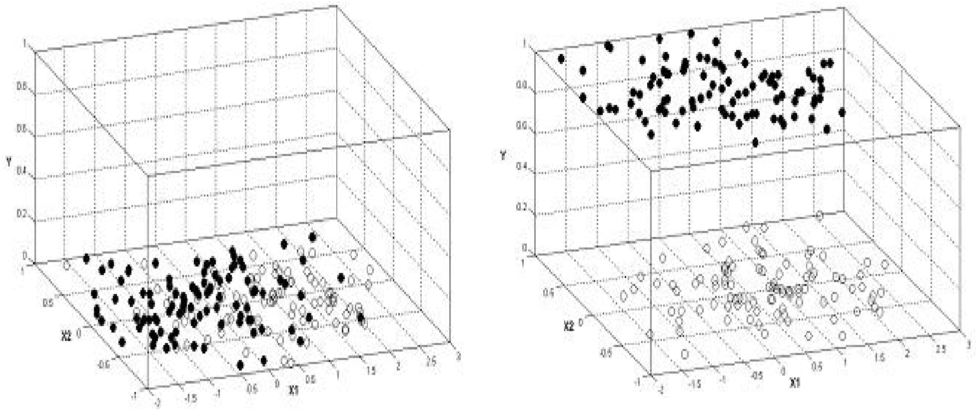
$\alpha = 0$ $\alpha > 0$

Figure3-4– Effect of α *to example 1 (separable case)*



$\alpha = 0$ $\alpha > 0$

Figure 3-5 – Effect of α *to example 2 (half-separable case)*



$\alpha = 0$ $\alpha > 0$

Figure 3-6– Effect of α to example 3 (not-separable case)

3.3. Center Based Algorithm

Algorithm 3.1. - Center Based Algorithm

```
Step 0. Initialization – Assign # of clusters, α value and normalize data matrix
Step 1. Define training and test data sets
Step 2. Learning - Find the clusters and their centers by using training data
Step 3. Prediction – Assign labels to test data
Step 4. Compare the predicted labels with real labels and find the error rate
Step 5. If all partitions of data set are used once as test set go to step 6
            Otherwise change the test set and go to Step 2
Step 6. Find the average error rate and stop
```

Before working with data set, it might have to be normalized in order to avoid any parameter to dominate the classification. Number of clusters that will be used in training part is important and set in initialization step. Optimum number for clusters changes depend on the structure of data set. Addition to that, as it is explained in **section 3.2**, the value α plays an important role. Choosing α as a very small number reduces the effect of labels, and the **x-space** becomes dominant. On the contrary, choosing α as very large number become **y-space** dominant and **x-space** negligible. A suitable value of α is crucial for using the information of both **x-space** and **y-space**.

Splitting data set into training and test sets is a part of the methodology. The normalized data set split into ten parts. Each of them used as test set once and remaining parts are used as training set. So the steps 2,3,4 are repeated 10 times in the algorithm. This methodology is called ten-fold-cross-validation, which is previously explained in **section 2.5.1**.

In the learning part, the aim is forming the clusters and giving labels to each one. The methodology in this step is k-means clustering which is previously explained in **section 2.4.2.1**. Firstly, we randomly set values to centers of clusters, according to the defined number of clusters. Then, assign each data point to the center which is the closest one. In order to find the closest center, the algorithm finds the distances to the centers by using **equation (3.1)** and accepts the smallest one. In the case of an equation, it assigns the data point to any of the clusters that have the smallest distance. Secondly the centers are updated with the information of its new data elements. After that, a reassignment of data points to new centered clusters takes place. This cycle ends when no data point changes its cluster in the reassignment phase. The last process of the learning part is the assignment of labels to the clusters. A cluster is labeled the same value with label of data points which it contains mostly.

The previously determined test data is used in prediction part. Only variables in **x-space** are considered and algorithm tries to predict the labels (**y-space** values) of the points. The distances to the cluster centers are found by using **x-space** distance. The label of the closest cluster is assigned the data point as predicted value. All data points in the test set are processed in the same way.

The original labels and the predicted ones are compared in order to find the error. The error is then classified type-I error and type-II error. When all the repetitions of cross-validation are completed, the average error, type-I error and type-II error rates are calculated. These error rates are then analyzed to interpret the efficiency of the algorithm with the determined number of clusters and α value.

3.4. KNN Based Algorithm

Algorithm 3.2. - KNN Based Algorithm

```
Step 0. Initialization – Assign α value, k value of KNN and normalize data
        matrix
Step 1. Define training and test data sets
Step 2. Learning – Assign new label to each data point according to its k nearest
        neighbors
Step 3. If none of the label is changed go to Step 4.
        Otherwise go to Step 2.
Step 4. Prediction – Assign labels to test data according to its k nearest neighbor
Step 5. Compare the predicted labels with real labels and find the error rate
Step 6. If all partitions of data set are used once as test set go to step 7
        Otherwise change the test set and go to Step 2
Step 7. Find the average error rate and stop
```

In the algorithm equation **(3.1)** and **(3.2)** are used as distance measure, same with center based algorithm. Because of that, the assignment of α has a significant effect on the result. Different from the center based algorithm, this algorithm requires the value of k for the number of neighborhood. By this assignment the algorithm assigns the label to a data point according to the labels of its k nearest neighbors. The structure of the data set may require normalizing operation in initializing phase.

Splitting data set into training and test sets is a part of this methodology, too. Similar with center based algorithm, the normalized data set split into ten parts. Each of them used as test set once and remaining parts are used as training set. So the steps 2, 3, 4 and 5 of the algorithm are repeated 10 times in the algorithm. This means that ten-fold-cross-validation is used here which is previously explained in **section 2.5.1**.

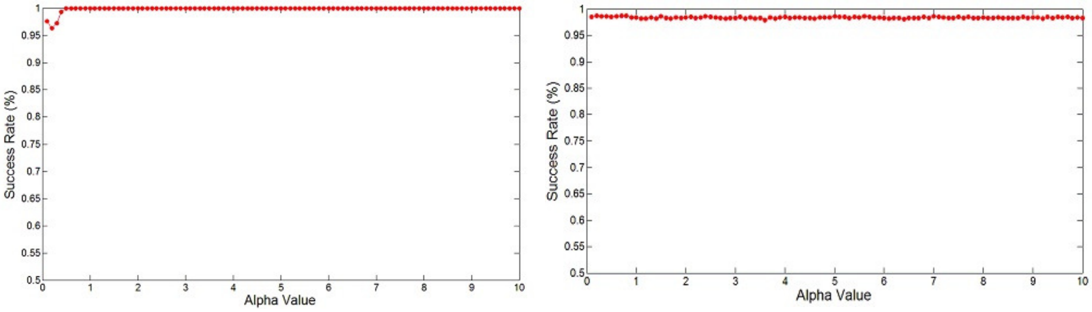
Each data point in data set has an original label. This methodology requires assigning a new label to each data point, assigned label. k nearest neighbors of each data point are taken into consideration and the dominated label is assigned to the data point as assigned label. After completing the process for all the data points in the data set, we control the number of data points that change its label. If there is no data point that changes its label, algorithm continues with the next step. Otherwise algorithm repeats the learning phase until the number of data points that change its label drops to zero.

The prediction phase occurs similar with the learning phase, but executed once. All data points in the learning phase gather an assigned label from the assigned labels of its k nearest neighbors of training set. The difference between the assigned labels and the original labels gives the error rate for current loop of cross-validation process. After all loops are completed the average error rate can be calculated to evaluate the performance of the algorithm.

CHAPTER 4

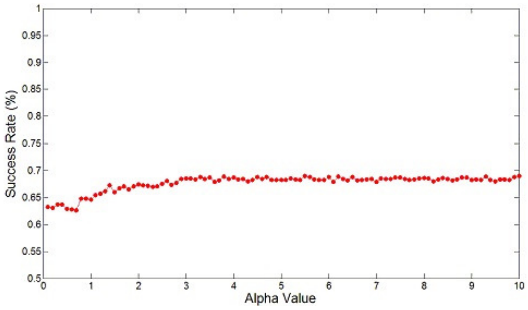
APPLICATION

Both algorithms are tested with generated data sets presented in **Chapter 3**. These data sets are generated with MATLAB Version 7.5.0.342 (R2007b) by using the source code shown in **Appendix–B**. All cases, named “separated”, “half-separated”, “not-separated” are tested with different parameter values, using center based heuristic and *KNN based heuristic*. Below, the figure shows the classification success rate of center-based heuristic:



Center Based, Euclidean Distance, K = 2
Separable Case

Center Based, Euclidean Distance, K = 2
Half-Separable Case



Center Based, Euclidean Distance, K = 2
Not-Separable Case

Figure 4-1 Classification Success Rates of Center Based Heuristic with Euclidean Distance

The α value is not effective on classification success rate in separable and half-separable data sets. **Appendix-C** shows the success rates of both heuristics on the data sets for different parameters.

After testing the algorithms by using generated data sets, both heuristics applied to real biomedical data sets taken from University of California, Irvine. These data sets contain the observations of different parameters in case of disease or health. In addition to becoming real data sets, they have different number of dimensions and also different numbers of classes (labels). The properties of these data sets are shown in *Table 4-1.*

Table 4-1 Properties of biomedical data sets

Name	**Number of points**	**Dimensions**	**Labels**
Breast Cancer	699	9	2
Diabetis	768	8	2
Hepatitis	155	19	2
Liver Cancer	345	6	2
Voting	435	16	2
Wine	178	13	3

In order to test the algorithms with these data sets, both algorithms executed with different parameters. For center-based heuristic 2, 3 and 4 clusters are used with an α scale. In this scale, α is increasing by 1 from 0 to 100. For KNN based heuristic 3 nearest neighbors is used. In this algorithm 100 different α values are also examined incrementing between 0 and 100. These experiments are performed on a computer that is Pentium(R) Dual Core CPU with 2.20 GHz, 2GB installed memory(RAM) and 32-bit operating system. The execution times are shown in *Table 4-2.*

Table 4-2 Execution times with biomedical data sets

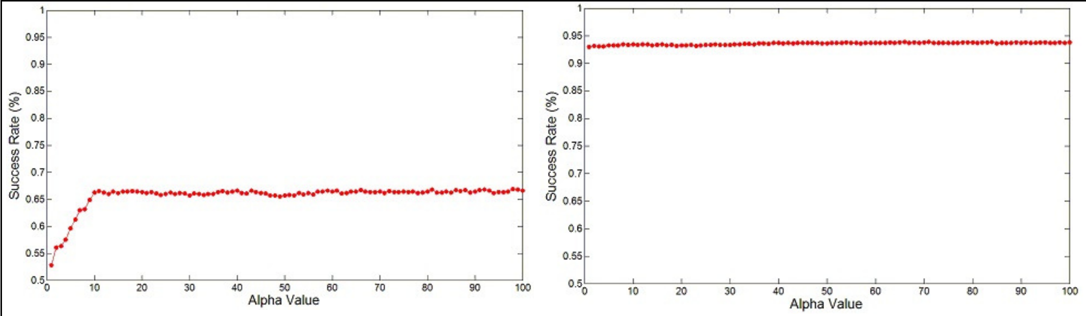
Data Set	**Time with Center-Based Algorithm (seconds)**	**Time with KNN-Based Algorithm (seconds)**
Breast Cancer	11.22	132.99
Diabetis	14.20	259.57
Hepatitis	2.88	13.77
Liver Cancer	5.30	32.70
Voting	9.25	90.38
Wine	3.88	8.94

Appendix–C gives the classification success rates of heuristics on these data sets.

CHAPTER 5

DISCUSSIONS AND EVALUATIONS

In **Chapter 4**, two heuristics are applied on real data sets, there are lots of experiments on generated data sets investigating the effects of parameters on classification success rates. One of these parameters for *center based heuristics* is the number of clusters, K. Although the success rates are changing according to K, there is no pattern to conclude for number of clusters; but the only important thing is choosing a cluster number greater than or equal to number of labels in the data set. If not, there will be at least one label that is not assigned to any of the clusters. It means that all data points which should have this particular label will be assigned to another label and it cause incorrect predictions. One of the biomedical data set "Wine" is a good example for this issue.



Wine Data Set, Mahalanobis Distance
K = 2

Wine Data Set, Mahalanobis Distance,
K = 3

Figure 5-1 Classification Success Rates of Wine Data Set (Center Based Heuristic with Mahalanobis Distance)

Wine data set contains three labels. When two clusters are used in the algorithm, the minimum error is around 34%, because all clusters are labeled with dominated data points and at the end there are two labeled clusters. So, one or two labels are used for labeling the clusters. It means that at least one label is not assigned to a cluster. Any data point which has this label is assigned to one of the other labels, causing high classification error rate. On the contrary, when 3 clusters are used in the algorithm, all labels can be used for labeling the clusters. It provides an opportunity to assign all data points to its real clusters. In this case error is reduced to 7% (*Figure 5-1*).

Similarly choice of K in *KNN based heuristic* is also important. If K is an even number, it can be difficult to find dominated label in a data point's neighborhood. When K is an even number, the points forced to be assigned arbitrarily in the case of tie. For this reason the choice of odd number for K, is a better choice in *KNN based heuristics* and K = 3 is used in this thesis. It is also possible to work with bigger odd numbers instead of 3, but since all the neighbors have the same importance in the heuristic, bigger K values lead to loose the local structure. This would be against the logic of *KNN based algorithm*.

Since Mahalanobis distance takes the correlations within a data set between the variable into consideration, this distance is used in both of the algorithms. The main reason for this choice is the structure of biomedical data sets. Correlations within the biomedical data sets make this distance type a better option for heuristics. In addition to this, Euclidean distance is also used for testing the heuristics in generated data sets.

The most important part of the algorithm, α value, has a strong effect up to a level. The main effect of α is to help the clustering in training phase. It maps the different labels to different areas in the new space, so classification becomes easy comparing with the original space (*Figure 3-6*). Small α values means small distances, large α values means large distances between these areas. This is why the clustering error reduces while α is increasing. In some value of α, the distance between these areas becomes so large which makes the clustering error zero. After that value increasing α has no effect on clustering, since clustering error already reaches zero. After that point the cluster centers and cluster labels can easily be found without any error. This effect can also be seen on the result diagrams of the algorithms. Error rates reduce up to a value and after that value, error rates get settled down. (See **Appendix-C**)

It is also valid for *KNN based heuristics*. While α maps different labeled data groups to different spaces, it increases the distances between different labeled data points. This reduces the probability of including any data points to a neighborhood of different labeled data point. When α reaches an optimal value, this probability and also training error becomes zero.

The particular value of alpha that makes the training error zero varies according to the structure of data set. If the data set contains separable classes, small alpha values may be sufficient, since the training error is already very small without any α value. On the contrary, half-separable or not-separable cases need higher α values to decrease the classification error in the training set.

Dimensions of data set also affect the optimal value of α. The way that α supports the training phase is adding a new dimension to data set. Adding a new dimension to 2-dimensional data set is more effective than adding a new dimension to 20-dimensional space. Because in the second case there are many other parameters that affect the distance calculation, so this additional dimension should have more weight to make the same affect with first case, and this weight is α.

To sum up, α value decreases the error rate in the testing data but it may take different values for different sets. Overall, higher the α value is, better the classification success rate is. In six biomedical data sets, the error rates are reduced by the help of α up to 8% comparing with the algorithms without α value (or $\alpha = 0$).

Table 5-1 Enhancement in Center Based Heuristic by α with biomedical data sets

Data Set	**α = 0**	**α = 100**	**Δ Error**
Breast Cancer	3,86%	3,83%	0,03%
Wine	7,02%	6,26%	0,76%
Voting	13,70%	11,46%	2,24%
Diabetis	34,50%	31,89%	2,61%
Hepatitis	48,88%	42,71%	6,17%
Liver Cancer	41,89%	33,77%	8,12%

Table 5-2 Enhancement in KNN Based Heuristic by α with biomedical data sets

Data Set	**α = 0**	**α = 100**	**Δ Error**
Breast Cancer	3,92%	3,53%	0,39%
Wine	5,77%	4,26%	1,51%
Voting	10,71%	9,77%	0,94%
Diabetis	26,48%	26,42%	0,06%
Hepatitis	42,49%	42,31%	0,18%
Liver Cancer	36,91%	34,73%	2,18%

CHAPTER 6

CONCLUSION AND FURTHER STUDIES

In this study, a new classification approach is examined. Information from class labels is combined with information from variables (features) by mapping the original space to a high dimensional space. In other words, a new kernel function is created by using a distance measure combining the feature space and class labels. This measure not only considers the distances between features but also the distance between class labels with a predefined weight value, α. This approach is implemented to two new heuristics which are tested with generated data sets and real biomedical data sets.

In "*center based heuristic*", α value does not affect the classification error rates significantly in separable data sets. In contrary, α value affects the results on half-separable and not-separable cases. Up to 8% of enhancement in classification error rate is observed in biomedical data sets with *center based heuristics*. In Breast Cancer data set even with zero value for α, high success classification rate is obtained and incremented α value is not improving success rate. In Liver Cancer data set with $\alpha = 0$ classification success rate equals to 58% which is improved up to 66% with high α values. Although Voting data set has high classification success rate (86%) when $\alpha = 0$, it also shows similar behavior with high α values.

Changing distance basis from Euclidean distance to Mahalanobis distance also increases the classification success rate, since the features are correlated in the biomedical data sets. Mahalanobis Distance considering the correlations, works better. On the contrary, for generated data sets, the effect of distance basis becomes less important since there is no correlation. Unlike α value and distance basis, number of clusters has no significant effect on classification success rates. While the classification success rate improves with increasing K (number of clusters) in Hepatitis data set, the classification success rate is affected negatively with increasing K in Breast Cancer data set.

In *KNN based heuristic*, success rates are relatively high for low α values comparing with center based algorithm. But the change with α value is not as high as the previous algorithm. Similarly in the separable case, it is hard to say that there is an effect of α on classification success rates. For not separable case, an improvement in success rate is observed by increasing α value, but it is not as effective as center based algorithm. The enhancement is up to 2% in biomedical data sets. Because of the data structure, changing distance basis from Euclidean to Mahalanobis also affects the results on biomedical data sets. Changing number of neighbors, determined by the user in advance, in *KNN based heuristic*, has no significant effect. But it is better to choose an odd number for the number of neighbors.

In this study, a projection approach to a higher space (in training set) using a compound distance measure combined feature space and class labels is developed. The effect of label information, represented by α value, is investigated in classification success rate. Although effect of label information measured with α is different for center-based and *KNN based heuristic*, there is a common behaviour in both algorithms. The improvement of the classification success rate depends on the complexity of data set. In other words, α affects non-separable sets more than separable sets. This common behaviour creates a question that should be examined in further studies. Can α value be a measure for separability?

It is observed that only α value is not enough to define separability, but a function of α with some other properties of data set, may produce meaningful results for this issue. This study shows that the dimensions of data, or number of variables in the data set, are important for effect of α. In addition to this, algorithm used for error calculation is also important for effect of α. These observations give a clue to find a separability measure for future research.

REFERENCES

Berry, M.J.A., Linoff, G.S., (2009), *Data Mining Techniques: For Marketing, Sales and Customer Relationship Management*, 2nd edition, New York: Wiley Publishing

Besset, D.H., (2001), *Object-Oriented Implementation of Numerical Methods: An Introduction with Java and Smalltalk*, California: Morgan Kaufmann

Bock, R.K., Krischer, W., (1998), *The Data Analysis Briefbook*, New York: Springer-Verlag

Camps-Valls, G., Bruzzone, L., (2009), *Kernel methods for Remote Sensing Data Analysis*, New Jersey: John Wiley and Sons

Cerrito, P.B., (2007), *Introduction to Data Mining Using SAS Enterprise Miner*, North Carolina: SAS Publishing

Cios, K.J., Pedrycz, W., Swiniarski, R.W., Kurgan, L.A., (2007), *Data Mining: A Knowledge Discovery Approach*, New York: Springer

Cumby, C., Roth, D., (2003), "On Kernel Methods for Relational Learning", *Proceedings of the Twentieth International Conference on Machine Learning (ICML-2003)*, Washington DC, Article accessed on 16th April 2009, http://l2r.cs.uiuc.edu/~danr/Papers/CumbyRo03.pdf

Ertöz, L., Steinbach, M., Kumar, V., (2003), "Finding Clusters of Different Sizes, Shapes, and Densities in Noisy, High Dimensional Data", January 24 2003,

D. Barbara, C. Kamath, (Eds.), *Proceedings of the Third SIAM International Conference on Data Mining, Volume 3*, 2003, San Francisco: SIAM

Eyob, E., (2009), *Social Implications of Data Mining and Information Privacy: Interdisciplinary Frameworks and Solutions*, Pennsylvania: Idea Group Inc.

Gallus, D., Abecker, A., Richter, D., (2008), "Classification of Landslide Susceptibility in the Development of Early Warning Systems", A. Ruas, and C. Gold, (Eds), *2008Headway in Spatial Data Handling, 13th International Symposium*, Berlin Heidelberg: Springer-Verlag

Han, J., Kamber, M., (2006), *Data Mining: Concepts and Techniques*, 2nd edition, California: Morgan Kaufmann

Hand, D.J., Mannila, H., Smyth, P., (2001), *Principles of Data Mining*, Massachusetts: MIT Press

Hearst, M.A., (1998), "Support Vector Machines", *IEEE Intelligent Systems and Their Applications*, July/August 1998, Vol. 13, Issue 4, pp. 18-28, ISSN 1094-

Hill, T., Lewicki, P., (2006), *Statistics: Methods and Applications, A Comprehensive Reference for Science*, Tulsa: StatSoft Inc.

Iyigun, C., (2011), *Clustering,* The Wiley Encyclopedia of Operations Research and Management Science (in print).

Kamen, E.W., Su, J.K., (1999), *Introduction to optimal estimation,* pp. 1, 1999, Berlin Heidelberg: Springer-Verlag

Larose, D.T., (2005), *Discovering Knowledge in Data: An Introduction to Data Mining*, New Jersey: John Wiley and Sons

Lee, D., Kim, M.H., (2002), "Data Mining", Published in Leondes, C.T., *Database and Data Communication Network Systems*, Vol. 1, Copyright 2002, California: Elsevier Science (U.S.A.)

Leondes, C.T., (2005), *Intelligent Knowledge-Based Systems: Volume 1: Knowledge-based Systems*, Norwell, Massachusetts; Birkhäuser & Kluwer Academic Publishers

Li, A., Shi, Y., (2005), "An Integrated Classification Method: Combination of LP and LDA", X. Deng and Y. Ye, (Eds.): *Internet and Network Economies: First International Workshop, WINE 2005*, LNCS 3828, pp. 758-767, 2005, Berlin Heidelberg: Springer-Verlag

Maimon, O.Z., Rokach, L., (2005), *Data Mining and Knowledge Discovery Handbook*, New York: Springer Science & Business

McLachlan, G.J., (1999), "Mahalanobis Distance", *RESONANCE*, June 1999, pp. 20-26, Article accessed on 16th April 2009, http://www.ias.ac.in/resonance/June1999/pdf/June1999p20-26.pdf

Minh, L.H., An, L.T.H., Tao, P. D., (2006), "Hierarchical Clustering Based on Mathematical Optimization", W. K. Ng, M. Kitsuregawa, and J. Li, (Eds): *Advances in Knowledge Discovery and Data Mining: 10th Pacific-Asia Conference, PAKDD 2006*, LNAI 3918, pp. 160-173, 2006, Berlin Heidelberg: Springer-Verlag

Pedrycz, W., (2005), *Knowledge-Based Clustering: From Data to Information Granules*, New Jersey: John Wiley & Sons

Priddy, K.L., Keller, P.E., (2005), *Artificial Neural Networks*, Washington: SPE Press

Principe, J.C., Liu, W., Haykin S., (2010), *Kernel Adaptive Filtering: A Comprehensive Introduction*, New Jersey: John Wiley and Sons

Rastegar, R., Rahmati, M., Meybodi, M.R., (2005), "A Clustering Algorithm using Cellular Learning Automata Based Evolutionary Algorithm", B. Riberio, R.F. Albrecht, A. Dobnikar, (Eds), *Adaptive and Natural Computing Algorithm*, New York: Springer-Verlag

Seber, G.A.F., (2004), *Multivariate Observations*, New Jersey: John Wiley and Sons.

Shmueli. G., Patel, N.R., Bruce, P.C., (2008), *Data Mining for Business Intelligence: Concepts, Techniques, and Application in Microsoft Office Excel with XLMiner*, New York: John Wiley & Sons

Taylor, C.M., Agah, A., (2008), "Data Mining and Genetic Algorithms: Finding Hidden Meaning in Biological and Biomedical Data", T.G. Simolinski, M.G. Milanova, A.E. Hassanien, (Eds.): *Computational Intelligence in Biomedical and Bioinformatics: Current Trends and Applications*, SCI 151, pp. 49-68, 2008, Berlin Heidelberg: Springer-Verlag

Thuraisingham, B., Awad, M., Khan, L., Wang, L., (2009), *Design and Implementation of Data Mining Tools*, Florida: CRC Press.

Wrobel, S., Gärtner, T., Horváth, T., (2005), "Kernels for Predictive Graph Mining", *From Data and Information Analysis to Knowledge Engineering, Volume 2005-2006*, New York: Springer-Verlag

Wübben, M., (2008), *Analytical CRM: Developing and Maintaining Profitable Customer Relationships in Non-Contractual Setting*, 1st edition, Frankfurt: Gabler Verlag

Zhang, Y., Su, H.Y., Jia, T., Chu, J., (2005), "Rule Extraction from Trained Support Vector Machines", T.B. Ho., D. Cheung, H. Liu, (Eds.): *Advances in Knowledge Discovery and Data Mining: 9th Pacific-Asia Conference PAKDD 2005*, LNAI 3518, pp. 61-70, 2005, Berlin Heidelberg: Springer-Verlag

APPENDICES

APPENDIX A

Algorithms in MATLAB

Center Based Algorithm

```
clear all
gennum = 500;
mu = [0 0];
SIGMA = [1 0; 0 0.2];
data1 = mvnrnd(mu,SIGMA,gennum);
unit = ones(gennum,1);
data1 = [data1 unit];
mu2 = [1 0];
data2 = mvnrnd(mu2,SIGMA,gennum);
unit = zeros(gennum,1);
data2 = [data2 unit];
data3 = [data1 ; data2] ;

[B,C] = size(data3);                    %% B==number of CMUPDATE = [];
%% Matrix for CMUPDATE2 = [];                        %% Matrix for
TRERROR = [];
TRAVER = [];
V = 10;                              %% Number of parts (Cross validation)
N = 10;                              %% Number of repeats  (Cross validation)

%% 1) Variables
K = 3;                           %% K==number of clusters
for alfverr = 1 : 100

alf = alfverr / 10;
```

```
KONTROLX = alfverr

%% 2) Keep The Labels


data = data3 ;
for i = 1:B
LABEL(i,1) = i;
LABEL(i,2) = data(i,C);
data(i,C) = 0 ;
end

%% 3) Find STD Of Attributes


   STD_MAT = std(data);

%% 4) Normalize Matrix


for i= 1:C
   if STD_MAT(1,i)~= 0                    %% To avoid dividing 0.
      NORM_DATA(:,i) = data(:,i)/STD_MAT(i) ;
   else
      NORM_DATA(:,i) = 0 ;
   end
end

%% 5) Repeat Cross Vaidation N Times


for h = 1 : N

%% 6)Divide The Set For Cross Validation
```

```
   part = round(B / V) ;                    %% Find the number of data in each part(Total data / # of parts)
    for dim = 1 : V
       DUM(1,dim) = part ;                  %% Matrix controls the # of data in each part.
    end
   for k = 1 : B
   CVM (k,2) = 0 ;                          %% CVM (Cross Validation Matrix), keeps the part number that the data belongs to
      while CVM(k,2) == 0
        num = round(0.5 + V * rand) ;       %% produce random number between 0.5 and V + 0.5 round it to a number between 1 and V+1.
        if DUM (1,num) > 0 & num < (V + 1)  %% Controls the # of data in each part and get over the risk of producing V+1.
          CVM (k,1) = k;
          CVM (k,2) = num;
          DUM (1,num) = DUM (1,num) - 1;
        end
      end
   end                                      %% End of producing the parts.



%% 7)Cross Validation:  Loop V times, in each loop one of V sets will be test set.

for t = 1 : V
   r = 1 ;
   s = 1 ;
   for z = 1 : B
      if CVM (z,2) ~= t                     %% In each loop all the parts except t. part will form the training set
```

```
            TRAINING (r,:) = NORM_DATA (z,:) ;     %% TRAINIG matrix
contains training data without labels.
            TRAINING2 (r,:) = TRAINING (r,:) ;
            TRAINING2 (r,C) = LABEL (z,2) ;        %% TRAINIG2 matrix contains
training data with labels.
            r = r + 1 ;
        else                                  %% t. part will be the test set
            TEST (s,:) = NORM_DATA (z,:) ;         %% TEST matrix contains test
data without labels.
            TEST2 (s,:) = TEST (s,:) ;
            TEST2 (s,C) = LABEL (z,2) ;            %% TEST2 matrix contains test data
with labels.
            s = s + 1 ;
        end
    end
    r = r - 1;                                %% # of data in the training set
    s = s - 1;                                %% # of data in the test set

%% 8)Initialine The Centers Of The Clusters

    for u = 1 : K                             %% Initializing the centers or K clusters
        CENTERS2(u,:) = TRAINING2 (u,:) ;          %% CENTERS2 matrix
contains centers of clusters with labels.
        CENTERS(u,:) = CENTERS2(u,:) ;
        CENTERS(u,C) = 0 ;                         %% CENTERS matrix contains centers
of clusters without labels.
    end

    for v = 1 : r
        CLUSTER(v,2) = 0 ;                         %% Initialize CLUSTER matrix.
    end
```

```
%% 9)Produce The Distance Matrix (Initially Covariance Matrix = I)

  CM = eye (C);                    %% Initialize Covariance Matrix as I.

  for v = 1 : r                    %% Find the distances by using initial centers
and I as Covariance Matrix.
    for w = 1 : K
    DISTANCE (v,w) = sqrt(abs((TRAINING(v,:) -
CENTERS(w,:))*(TRAINING(v,:) - CENTERS(w,:))') + alf *
abs(TRAINING2(v,C) - CENTERS2(w,C)));
    end
  end

  counter = 1 ;

%% 10)Determine The Centers Of Clusters


  while counter ~= 0               %% Loop until the centers of clusters will
be determined.
  counter = 0 ;
  for v = 1 : r                    %% Assign data to the clusters.
    [dis,cls] = min (DISTANCE (v,:)) ;     %% Find the closest cluster.
    CLUSTER (v,1) = v ;
    if CLUSTER (v,2) ~= cls              %% Control if the data transfers to
another cluster or not.
    CLUSTER (v,2) = cls ;                %% Assing new cluster number to the
data.
    counter = counter + 1 ;             %% Count the changes.
    end
```

```
    end                                        %% End of assignments.

    for w = 1 : K                                  %% Update the centers.
        for z = 1 : C
        SUM(1,z) = 0 ;
        end
        NUMSUM = 0;
        for v = 1 : r                          %% Find the new center by taking average of
the dimensions.
           if CLUSTER (v,2) == w
            SUM(1,:) = SUM(1,:) + TRAINING2(v,:) ;
            NUMSUM = NUMSUM + 1;
            CMUPDATE(NUMSUM,:) = TRAINING(v,:) ;
                for m = 1 : (C-1)
                    CMUPDATE2(NUMSUM,m) = CMUPDATE(NUMSUM,m) ;
                end
            end
        end
        CENTERS2(w,:) = SUM(1,:) / NUMSUM ;       %% Update the centers.
        CENTERS2(w,C) = round (CENTERS2(w,C)) ;    %% Find the labels of the
centers.
        CENTERS (w,:) = CENTERS2 (w,:) ;
        CENTERS (w,C) = 0 ;                     %% Unlabeled center matrix for
calculations.

        for z = 1 : (C - 1)
            TRAINING3(:,z) = TRAINING2(:,z) ;      %% Unlabeled training matrix
for distance calculations.
            CENTERS3(:,z) = CENTERS2(:,z) ;        %% Unlabeled center matrix for
distance calculations.
```

```
      TEST3(:,z) = TEST2(:,z) ;            %% Unlabeled test matrix for distance
calculations.
    end
    COVMAT (:,:,w) = cov (CMUPDATE2) ;        %% Update Covariance
Matrix for each cluster w.
  end

  for v = 1 : r                            %% Update DISTANCE matrix.
    for w = 1 : K
    DISTANCE (v,w) = sqrt(abs((TRAINING3(v,:) -
CENTERS3(w,:))*(TRAINING3(v,:) - CENTERS3(w,:))') + alf *
abs(TRAINING2(v,C) - CENTERS2(w,C)));
    end
  end
 end                                       %% Return line 106 until the centers of clusters
will be determined.

 cntr = 0;
 terr = 0;
 TRERROR(alfverr,t) = 0;

 for v = 2 : r
 if CLUSTER(v,2) == CLUSTER ((v-1),2)
 else
   terr = terr + 1;
 end
 end
 TRERROR(alfverr,t) = terr - K + 1;

%% 11)Test: Predict The Classes
```

```
 for v = 1 : s
     for w = 1 : K
     CONTROL (v,w) = sqrt(abs((TEST3(v,:) - CENTERS3(w,:))*(TEST3(v,:) - CENTERS3(w,:))'));
     end
 end

 for v = 1 : s
     [dis,cls] = min (CONTROL (v,:)) ;          %% Find the minimum distance.
     PREDIC (v,1) = v ;
     PREDIC (v,2) = CENTERS2(cls,C) ;          %% Predict the class according to the label of cluster.
 end

%% 12)Find The Errors For The Current Cross Validation

 error = 0 ;
 type1 = 0 ;
 type2 = 0 ;

 for v = 1 : s                                  %% Compare the predictions with the real data.
    if PREDIC (v,2) ~= TEST2 (v,C)
     error = error + 1;                         %% Add the error if there is a mismatch.
    end
    if PREDIC (v,2) > TEST2 (v,C)
     type1 = type1 + 1;                         %% Add the error if there is an overestimation.
    end
    if PREDIC (v,2) < TEST2 (v,C)
```

```
      type2 = type2 + 1;                  %% Add the error if there is an
underestmation.
    end
 end

 PERROR(h,t) = error / s ;                 %% Keep the errors for each run.
 PTYPE1(h,t) = type1 / s ;                 %% Keep the errors for each run.
 PTYPE2(h,t) = type2 / s ;                 %% Keep the errors for each run.

end
  TRAVER(alfverr,2) = 0;
  TRAVER(alfverr,1) = alfverr;
  for v = 1 : V
  TRAVER(alfverr,2) = TRAVER(alfverr,2)+ TRERROR(alfverr,V) ;
  end
  TRAVER(alfverr,2) = TRAVER(alfverr,2) / (V * r) ;
end

%% 13)Find The Average Errors

 Avererror = (sum(PERROR(:)) / V) /N ;          %% Find the averages of the
errors.
 Avertype1 = (sum(PTYPE1(:)) / V) /N ;          %% Find the averages of the
errors.
 Avertype2 = (sum(PTYPE2(:)) / V) /N ;          %% Find the averages of the
errors.
 TOTERROR = [Avererror Avertype1 Avertype2];       %% Result Matrix

 Log(alfverr,:) = [alf ([1 1 1] - TOTERROR)] ;
end
```

```
plot(Log(:,1)',Log(:,2)',':dg','MarkerFaceColor','g');
hold on ;
plot(Log(:,1)',Log(:,3)',':*b','MarkerFaceColor','b');
plot(Log(:,1)',Log(:,4)',':or','MarkerFaceColor','r');
hold off;
```

KNN Based Algorithm:

```
%% 0) Initialization
 clear all;
gennum = 500;
mu = [0 0];
SIGMA = [1 0; 0 0.2];
data1 = mvnrnd(mu,SIGMA,gennum);
unit = ones(gennum,1);
data1 = [data1 unit];
mu2 = [8 0];
data2 = mvnrnd(mu2,SIGMA,gennum);
unit = zeros(gennum,1);
data2 = [data2 unit];
data3 = [data1 ; data2] ;
 [B,C] = size(data3);                    %% B==number of data points &
C==dimension of data set
CMUPDATE = [];                           %% Matrix for Updating Covariance
Matrix (with labels)
CMUPDATE2 = [];                          %% Matrix for Updating Covariance
Matrix (without labels)
TRERROR = [];
TRAVER = [];
V = 10;                              %% Number of parts (Cross validation)
N = 10;                              %% Number of repeats  (Cross validation)
%% 1) Variables
K = 3;                               %% K==number of clusters (KNN)
%% alf= coefficient in the distance
for alfverr = 1 : 100
 alf = alfverr / 10;
 %% alf = alfverr ;
```

```
KONTROLX = alfverr
%% 2) Keep The Labels
data = data3 ;
for i = 1:B
LABEL(i,1) = i;
LABEL(i,2) = data(i,C);
data(i,C) = 0 ;
end
%% 3) Find STD Of Attributes
   STD_MAT = std(data);
%% 4) Normalize Matrix
for i= 1:C
   if STD_MAT(1,i)~= 0                          %% To avoid dividing 0.
      NORM_DATA(:,i) = data(:,i)/STD_MAT(i) ;
   else
      NORM_DATA(:,i) = 0 ;
   end
end
%% 5) Repeat Cross Vaidation N Times
for h = 1 : N
%% 6)Divide The Set For Cross Validation
   part = round(B / V) ;                        %% Find the number of data in each
part(Total data / # of parts)
    for dim = 1 : V
       DUM(1,dim) = part ;                      %% Matrix controls the # of data in each
part.
    end
   for k = 1 : B
   CVM (k,2) = 0 ;                              %% CVM (Cross Validation Matrix), keeps
the part number that the data belongs to
      while CVM(k,2) == 0
```

```
           num = round(0.5 + V * rand) ;          %% produce random number between
0.5 and V + 0.5 round it to a number between 1 and V+1.
           if DUM (1,num) > 0 & num < (V + 1)     %% Controls the # of data in each
part and get over the risk of producing V+1.
              CVM (k,1) = k;
              CVM (k,2) = num;
              DUM (1,num) = DUM (1,num) - 1;
           end
        end
    end                                   %% End of producing the parts.
%% 7)Cross Validation:  Loop V times, in each loop one of V sets will be test set.
for t = 1 : V
    r = 1 ;
    s = 1 ;
    for z = 1 : B
        if CVM (z,2) ~= t                  %% In each loop all the parts except t. part
will form the training set
            TRAINING (r,:) = NORM_DATA (z,:) ;     %% TRAINIG matrix
contains training data without labels.
            TRAINING2 (r,:) = TRAINING (r,:) ;
            TRAINING2 (r,C) = LABEL (z,2) ;       %% TRAINIG2 matrix contains
training data with labels.
            r = r + 1 ;
        else                               %% t. part will be the test set
            TEST (s,:) = NORM_DATA (z,:) ;        %% TEST matrix contains test
data without labels.
            TEST2 (s,:) = TEST (s,:) ;
            TEST2 (s,C) = LABEL (z,2) ;           %% TEST2 matrix contains test data
with labels.
            s = s + 1 ;
        end
```

```
   end
   r = r - 1;                              %% # of data in the training set
   s = s - 1;                              %% # of data in the test set
%% 8)Find the labels according to KNN
          TRAINKNN2 (:,:) = TRAINING2 (:,:) ;
          for b = 1 : r
          for a = 1 : C
          TRAINKNN (b,a) = TRAINKNN2 (b,a) ;
          end
          TRAINKNN (b,C+1) = TRAINKNN2 (b,C) ;
          end
          for b = 1 : r
          for a = 1 : (C - 1)
          TRAINXS (b,a) = TRAINKNN (b,a);
          end
          end
          for i = 1 : r
             for j = 1 : r
          KNN(i,j) = 0 ;
             end
          end
  m = 1 ;
  while m ~= 0
   i = 0 ;
   j = 0 ;
   m = 0 ;
   COVKNN (:,:) = cov (TRAINXS) ;
          for i = 1 : r
             for j = 1 : r
 KNN(i,j) = sqrt(abs((TRAINXS(i,:) - TRAINXS(j,:)) *(TRAINXS (i,:) -
TRAINXS (j,:))') + alf * abs(TRAINKNN(i,C+1) - TRAINKNN(j,C+1))) ;
```

```
        end
      end
i = 0 ;
j = 0 ;
u = 0 ;
w = 1 ;
   for i = 1 : r
      x = 0 ;
        for u = 1 : K
           v = 1000000 ;
            for j = 1 : r
               if i ~= j
                  if KNN (i,j) >= 0
                     if KNN (i,j) < v
                        v = KNN (i,j) ;
                        w = j;
                     end
                  end
               end
            end
            if i ~= w
            x = x + TRAINKNN (w,C+1) ;
            end
            KNN (i,w) = -1 ;
        end
        x = round (x / K) ;
        if TRAINKNN (w,C+1) ~= x
           m = m + 1 ;
           TRAINKNN (w,C+1) = x ;
        end
   end
```

```
  end
%% 11)Test: Predict The Classes
          TESTKNN2 (:,:) = TEST2 (:,:) ;
          for a = 1 : C
          TESTKNN (:,a) = TESTKNN2 (:,a) ;
          end
          TESTKNN (:,C+1) = TESTKNN2 (:,C) ;
          for b = 1 : s
          for a = 1 : (C - 1)
          TESTXS (b,a) = TESTKNN(b,a);
          end
          end
          COVKNN (:,:) = cov ([TRAINXS;TESTXS]) ;
          for i = 1 : s
             for j = 1 : r
                 TKNN(i,j) = sqrt(abs((TESTXS(i,:) - TRAINXS (j,:))
*(TESTXS(i,:) - TRAINXS (j,:))'));
             end
          end
   i = 0 ;
   j = 0 ;
   u = 0 ;
   w = 1 ;
          for i = 1 : s
          x = 0 ;
             for u = 1 : K
                 v = 1000000 ;
                 for j = 1 : r
                    if TKNN (i,j) >= 0
                      if TKNN (i,j) < v
                        v = TKNN (i,j) ;
```

```
                    w = j;
                  end
                end
             end
             x = x + TRAINKNN (w,C+1) ;
             TKNN (i,w) = -1 ;
          end
          x = round (x / K) ;
          TESTKNN (i,C+1) = x ;
          end
%% 12)Find The Errors For The Current Cross Validation
 error = 0 ;
 type1 = 0 ;
 type2 = 0 ;
 for v = 1 : s                              %% Compare the predictions with the real
data.
   if TESTKNN (v,C) ~= TESTKNN (v,C+1)
     error = error + 1;                     %% Add the error if there is a mismatch.
   end
   if TESTKNN (v,C) > TESTKNN (v,C+1)
     type1 = type1 + 1;                     %% Add the error if there is an
overestimation.
   end
   if TESTKNN (v,C) < TESTKNN (v,C+1)
     type2 = type2 + 1;                     %% Add the error if there is an
underestmation.
   end
 end
 % Training error
 terror = 0 ;
 ttype1 = 0 ;
```

```
  ttype2 = 0 ;
  for v = 1 : r                            %% Compare the predictions with the real
data.
     if TRAINKNN (v,C) ~= TRAINKNN (v,C+1)
        terror = terror + 1;                  %% Add the error if there is a mismatch.
     end
     if TRAINKNN (v,C) > TRAINKNN (v,C+1)
        ttype1 = ttype1 + 1;                  %% Add the error if there is an
overestimation.
     end
     if TRAINKNN (v,C) < TRAINKNN (v,C+1)
        ttype2 = ttype2 + 1;                  %% Add the error if there is an
underestmation.
     end
  end
  TPERROR(h,t) = terror / r ;                  %% Keep the errors for each run.
  TPTYPE1(h,t) = ttype1 / r ;                  %% Keep the errors for each run.
  TPTYPE2(h,t) = ttype2 / r ;                  %% Keep the errors for each run.
  % End of training error
  PERROR(h,t) = error / s ;                   %% Keep the errors for each run.
  PTYPE1(h,t) = type1 / s ;                   %% Keep the errors for each run.
  PTYPE2(h,t) = type2 / s ;                   %% Keep the errors for each run.
end
end
%% 13)Find The Average Errors
  % training error
 Trainerror = (sum(TPERROR(:)) / V) /N ;          %% Find the averages of the
errors.
 Traintype1 = (sum(TPTYPE1(:)) / V) /N ;          %% Find the averages of the
errors.
```

```
 Traintype2 = (sum(TPTYPE2(:)) / V) /N ;            %% Find the averages of the errors.
 TTRERROR = [Trainerror Traintype1 Traintype2];      %% Result Matrix
 TLog(alfverr,:) = [alf TTRERROR] ;
   % training error
 Avererror = (sum(PERROR(:)) / V) /N ;            %% Find the averages of the errors.
 Avertype1 = (sum(PTYPE1(:)) / V) /N ;            %% Find the averages of the errors.
 Avertype2 = (sum(PTYPE2(:)) / V) /N ;            %% Find the averages of the errors.
 TOTERROR = [Avererror Avertype1 Avertype2];       %% Result Matrix
Log(alfverr,:) = [alf ([1 1 1] - TOTERROR)] ;
   %%Log(alfverr,:) = [alf TOTERROR] ;
end
plot(Log(:,1)',Log(:,2)',':dg','MarkerFaceColor','g');
hold on ;
plot(Log(:,1)',Log(:,3)',':*b','MarkerFaceColor','b');
plot(Log(:,1)',Log(:,4)',':or','MarkerFaceColor','r');
hold off;
```

APPENDIX B

Source Code for Data Set Generation

a. Separated Data:

```
clear all
gennum = 500;
mu = [0 0];
SIGMA = [1 0; 0 0.2];
data1 = mvnrnd(mu,SIGMA,gennum);
unit = ones(gennum,1);
data1 = [data1 unit];
mu2 = [8 0];
data2 = mvnrnd(mu2,SIGMA,gennum);
unit = zeros(gennum,1);
data2 = [data2 unit];
data3 = [data1 ; data2] ;
```

b. Half-Separated Data:

```
clear all
gennum = 500;
mu = [0 0];
SIGMA = [1 0; 0 0.2];
data1 = mvnrnd(mu,SIGMA,gennum);
unit = ones(gennum,1);
data1 = [data1 unit];
mu2 = [4 0];
data2 = mvnrnd(mu2,SIGMA,gennum);
unit = zeros(gennum,1);
data2 = [data2 unit];
data3 = [data1 ; data2] ;
```

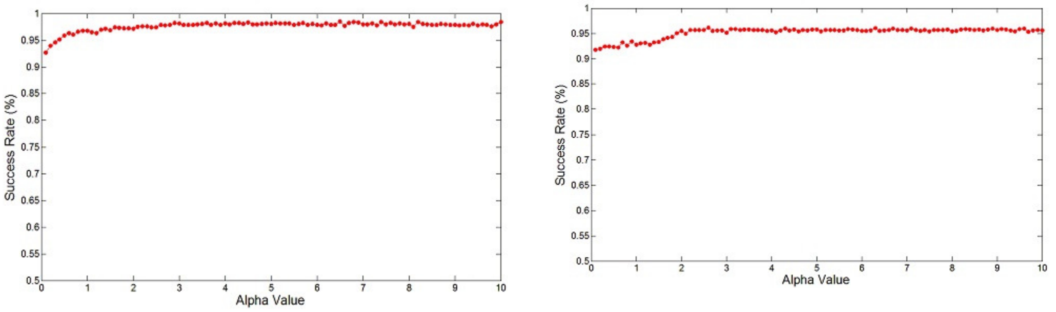
c. Not-Separated Data:

```
clear all
gennum = 500;
mu = [0 0];
SIGMA = [1 0; 0 0.2];
data1 = mvnrnd(mu,SIGMA,gennum);
unit = ones(gennum,1);
data1 = [data1 unit];
mu2 = [1 0];
data2 = mvnrnd(mu2,SIGMA,gennum);
unit = zeros(gennum,1);
data2 = [data2 unit];
data3 = [data1 ; data2] ;
```

APPENDIX C

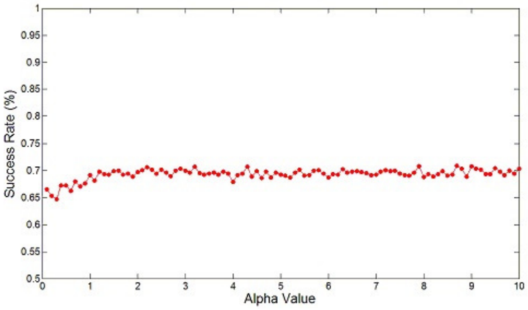
Application in MATLAB

C.1. Center Based Algorithm



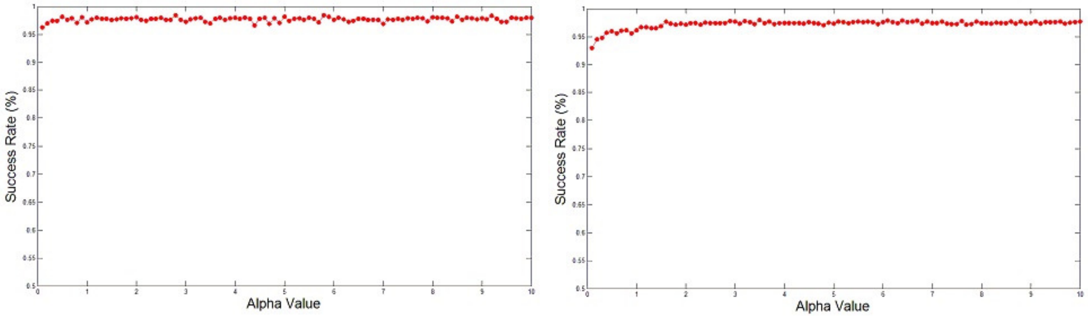
Center Based, Euclidean Distance, K = 3
Separable Case

Center Based, Euclidean Distance, K = 3
Half-Separable Case



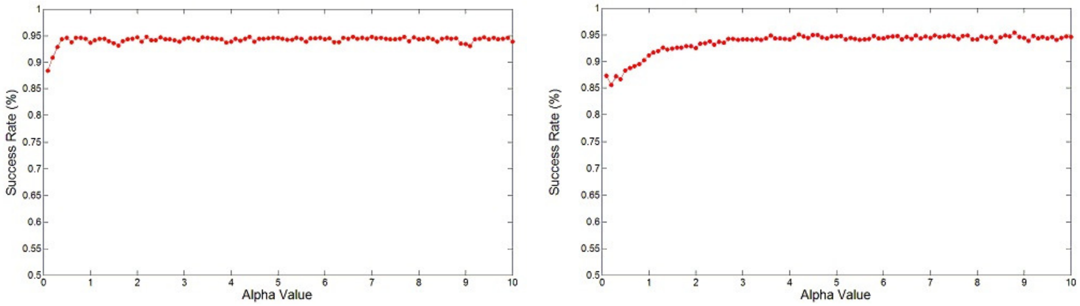
Center Based, Euclidean Distance, K = 3
Not-Separable Case

Figure C-1 - Success Rate vs. α value, Center Based Algorithm with Euclidean Distance



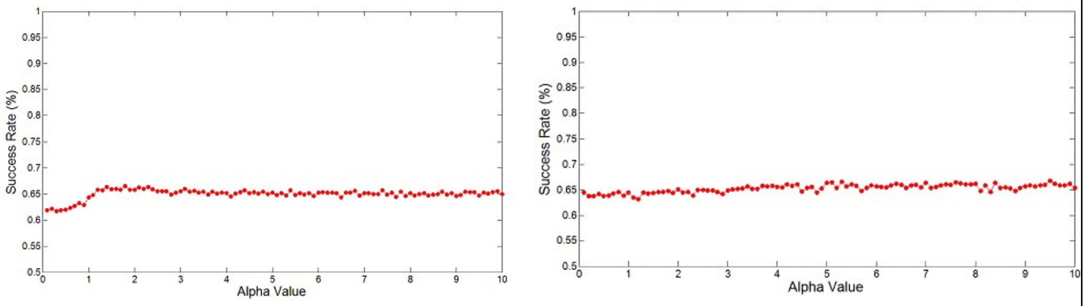
Success Rate of Separated, Mahalanobis Distance, K = 2

Success Rate of Separated, Mahalanobis Distance, K = 3.



Success Rate of Half - Separated, Mahalanobis Distance, K = 2

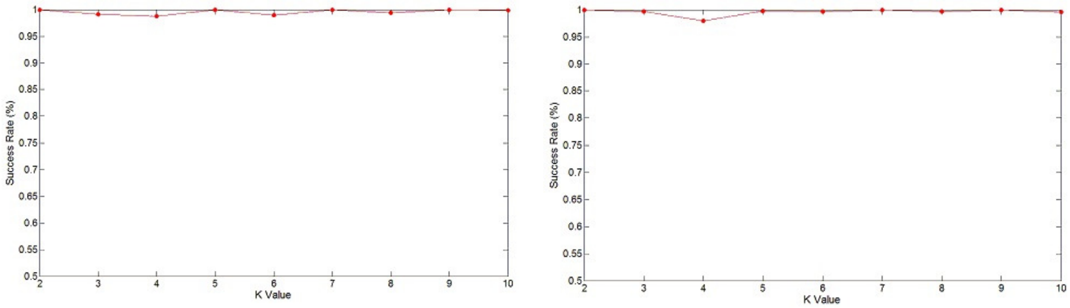
Success Rate of Half - Separated, Mahalanobis Distance, K = 3



Success Rate of Not-Separated, Mahalanobis Distance, K = 2

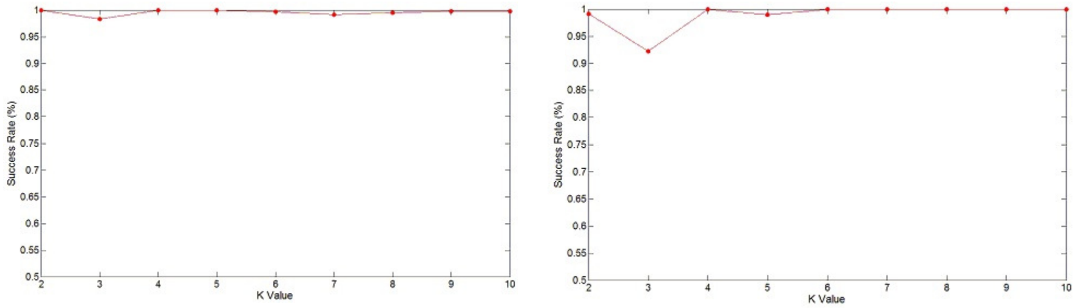
Success Rate of Not-Separated, Mahalanobis Distance, K = 3

Figure C-2 - Success Rate vs. α value, Center Based Algorithm with Mahalanobis Distance



Success Rate of Separated, Euclidean Distance, $\alpha = 10$

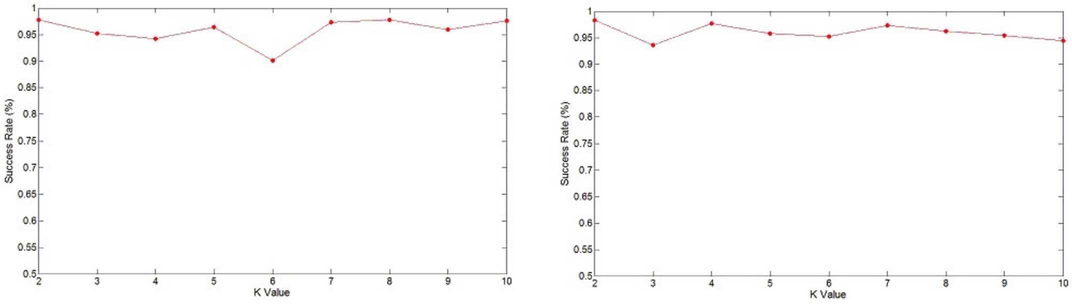
Success Rate of Separated, Euclidean Distance, $\alpha = 3$



Success Rate of Separated, Euclidean Distance, $\alpha = 1$

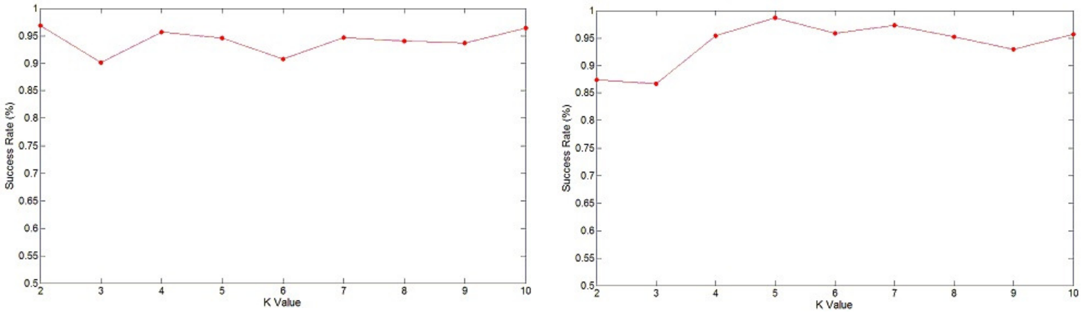
Success Rate of Separated, Euclidean Distance, $\alpha = 0.1$

Figure C-3 - Success Rate vs. Number of Clusters, Center Based Algorithm on Separated Data with Euclidean Distance



Success Rate of Half-Separated, Euclidean Distance, $\alpha = 10$

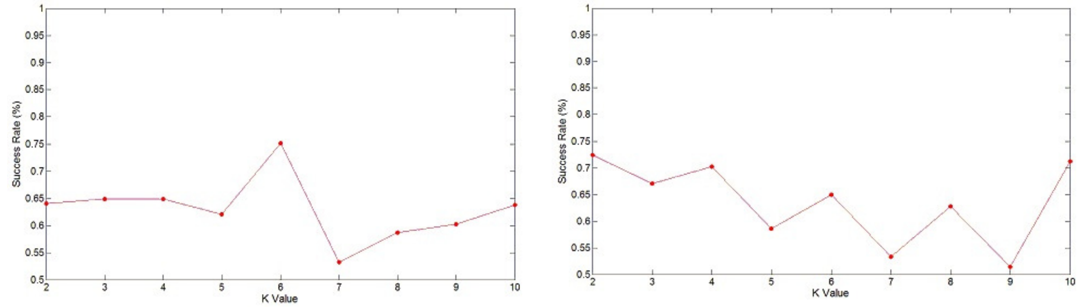
Success Rate of Half-Separated, Euclidean Distance, $\alpha = 3$



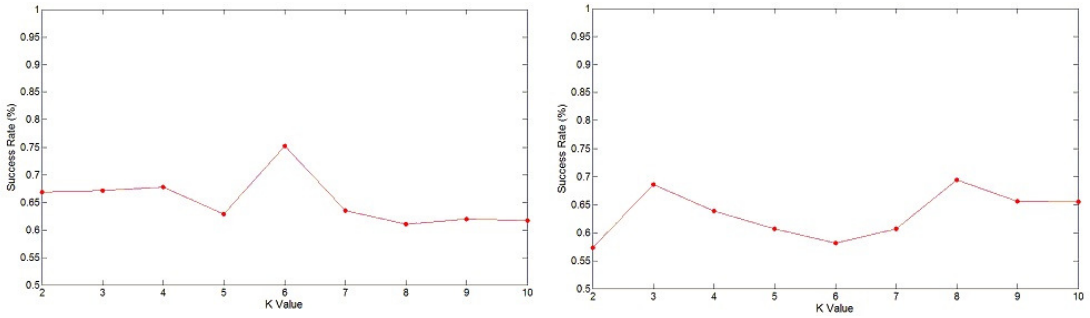
Success Rate of Half-Separated, Euclidean Distance, $\alpha = 1$

Success Rate of Half-Separated, Euclidean Distance, $\alpha = 0.1$

Figure C-4 - Success Rate vs. Number of Clusters, Center Based Algorithm on Half-Separated Data with Euclidean Distance

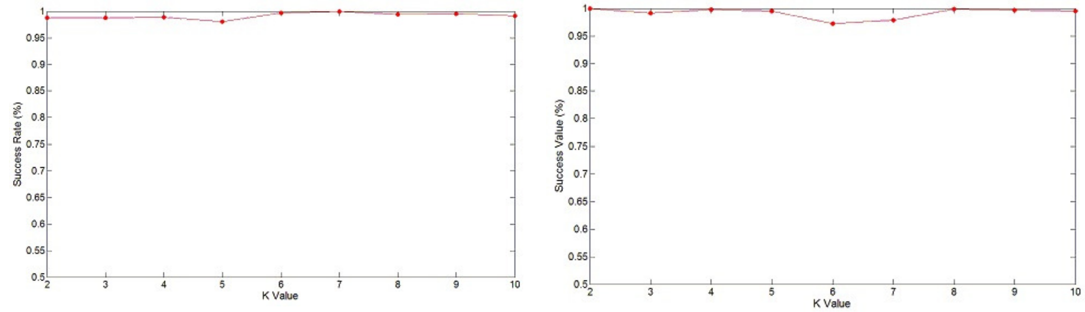


Success Rate of Not -Separated, Euclidean Distance, $\alpha\ = 10$ *Success Rate of Not -Separated, Euclidean Distance,* $\alpha\ = 3$



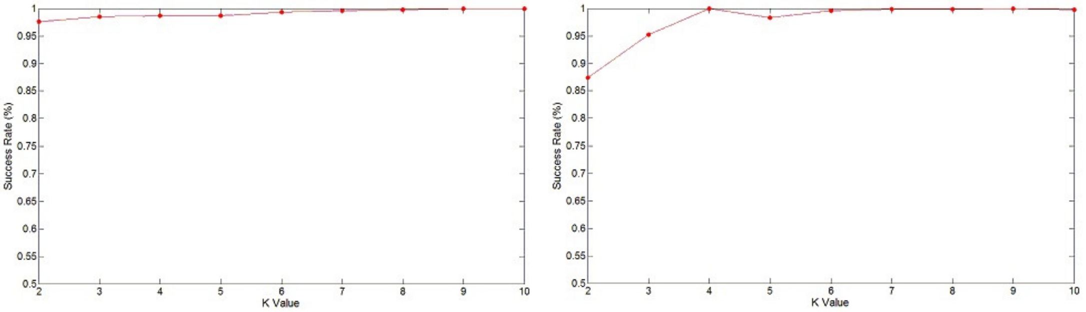
Success Rate of Not -Separated, Euclidean Distance, $\alpha\ = 1$ *Success Rate of Not -Separated, Euclidean Distance,* $\alpha\ = 0.1$

Figure C-5 - Success Rate vs. Number of Clusters, Center Based Algorithm on Not-Separated Data with Euclidean Distance



Success Rate of Separated, Mahalanobis Distance, $\alpha = 10$

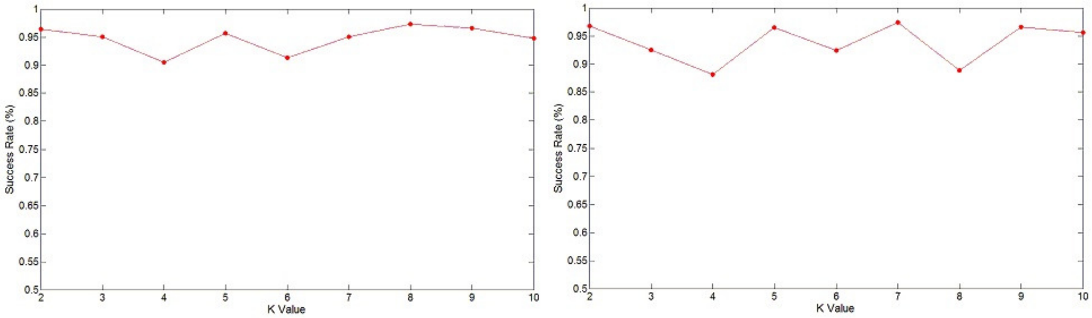
Success Rate of Separated, Mahalanobis Distance, $\alpha = 3$



Success Rate of Separated, Mahalanobis Distance, $\alpha = 1$

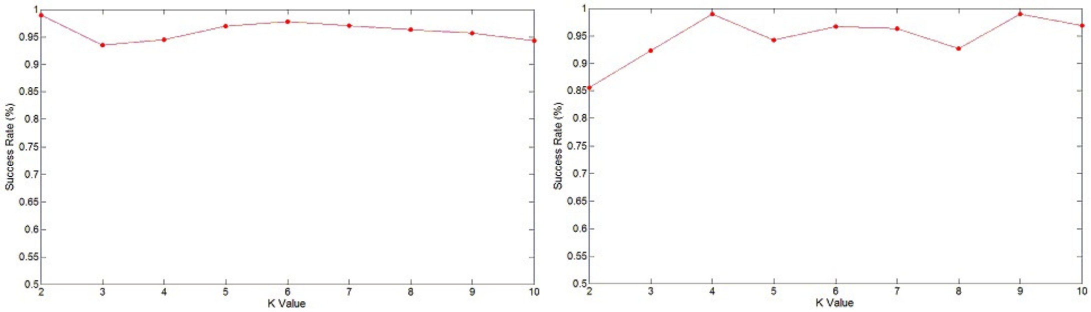
Success Rate of Separated, Mahalanobis Distance, $\alpha = 0.1$

Figure C-6 - Success Rate vs. Number of Clusters, Center Based Algorithm on Separated Data with Mahalanobis Distance



Success Rate of Half-Separated, Mahalanobis Distance, $\alpha = 10$

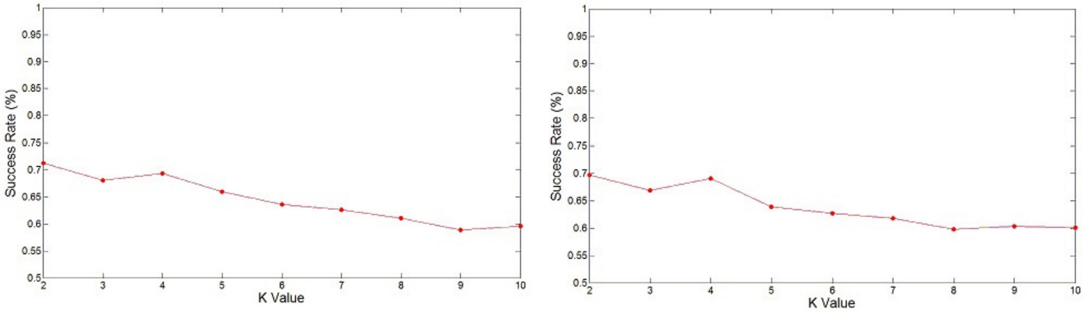
Success Rate of Half-Separated, Mahalanobis Distance, $\alpha = 3$



Success Rate of Half-Separated, Mahalanobis Distance, $\alpha = 1$

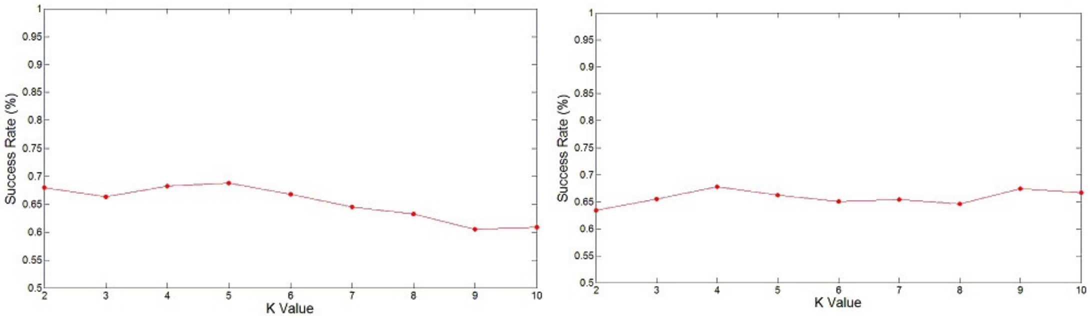
Success Rate of Half-Separated, Mahalanobis Distance, $\alpha = 0.1$

Figure C-7 - Success Rate vs. Number of Clusters, Center Based Algorithm on Half-Separated Data with Mahalanobis Distance



Success Rate of Not-Separated, Mahalanobis Distance, $\alpha = 10$

Success Rate of Not-Separated, Mahalanobis Distance, $\alpha = 3$

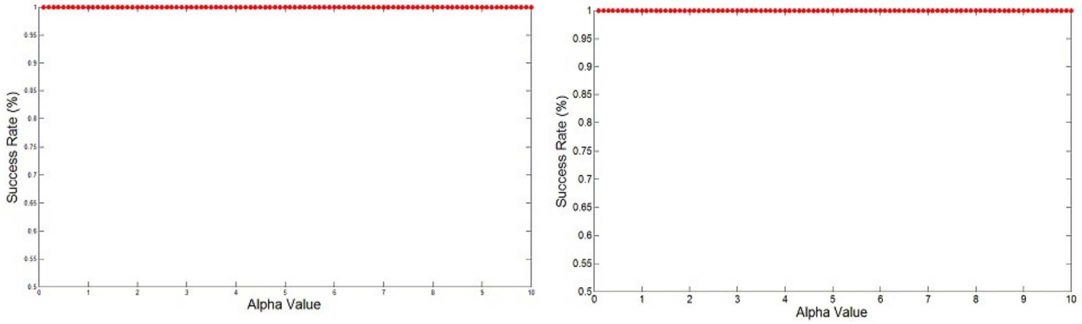


Success Rate of Not-Separated, Mahalanobis Distance, $\alpha = 1$

Success Rate of Not-Separated, Mahalanobis *Distance,* $\alpha = 0.1$

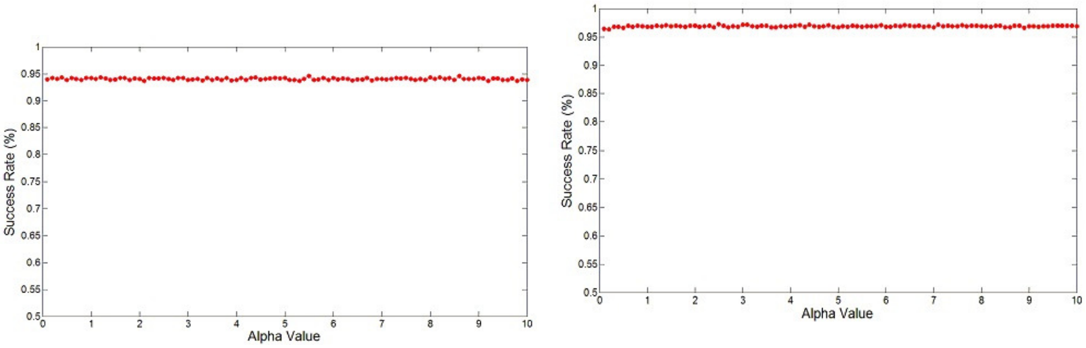
Figure C-8 - Success Rate vs. Number of Clusters, Center Based Algorithm on Not-Separated Data with Mahalanobis Distance

C.2. KNN Based Algorithm



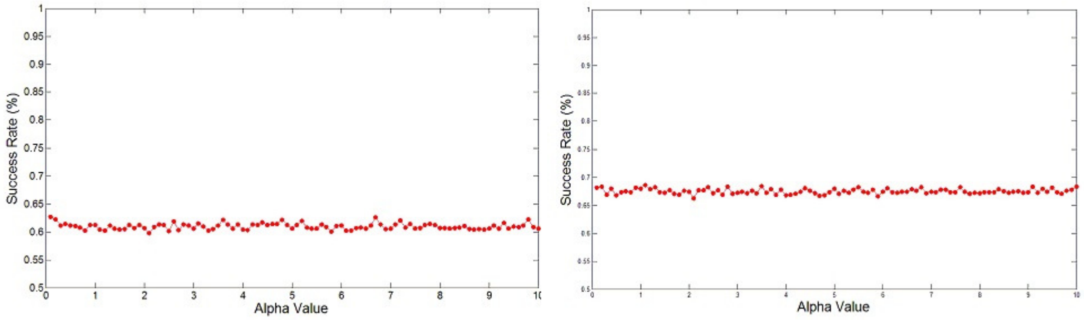
Success Rate of Separated, Euclidean Distance, K = 3

Success Rate of Separated, Mahalanobis Distance, K = 3



Success Rate of Half-Separated, Euclidean Distance, K = 3

Success Rate of Half-Separated, Mahalanobis Distance, K = 3



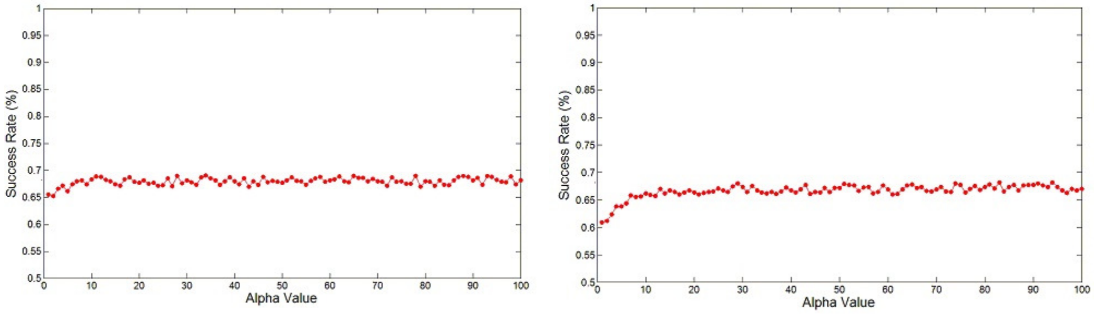
Success Rate of Not-Separated, Euclidean Distance, K = 3

Success Rate of Not-Separated, Mahalanobis Distance, K = 3

Figure C-9 - Success Rate vs. α Value, KNN Based Algorithm

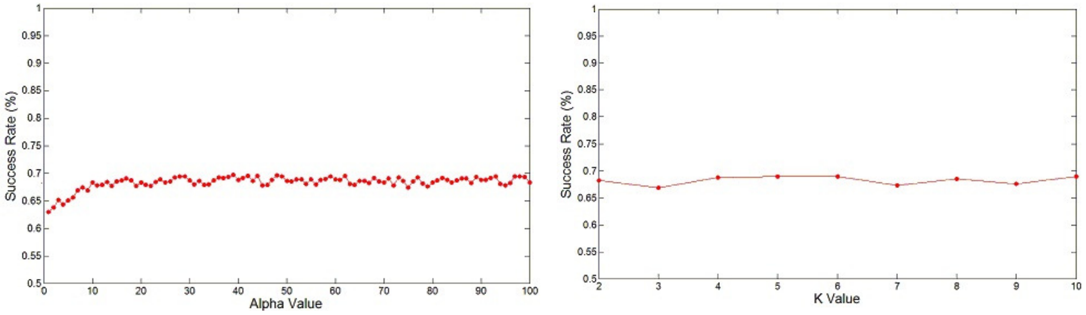
C.3. Center Based Algorithm Results on Biomedical Data sets

i. Diabetis:



Success rate of Diabetis, Mahalanobis Distance, $K = 2$, $\alpha \in [0\ 100]$

Success rate of Diabetis, Mahalanobis Distance, $K = 3$, $\alpha \in [0\ 100]$

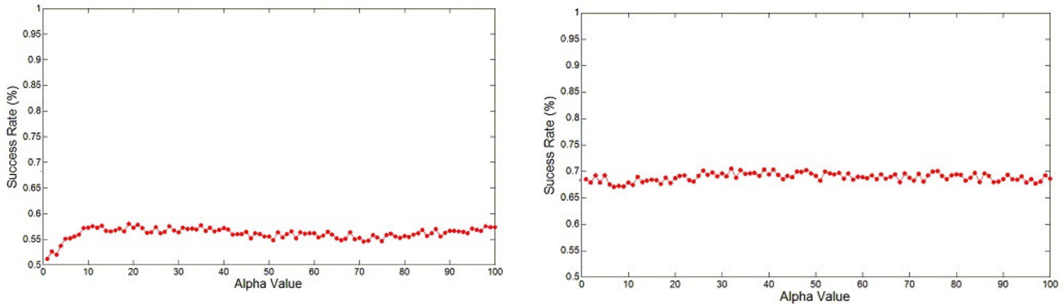


Success rate of Diabetis, Mahalanobis Distance, $K = 4$, $\alpha \in [0\ 100]$

Success rate of Diabetis, Mahalanobis Distance, $\alpha = 50$

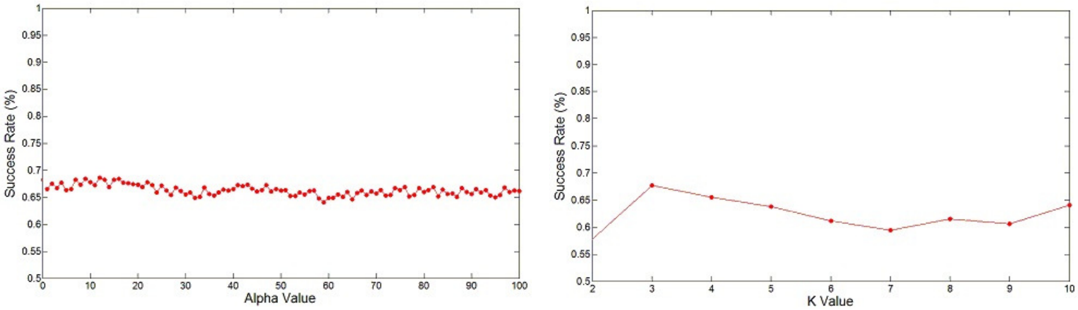
Figure C-10 - Success Rate of Diabetis Data Set, Center Based Algorithm with Mahalanobis Distance

ii. Hepatitis:



Success rate of Hepatitis, Mahalanobis Distance, $K = 2$, $\alpha \in [0\ 100]$

Success rate of Hepatitis, Mahalanobis Distance, $K = 3$, $\alpha \in [0\ 100]$

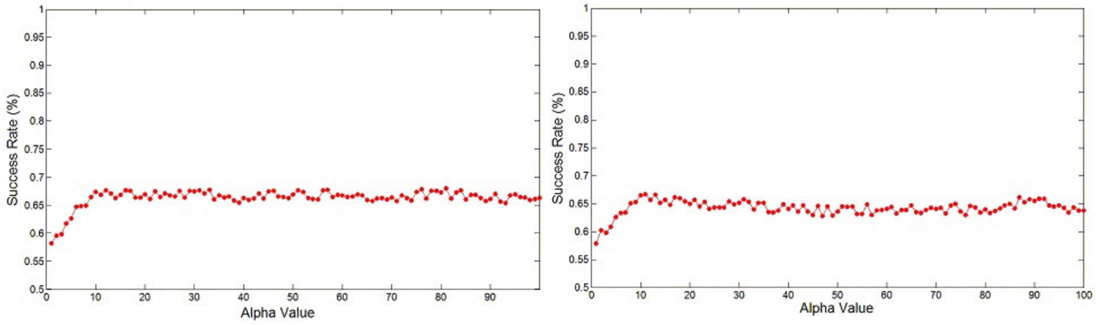


Success rate of Hepatitis, Mahalanobis Distance, $K = 4$, $\alpha \in [0\ 100]$

Success rate of Hepatitis, Mahalanobis Distance, $\alpha = 50$

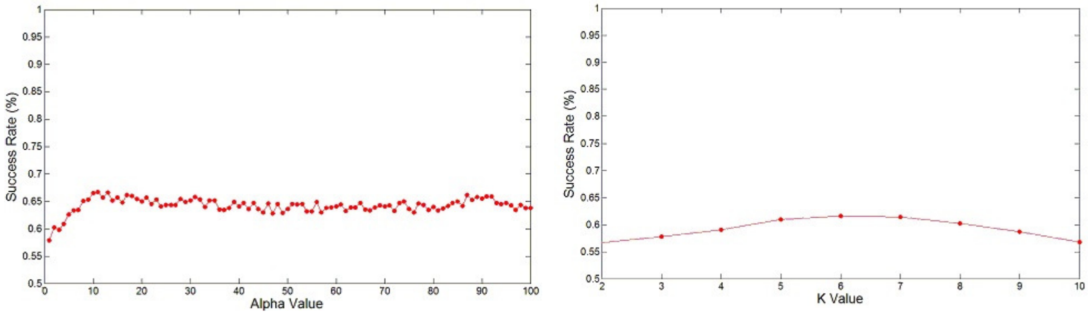
Figure C-11 - Success Rate of Hepatitis Data Set, Center Based Algorithm with Mahalanobis Distance

iii. Liver Cancer:



Success Rate of Liver Cancer, Mahalanobis Distance, $K = 2$, $\alpha \in [0\ 100]$

Success Rate of Liver Cancer, Mahalanobis Distance, $K = 3$, $\alpha \in [0\ 100]$

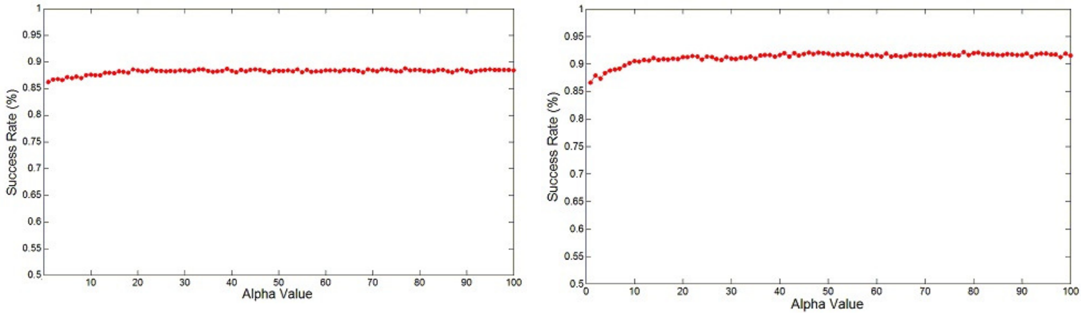


Success Rate of Liver Cancer, Mahalanobis Distance, $K = 4$, $\alpha \in [0\ 100]$

Success Rate of Liver Cancer, Mahalanobis Distance, $\alpha = 50$

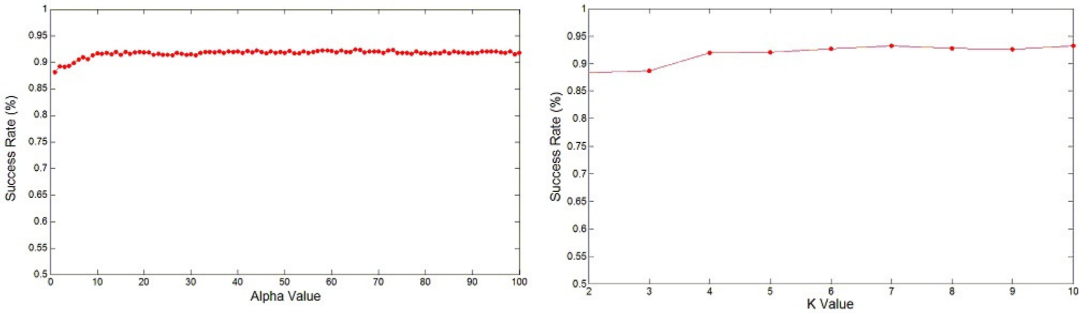
Figure C-12 - Success Rate of Liver Cancer *Data Set, Center Based Algorithm with Mahalanobis Distance*

iv. Voting:



Success Rate of Voting, Mahalanobis Distance, $K = 2$, $\alpha \in [0\ 100]$

Success Rate of Voting, Mahalanobis Distance, $K = 3$, $\alpha \in [0\ 100]$

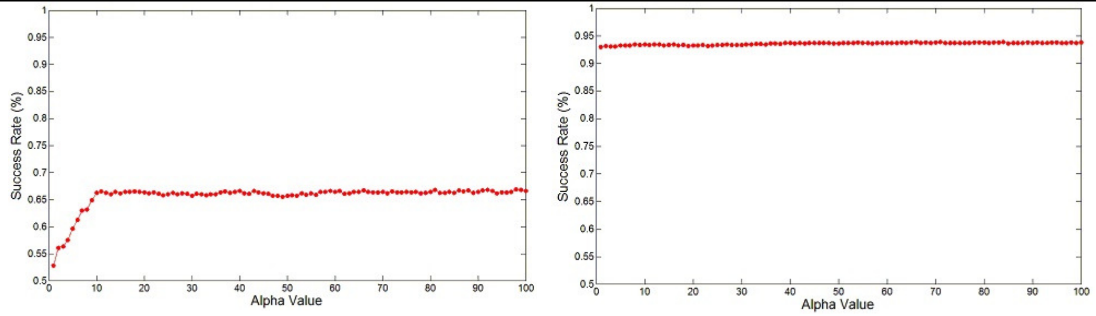


Success Rate of Voting, Mahalanobis Distance, $K = 4$, $\alpha \in [0\ 100]$

Success Rate of Voting, Mahalanobis Distance, $\alpha = 50$

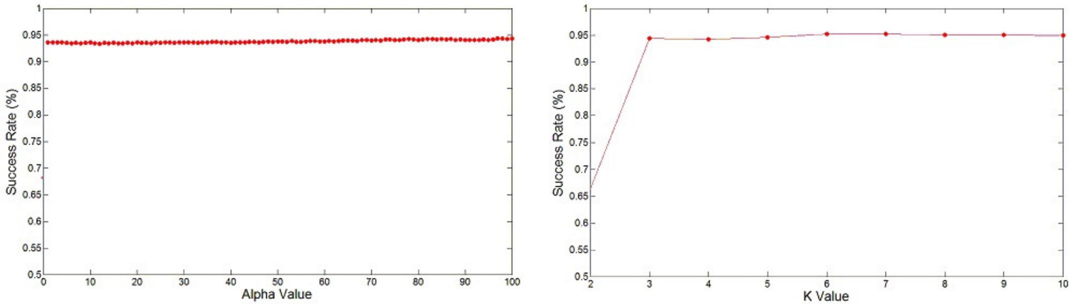
Figure C-13 - Success Rate of Voting Data Set, Center Based Algorithm with Mahalanobis Distance

v. Wine:



Success Rate of Wine, Mahalanobis Distance, $K = 2$, $\alpha \in [0\ 100]$

Success Rate of Wine, Mahalanobis Distance, $K = 3$, $\alpha \in [0\ 100]$

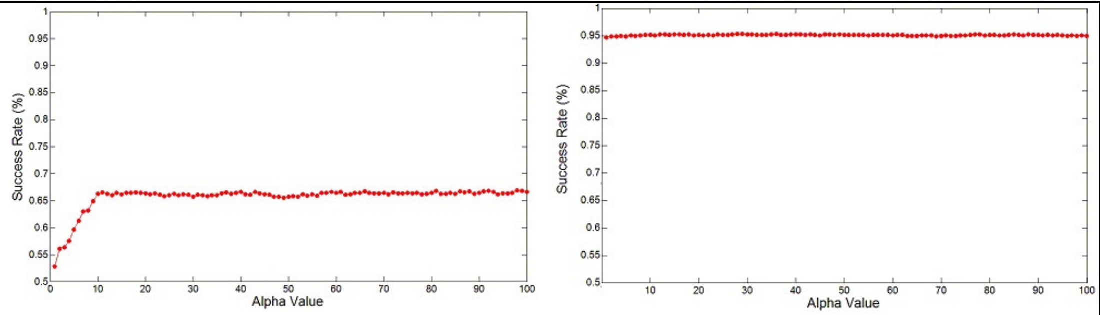


Success Rate of Wine, Mahalanobis Distance, $K = 4$, $\alpha \in [0\ 100]$

Success Rate of Wine, Mahalanobis Distance, $\alpha = 50$

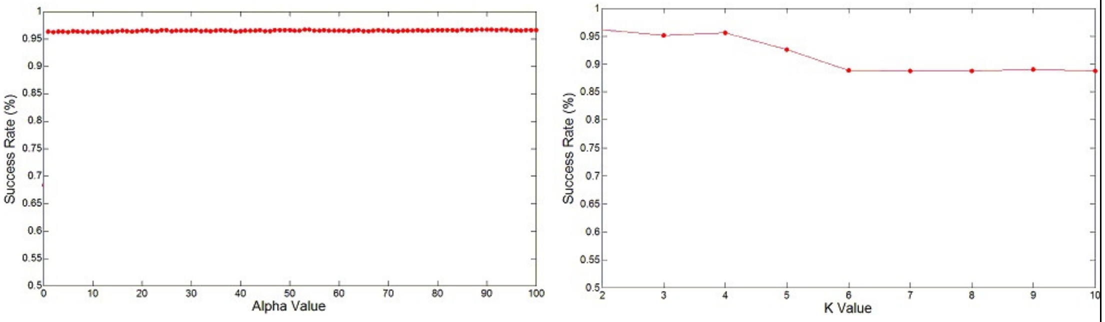
Figure C-14 - Success Rate of Wine Data Set, Center Based Algorithm with Mahalanobis Distance

vi. Breast Cancer:



Success Rate of Breast Cancer, Mahalanobis Distance, K = 2, $\alpha \in [0\ 100]$

Success Rate of Breast Cancer, Mahalanobis Distance, K = 3, $\alpha \in [0\ 100]$

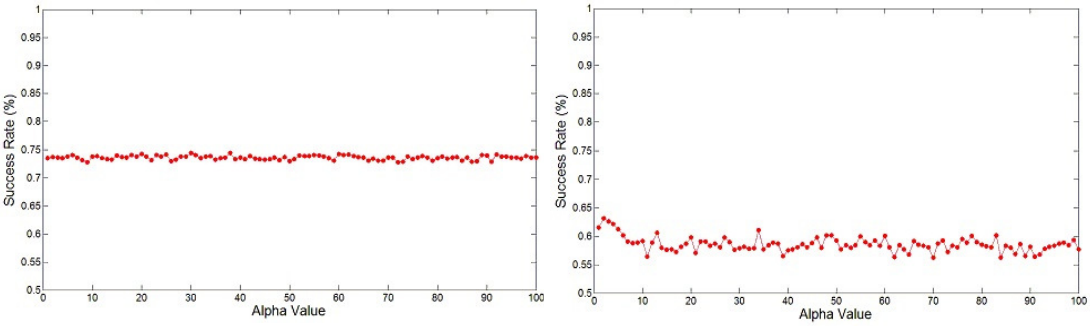


Success Rate of Breast Cancer, Mahalanobis Distance, K = 4, $\alpha \in [0\ 100]$

Success Rate of Breast Cancer, Mahalanobis Distance, $\alpha = 50$

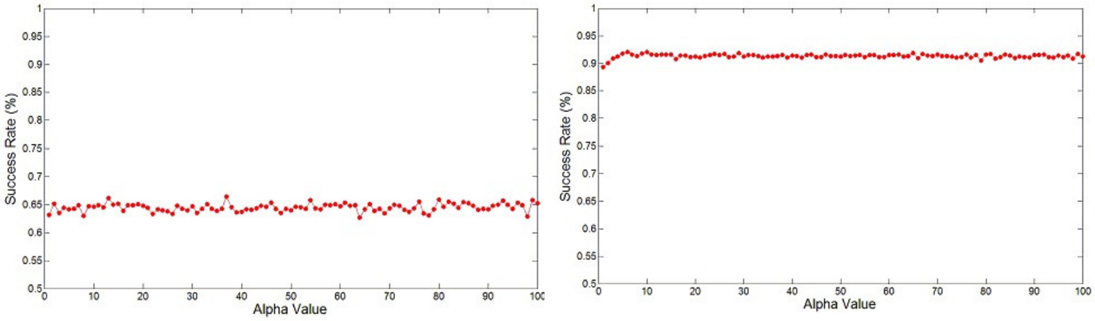
Figure C-15 - Success Rate of Breast Cancer Data Set, Center Based Algorithm with Mahalanobis Distance

C.4. KNN Based Algorithm Results on Biomedical Data Sets



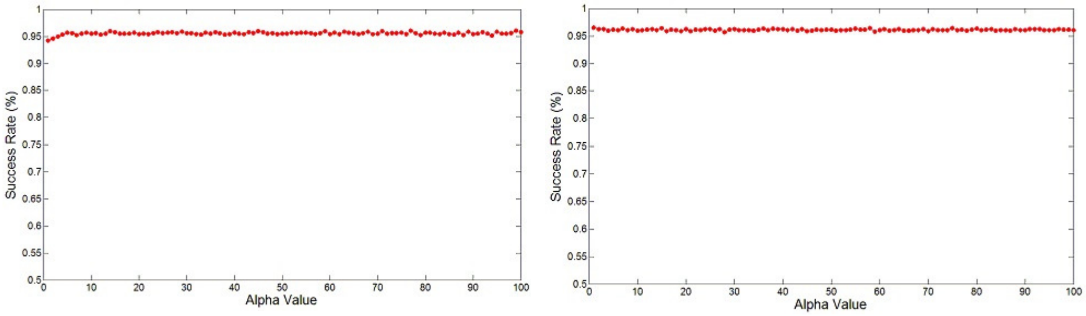
Success Rate of Diabetis, Mahalanobis Distance, K = 3, $\alpha \in [0\ 100]$

Success Rate of Hepatitis, Mahalanobis Distance, K = 3, $\alpha \in [0\ 100]$



Success Rate of Liver Cancer, Mahalanobis Distance, K = 3, $\alpha \in [0\ 100]$

Success Rate of Voting, Mahalanobis Distance, K = 3, $\alpha \in [0\ 100]$



Success Rate of Wine, Mahalanobis Distance, K = 3, $\alpha \in [0\ 100]$

Success Rate of Breast Cancer, Mahalanobis Distance, K = 3, $\alpha \in [0\ 100]$

Figure C-16 - Success Rate of Biomedical Data Sets, KNN Based Algorithm with Mahalanobis Distance