

Improving the discovery of Motifs in high-dimensional sequences of varying length

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Abstract

Acknowledgements

Many thanks to my mummy for the numerous packed lunches; and of course to Igor, my faithful lab assistant.

Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

(M. Adnan Haider)

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Chapter 1

Introduction

Over the course of the last decade, the mining of time-series data have received considerable attention within the data mining and machine learning community. The term 'time series' denotes a set of observations concurring any activity against different periods of time. The duration of time period may be either in the order of milliseconds or monthly or even annually depending on the domain.

Mathematically, a time series is defined by the values $y_1, y_2 \dots y_n$ at times $t_1, t_2 \dots t_n$ where $y = f(t)$. The time t_i acts as an independent variable to estimate dependent variables y_i . The dimensionality of the series is denoted as \mathbf{n} where ' \mathbf{n} ' denotes the length of the sequence.

Time series analysis is used in many applications ranging from sales forecasting, budgetary analysis to stock market analysis and many more. One particular domain where the application of time series analysis is currently very popular is *motif* discovery- the problem of efficiently locating frequent/interesting sub-patterns in the data. The knowledge of motifs has been seen to have important applications in various aspects of data mining tasks. For instance motifs can use applied :

- to discover association rules [1]. the reflect information of 'primitive shapes.
- to specify the number of clusters for unsupervised clustering algorithms. Clustering is one of the most frequently used data mining tasks. It involves an unsupervised process for partitioning a dataset into a specified number of meaningful groups. The knowledge of motifs give a good approximation on the number of meaningful groups that are present in the data. [2].
- to identify important sub-patterns in DNA and gene sequences [3]

In the analysis of speech data, motifs also play a very important role. Recent

research have shown that detecting and isolating motifs in speech utterances is equivalent to extracting frequently spoken words spoken by the speaker(s) [4, 5]. The methodology proposed in these papers is based on constructing a framework that is entirely data driven i.e there is no intermediate recognition stage that maps an audio signal to a symbolic representation such as the 'phone' states in the HMM model. This results in the word acquisition process to be unsupervised which presents a completely different approach to the current speech recognition systems that are built using a supervised training methodology employing manually transcribed speech to model the underlying speech process.

To identify and extract motifs from time series data, various clustering algorithms have been proposed. The two most commonly used approaches are:

1. Dynamic time warping algorithm(DTW) [6, 7, 8, 9, 10, 11] that clusters similar sequences separated by time shifts and/or scale.
2. Single value decomposition(SVD)[12]. The entire time series data is approximated by a low-rank approximation matrix achieved through mapping the data onto a low dimensional orthogonal feature space.

Both these algorithms suffer from severe setbacks when applied directly on the 'raw' time series data. The DTW algorithm for example, suffers from large run-times when the length of the time series sequences are very long. This is because the time complexity of the algorithm is quadratic and is dependent on the dimensionality of the sequences i.e the length of the sequences. To address this issue window constraints (Itakura parallelogram[13], Sakoe-Chiba band[7]) are imposed that reduces size of the search space by forcing the algorithm to look for optimal path that are along the diagonal. Although introducing the window constraint does improve the time complexity but the reduction the search space leads to a substantial decrease in the accuracy of the algorithm[11].

The SVD on the other hand also suffers from high computational cost when the number of samples \ll the size of the dimension of the data. For long time sequences, the high computational cost incurred by the SVD is therefore quite pronounced as each point in the time series corresponds to a feature/attribute. However, the main drawback of SVD is that it cannot be applied to time-series datasets where the length of the sequences vary. This constraint greatly reduces the type of time series domains to which SVD can be applied to. The speech corpus is an prime example of one such domain where SVD cannot be applied directly. Data sets comprised of speech utterances are a good example where recorded utterances do not share the same dimensionality (i.e the same length) as acoustically similar signals may be contracted/expanded versions of each other due to speaker variations, context etc.

The purpose of this project is to employ machine learning techniques to tackle and resolve the drawbacks incurred by both algorithms and thus improve their performance in handling long time series sequences that vary in length. In the first half of the project, I will be solely concentrating on improving the performance of the DTW algorithm in problem domains where the minimising the time complexity is a high priority. In the second half of the project, I will be investigating ways to successfully adapt the SVD to work on long sequences that vary in length.

For this project, I will be using 3 time series data sets (details in chapter 2):

- TIGITS
- INLINESKATE
- CINC_ECG_TORSO

The prime objective here is to improve the accuracy of the DTW and SVD algorithm in tackling high dimensional time series sequences that vary in length while minimising the run-time to a minimum. To evaluate and compare the merits of different proposed changes, I combined both algorithms with the K nearest neighbour classifier and partitioned each of the above data sets into two disjoint subsets: one to be used as a test set and the other as a training set. The reason for choosing the nearest neighbour classifier is because it shares almost the same methodology as the algorithms used to detect motifs. Motif detection algorithms are memory based i.e they rely on comparing each sequence with other sequences in the data set. K nearest neighbours differs from motif detection on two aspects: each sequence in the test set is compared with sequences that belong only to the training data set and the entire process is supervised i.e correct label information are available to check the accuracy of the algorithm. The availability of correct labels allow accuracy and run-time scores of the nearest neighbour methods to serve as a useful evaluation metric to compare and evaluate various adaptations of the DTW and SVD algorithm. Improvements in SVD and DTW that lead to greater classification accuracy scores and low run-times are mostly likely to result in better extraction of motifs in the unsupervised context.

The dissertation is organised as follows: Chapter 2 gives a description of the 3 time-series datasets used for this project. Chapter 4 provides a detailed background description of the DTW algorithm. Chapter 3 and 4 investigate methods to improve the performance of the DTW algorithm in terms of both accuracy and speed. Chapter 4...

Chapter 2

Datasets Used

There are two primary goals of this project :

- improve the performance of the DTW algorithm on long time series sequences.
- adapt SVD to create a unique ‘fingerprint’ scheme for each distinguished motif/time series pattern.

For each of these algorithms, the performance of different adaptations was evaluated by combining them with the 1 nearest neighbours classifier. As I have mentioned in the previous chapter, the 1 nearest neighbour classifier shares the same methodology as the algorithms used to detect motifs. Thus, if the proposed adaptations improve the performance of 1 nearest neighbour classifier then it is highly likely that they will achieve better performance in detecting motifs. The data sets used for evaluation were carefully chosen so that they contain time series sequences that have very long lengths.

The data sets used for this project are as follows:

1. TIDIGITS speech corpus
2. The UCR data set :CinC_ECG_torso
3. The UCR data set :InlineSkate

All 3 data sets were partitioned into two disjoint sets: test set and training sets. Each sample in the training and test data set corresponds to a particular pattern. The class information of the training samples were used to evaluate the accuracy of the nearest neighbours classifier.

The primary dataset that I have used for this project is the ‘TIGITS’ corpus. In comparison to the UCR datasets, the length of the time series sequences in the TIGITS corpus are on average 100 times longer than the time series sequences of the two UCR datasets. Description of the data sets is given below:

2.0.1 Brief description of TIDIGITS data set

The utterances in the TIDIGITS[14] data set correspond to digit sequences. The corpus consists of :

- 22 isolated digits (two tokens of each of the eleven digits)
- 11 two-digit sequences
- 11 three-digit sequences
- 11 four-digit sequences
- 11 five-digit sequences
- 11 seven-digit sequences

In this corpus, the motifs correspond to individual digits. Thus for my experiments, I have considered only the isolated digit sequences for classification, more specifically the digits from 0 to 9. The database as I have mentioned earlier is divided into two subsets, one to be used for algorithm design and one to be used only for evaluation. Both sets contain samples belonging to different speaker categories i.e (men,women,boy,girl) who in turn have different dialect classifications. The table below shows the partitioning of speakers from different speaker categories in the training and test data set.:

Subset	Man	Woman	Boy	Girl
Train	55	57	25	26
Test	56	57	25	25

For this project, the entire training set was used for nearest neighbour classification, although only samples from one production was taken. To ensure that the experiments completed with in a reasonable time, I have only used $\frac{1}{3}$ of the samples of the test set.

The test data subset used for evaluation consists of

- 162 random samples from boy category
- 162 random samples from girl category
- 326 random samples from men category
- 326 random samples from women category

Note: The samples were not chosen exactly randomly. When subsampling from each category, I have ensured that:

- the samples belong to a number of different speakers
- the chosen subset consists of enough examples of all 10 digits.

2.0.2 Brief description CinC_ECG_torso and InLineSkate dataset

The UCR data resource has been funded by an NSF(National Science Foundation) since 2003 and is the largest public collection of time series data sets that have been made available to the data mining/machine learning community, to encourage reproducible research for time series classification and clustering. To evaluate the performance of different adaptations of the two algorithms on high dimensional sequences, we require data sets that contain extremely long sequences. The UCR data sets 'CinC_ECG_torso'[15] and the 'InLineSkate'[15] therefore are an excellent choice as they contain time series sequences that have the longest lengths.

1. CinC_ECG_torso

- Length of the time series:1639
- Size of test set:1380
- Size of training set:40
- Number of classes:4

2. InLineSkate

- Length of the time series:1882
- Size of test set:550
- Size of training set:100
- Number of classes:7

Chapter 3

Background

3.1 Dynamic Time Warping Algorithm

The Dynamic Time Warping algorithm is a similarity metric that is used cluster similar time series sequences varying in length, scale and speed. The problem formulation [6] of the algorithm is stated as follows: Given two time series X , and Y , of lengths $|X|$ and $|Y|$,

$$X = x_1, x_2, \dots, x_{|X|} \quad (3.1)$$

$$Y = y_1, y_2, \dots, y_{|Y|} \quad (3.2)$$

construct a warping path W

$$W = w_1, w_2, \dots, w_k \text{ where } \max(|X|, |Y|) \leq k \leq |X| + |Y|$$

where

- k denotes the length of the warping path
- the l th element of the warping path is $w_l = (i, j) \in [1 : N] \times [1 : M]$ for $l \in [1 : k]$ where i is an index from the time series X and j is an index from the time series Y .

To properly understand the above formulation some key definitions must be stated:

1. Warping path [16]: An (N, M) -warping path (or simply referred to as warping path if N and M are clear from the context) is a sequence $w = (w_1, \dots, w_k)$ with $w_l = (i, j) \in [1 : N] \times [1 : M]$ for $l \in [1 : k]$ that satisfies the following three conditions.

- (a) Boundary condition [16, 7, 10, 13]: $w_1 = (1, 1)$ and $w_k = (N, M)$.

The boundary condition enforces that the first elements of the series

X and Y as well as the last elements of the series X and Y have to be aligned with each other. This prevents the alignment from missing any points.

(b) Monotonicity condition [16, 7, 13]:

$\forall i \in [1 : k - 1], [|w_{i+1} - w_i| = 1]$. In other words, $w_k = (i, j), w_{k+1} = (i', j'), i \leq i' \leq i + 1, j \leq j' \leq j + 1$

The condition requires that the path will not turn back on itself. Both the i and j indexes either stay the same or increase but they will never decrease.

(c) Step-size condition [16, 7, 13]: $w_{l+1} - w_l \in \{(1,0), (0,1), (1,1)\}, \forall l \in [1:k-1]$.

The step size condition expresses a kind of continuity condition: no element in X and Y can be omitted and there are no replications in the alignment

Intuitively speaking, the (N,M) warping path $w = (w_1, \dots, w_k)$ defines an alignment between two sequences $X = (x_1, x_2, \dots, x_N)$ and $Y = (y_1, y_2, \dots, y_M)$ by assigning each element of X to a unique element in Y.

2. Optimum Warping Path [10, 16]:

The optimal warp path corresponds to the minimum-distance warp path, where the distance of a warp path W is given as

$$Dist(W) = \sum_{m=1}^K dist(X, Y)_{|(w_m)}$$

where $w_m = (i, j) \in [1 : N] \times [1 : M]$

The $dist(X, Y)_{|(w_m)}$ represents the distance computed using an appropriate cost function between the value x_i of sequence X and the value y_j of sequence Y.

$$dist(X, Y)_{|(w_m)} = dist(x_{x_i}, y_{y_j})$$

The goal of the DTW algorithm is to compute the distance of the optimal warping path for given two time series sequences. Instead of attempting to solve the entire problem all at once, the algorithm utilises the technique of dynamic programming to find an optimum alignment between two sequences through the computation of local distances between the points in the temporal sequences. The algorithm proceeds by iteratively filling in values for each cell (i,j) in the $|X|$ by $|Y|$ cost matrix D . The value of the cell (i,j) is given by $D(x_i, y_j)$ which uses a cost metric to compute the distance of optimum warp

path from (1,1) to (i,j) :

$$D(i,j) = \text{Dist}(i,j) + \min(D(i-1,j), D(i-1,j-1), D(i,j-1))$$

The figure below illustrates the working of the DTW algorithm.

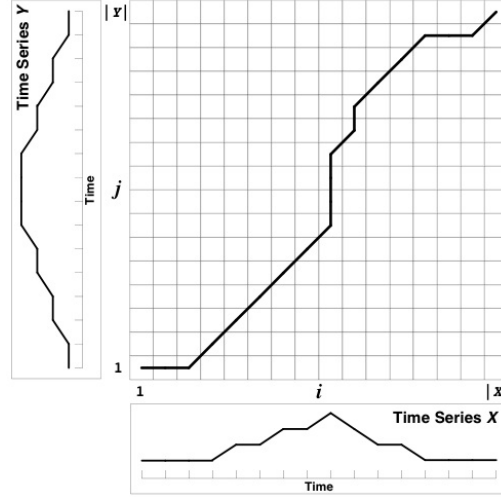


Figure 3.1: The DTW cost matrix with the minimum-distance warp path traced through it.

Generally as a cost metric, the euclidean metric is mostly widely used. For this project, I will hence consider the basic DTW algorithm equipped with the euclidean metric as my baseline model. An outline of the base line DTW algorithm is given below:

Algorithm 1 Value-Based DTW

```

1: procedure VALUE-BASED(seq1, seq2) ▷ two raw sequences
2:   DTW = zeros(length(seq1)+1, length(seq2)+1)
3:   for i=1: to length(seq1) do ▷ Initialise the DTW cost matrix
4:     DTW(i,0) = ∞
5:   end for
6:   for i=1 to length(seq2) do
7:     DTW(0,i) = ∞
8:   end for
9:   for i=2 to length(seq1) do
10:    for j=2 to length(seq2) do ▷ cost(a,b)≡euclid(a,b)
11:      DTW(i,j) = cost(seq1(i), seq2(j)) + min{ DTW(i-1,j)+DTW(i,j-1)+DTW(i-1,j-1) }
12:    end for
13:  end for
14:  return result =  $\frac{\text{DTW}(n,m)}{nm}$  ▷ n=length(seq1), m=length(seq2)
15: end procedure

```

The computational complexity of the DTW algorithm is $O(n^2)$ where n denotes the length of the sequences that are being compared. Thus for time series domains having high dimensions i.e. long lengths, the time and computational costs incurred by the algorithm are quite high. To address this issue, two well-known global window constraints are employed: the Sakoe-Chiba band [7] and the Itakura parallelogram [13]. Figure 3.2 gives an illustration of the use of both constraints:

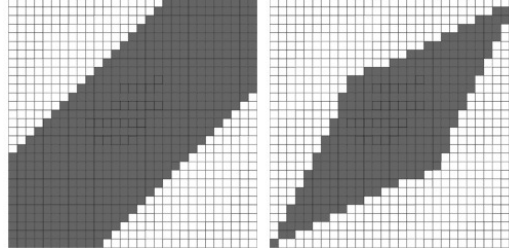


Figure 3.2: Two constraints: Sakoe-Chiba Band (left) and an Itakura Parallelogram (right), both have a width of 5.

The shaded areas in the above figure represent the cells of the cost matrix that are filled in by the DTW algorithm for each constraint. The width of each shaded area/window, is specified by a window parameter. When these constraints are used, the DTW algorithm finds the optimal warp path only through the constraint window. However, the globally optimal warp path will not be found if it is not entirely inside the window[6]. The window parameter therefore determines the accuracy of the DTW algorithm. Decreasing the width decreases the accuracy. If the width is 0 and the series are of equal length then the DTW generalises to the euclidean distance which is a notoriously inaccurate similarity measure for time series data[17]. To constraint the time complexity to a minimum, the vast majority of the data mining researchers use a Sakoe-Chiba Band with a 10% width. This reduces the time complexity from $O(n^2)$ to $O(wn)$ where w is the size of the window parameter.

3.2 Single Value Decomposition

The formal definition of SVD as stated in[18, 12] is given as follows:

Any $M \times N$ real matrix X can be factorized of the form $X = UDV^T$ where

- U is a $M \times M$ orthogonal matrix. The columns of U are the eigenvectors of XX^T

- D is a $M \times N$ rectangular matrix with :

$$D_{ij} = \begin{cases} \sigma^2, & \text{if } j = i \\ 0, & \text{otherwise} \end{cases}$$

Here D is a diagonal matrix where the diagonal entities are called singular values and are ranked from greatest to least. The number of non-zero singular values determine the rank of the original matrix.

- V is a $N \times N$ orthogonal matrix. The columns of V are the eigenvectors of $X^T X$. Since $X^T X$ is the covariance matrix, these eigenvectors span the linear subspace that maximises the variance of the data.

Dimensionality reduction is achieved by discarding the eigenvectors in V i.e the columns that are associated with the smallest or zero singular values. Thus, each sample can now be represented by fewer dimensions. For data matrices where $M \ll N$, there exists at most $M-1$ singular values. In such situations, considering only the non zero columns in the diagonal matrix D and the associated columns in V achieves dimensionality reduction without any loss of function. The data matrix X can be factorized as $X = U \times D' \times V'^T$ where D is now an M by K diagonal matrix containing only positive values on its diagonal and V' is the corresponding N by K matrix. The matrix $V'^T V$ captures the full covariance of the data.

Chapter 4

Optimising DTW

The Dynamic Time Warping(DTW) algorithm is the one of the oldest algorithm that is used to compare and cluster sequences varying in time, scale and speed. Given two temporal sequences, the algorithm utilises the technique of dynamic programming to compute the cost of the optimum alignment path between them. The computed cost gives an indication of the degree of similarity. The smaller the cost, the more similar the sequences are. Intuitively speaking, DTW can be seen as a clustering algorithm that clusters patterns that share roughly the same shape. As I have stated in the previous chapter, the time and computational complexity of this algorithm is $O(n^2)$ where n denotes the length of the sequences that are being compared. Thus for time series domains having high dimensions i.e long sequences, DTW becomes a very unattractive choice as it suffers from high computational and time costs.

To address the issue of the curse of dimensionality, DTW algorithms employ a window constraint to reduce the search space. The most commonly used are Sakoe-Chuba Band[7] and the Itakura window constraint [13]. Figure[3.2] gives an illustration of the nature of these window constraints. Such constraints determine the allowable shapes that a warping path can take by restricting the DTW to construct optimal warping paths only through a restricted number of cells around the diagonal region of the cost matrix. As the dimensionality(length) of the sequences increases, the size of the window is adjusted accordingly. Rigid window constraints impose a more rigid alignment that prevent an overly temporal skew between two sequences, by keeping frames of one sequence from getting too far from the other. The vast majority of the data mining researchers use a Sakoe-Chiba Band with a 10% width for the global constraint [19] to constraint the time complexity of DTW to a minimum. For finding motifs in data sets comprising of speech utterances, the use of rigid window constraints is highly undesirable. Utterances corresponding to the same lexical identity may suffer from large variations in speed, scale and time due to the word(s) being spoken in difference contexts, by different speakers, in different environments etc. Thus it is necessary to explore alternative tech-

niques to window constraints that can reduce the time complexity of DTW without degrading its accuracy.

Before investigating methods to improve the DTW algorithm itself, it is highly necessary to first understand the nature of the data sequences that the DTW is presented with. Achieving a thorough understanding of the data can result in the extraction of a smaller set of relevant features that can be used to achieve better discrimination between different classes/motifs. In this chapter, I investigate domain-dependent preprocessing techniques to improve the performance of the baseline DTW algorithms in clustering patterns that have long lengths.

There are presently two groups of preprocessing techniques commonly used to address this issue:

- Feature Selection
- Feature Extraction

Feature selection techniques involve selecting only a subset of attributes from the original data. With respect to the time series data, the technique is analogous to sub-sampling the sequence. To remove redundant features, one of the most popular feature selection approach is the exploratory data analysis(EDA). EDA is an approach to data analysis that postpones the usual assumptions about what kind of model the data follows with the more direct approach of allowing the data itself to reveal its underlying structure and models. The particular techniques employed in EDA are often quite simple, consisting of various techniques of:

1. Plotting the raw data such as data traces, histograms, histograms, probability plots, lag plots, block plots, and Youden plots.
2. Plotting simple statistics such as mean plots, standard deviation plots, box plots, and main effects plots of the raw data.
3. Positioning such plots so as to maximise our natural pattern-recognition abilities, such as using multiple plots per page.

Apart from removing redundant features, we can also construct more useful features from the existing ones. Feature extraction processes are concerned with the range of techniques that apply an appropriate functional mapping to the original attributes to extract new features. The intuition behind feature extraction is that the data vectors $\{x_n\}$ typically lie close to a non-linear manifold whose intrinsic dimensionality is smaller than that of the input space as a result of strong correlations between the input features. Hence by using appropriate functional mapping, we obtain a smaller set of features that capture the intrinsic correlation between the input features. By doing so, we move from working in high dimensional spaces to working in low dimensional spaces. The choice of appropriate functional mapping can also

improve the clustering of data. For example, let's consider figure 4.1: The left-hand plot represents the locations of two dimensional data points in the original input space. The colours red and blue denote the classes to which the data points belong to. To cluster the data with respect to their classes, it will be ideal if we can partition the input space into disjoint regions where intra class variation is small and inter class separation is large. For this example, this is achieved by mapping the points to a feature space spanned by two gaussian basis functions (shown on the right). Now, we can partition the feature space into two disjoint regions, one of each cluster.

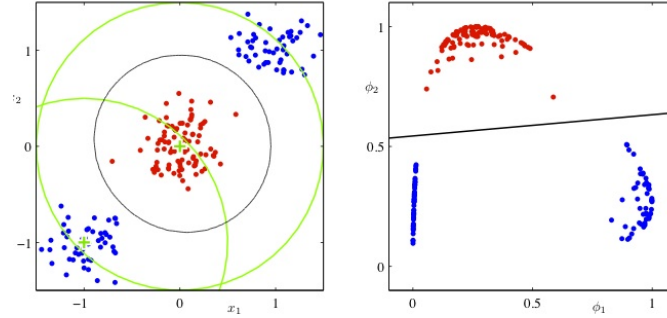


Figure 4.1: The figure on the right corresponds to location of the data points in the feature space spanned by gaussian basis functions $\phi_1(x)$ and $\phi_2(x)$

In the following sections, I investigate whether the application of exploratory data analysis and the construction of features that integrate metadata mainly knowledge of the domain can aid the baseline DTW algorithm in achieving low run times and good accuracy on long time series sequences. The primary data set that I will be using is the TIDIGITS corpus as the time series sequences of this data set have lengths that are in the order of 10^4 .

4.1 Feature Selection

The computational and time complexity associated with the DTW algorithm is governed by the length of the time series. Removing redundant features can result in a great reduction in the time complexity without any negative impact on the accuracy. To get an idea about the underlying structure of the data, I studied the plots of the time series sequences along with listening to the individual samples. Figure 4.2 shows the plot of raw signal corresponding to the word '8' by a speaker from the *boy* category.

From the visual and auditory analysis, I have made the following observations:

- Long durations of silence occupy the beginning and end of each utterance. The durations of the interesting regions that actually contain information

about the spoken digit is quite small in comparison to the durations of silence regions. Removing these silence segments allow reduction in the dimensionality of the time series sequences with minimal loss of information.

- The recordings are highly distorted when played in *matlab*. The distorted signals fail to provide any type of auditory clue about category of the speaker i.e whether the speaker belongs to { boy,girl, men,women} the signal has to be played multiple time to correctly identify the spoken word.

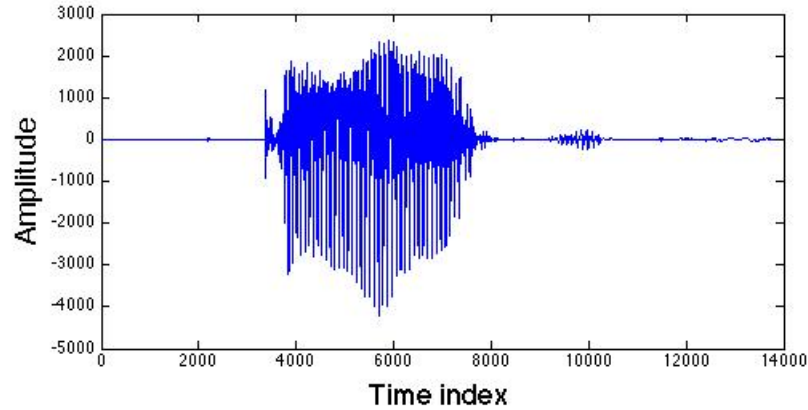


Figure 4.2: 'Raw' signal

4.1.1 Signal Filter

To remove the redundant attributes from the time series utterances, I have constructed the following algorithm: 'SignalFilter' that performs feature selection by removing segments corresponding to durations of silence. An outline of the algorithm is as follows:

Algorithm 2 SignalFilter

```

1: procedure SIGNALFILTER(signal) ▷ raw signal
2:   threshold = 0
3:   maxAmplitude = max(rawSignal)
4:   Adapt the threshold based on the value taken by the maximum amplitude
5:   output ← removeSilence(rawSignal, threshold)
6:   return output
7: end procedure

```

The algorithm employs an adaptive threshold to select and remove redundant attributes. The value of the threshold is dependent on the maximum amplitude of the sequence. The value set is comparatively higher for utterances of

speakers having a loud and deep voice and lower for utterances for speakers having gentle and low voice.

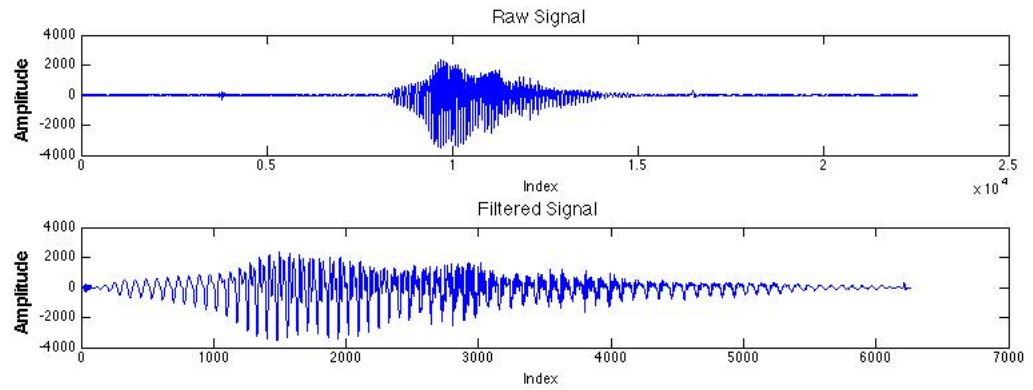


Figure 4.3: shows the raw acoustic signal corresponding to the utterances of the digit '8' alongside with the filtered signal at the bottom.

From figure 4.3, it can be observed that the filter preserves the interesting patterns associated with the utterance while succeeding in reducing the dimensionality of the data. To investigate the effect of introducing this prior feature selection step on the performance of the baseline DTW algorithm, I conducted the following experiment:

SETUP:

- Dataset used: TIDIGITS Test-set size : 976 samples

category	sample size
boy	162
girl	162
men	326
women	326

Training data set size: 1467

category	sample size
boy	225
girl	234
men	495
women	513

- An outline of DTW used algorithm used for this experiment is given below.

Algorithm 3 Value-Based DTW

```

1: procedure VALUE-BASED(seq1, seq2) ▷ two raw sequences
2:   DTW = zeros(length(seq1)+1, length(seq2)+1)
3:   w = max( $\lceil 0.1 * \max(n, m) \rceil$ , abs(n-m)) ▷ Window constraint
4:   for i=1: to length(seq1) do ▷ Initialise the DTW cost matrix
5:     DTW(i,0) =  $\infty$ 
6:   end for
7:   for i=1 to length(seq2) do
8:     DTW(0,i) =  $\infty$ 
9:   end for
10:  for i=2 to length(seq1) do
11:    for j=max(2, i-w) to min(length(seq2), i+w) do ▷
12:      cost(a,b)  $\equiv$  euclid(a,b)
13:      DTW(i,j) = cost(seq1(i), seq2(j)) + min{ DTW(i-1,j)+DTW(i,j-1)+DTW(i-1,j-1) }
14:    end for
15:  end for
16:  return result =  $\frac{DTW(n,m)}{nm}$  ▷ n=length(seq1), m=length(seq2)
17: end procedure

```

Note : The main objective of my research is to improve the accuracy of the DTW algorithm while reducing the time and computational cost to a **minimum**. Even after applying the feature selection process, from initial experiments on few samples, I have found that the computational cost incurred by the algorithm is still very high. Hence to minimise run time, I employed the Sakoe-Chuba band that has an adaptive window size of : $w = \max(\lceil 0.1 * \max(n, m) \rceil, \text{abs}(n-m))$. The lower bound of the window size is set to 10% of the size of the longest sequence which is the standard size that vast majority of the data mining researchers [19] use to keep the time complexity of DTW to a minimum.

- RESULTS:

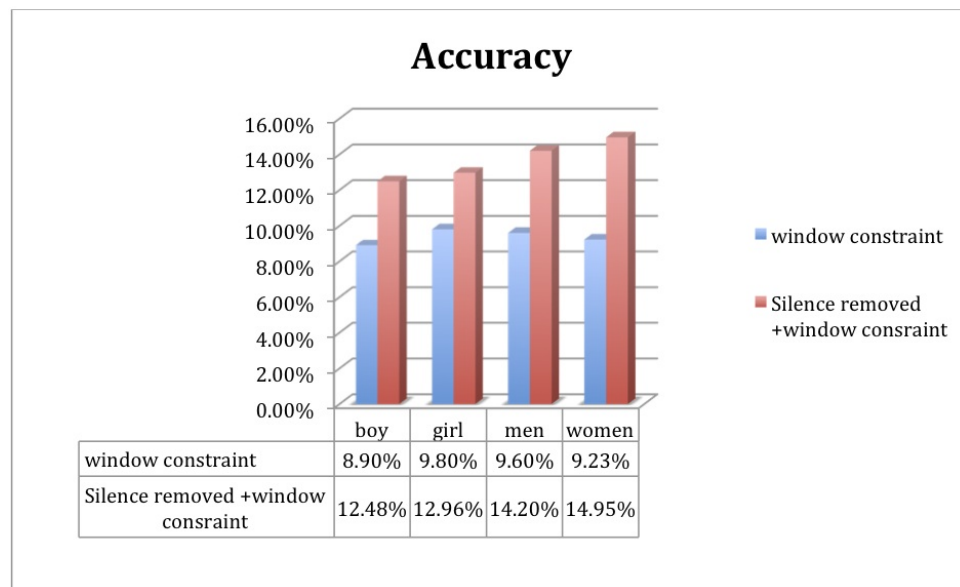


Figure 4.4

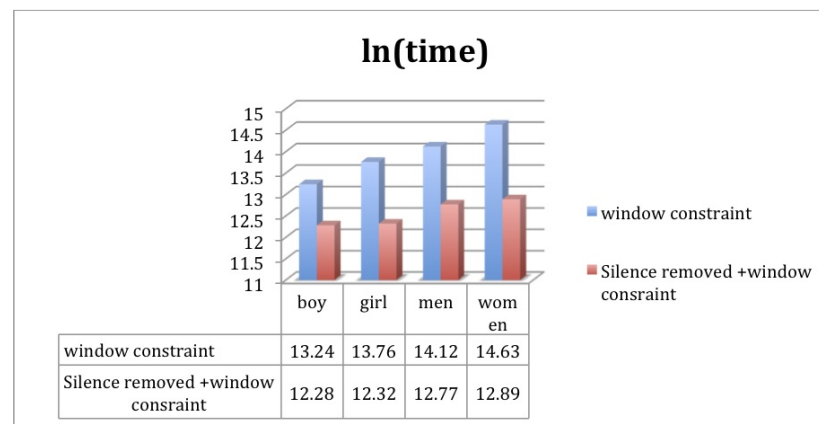


Figure 4.5

Observations:

- The DTW algorithm achieves very poor accuracy. The poor accuracy is a result of one or a combination of the following three factors:
 - the use of raw values as features: the numerical value associated with each time point is not a complete picture of the data point in relation to the rest of the sequence.
 - the use of the rigid window constraint- the low accuracy may be attributed to the optimum warping path between similar patterns lying outside boundaries of the Sakoe-Chuba bands[5, 4].
 - not integrating knowledge of the domain: The data set is comprised of speech utterances. It is a widely known fact that for speech data,

the MFCC feature vectors capture the information of phones that make up a word. Since different lexical identities are composed of different phones, these use of MFCC vectors can increase the inter class variance of the samples. (details of MFCC to follow)[4, 20, 5, 21, 22].

- Removing ‘silence’ segments improve **both** the accuracy and the run-time of the algorithm. While the decrease in run-time is quite obvious, the increase in accuracy is not. All utterances contain durations of silence. Taking the silence regions into account decreases the inter class variance and in turn increase intra class variance as they bring in an unwanted notion of similarity in dissimilar patterns.

4.1.2 Downsampling

From conducting further exploratory data analysis, I have observed that if I down-sample the utterances by $\frac{1}{2}$ which in other words corresponds to decreasing the sampling frequency by half, the global shape is still preserved even though some local information is lost as shown in figure 4.6. This results in further reduction in the dimensionality of the sequences i.e the length of the sequences.

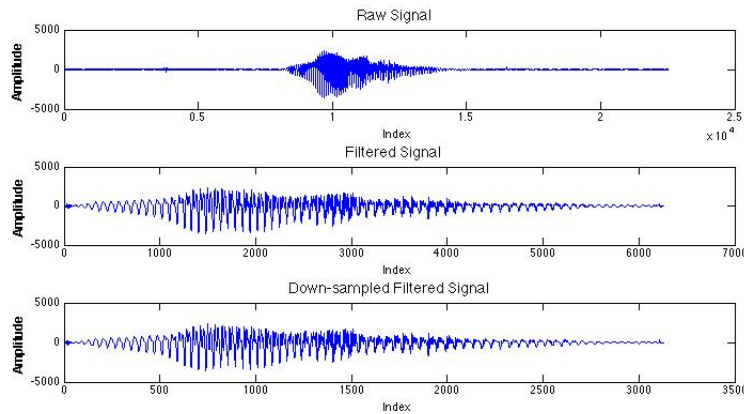


Figure 4.6: shows the raw acoustic signal of the digit ‘8’ (top figure), the silence removed version of the signal(middle) and the silence removed and down sampled version of the acoustic signal (bottom)

To investigate the effect of performing further dimensionality reduction on the time series sequences through down sampling on the accuracy of the DTW, I performed the following experiment:

Dataset: The TIDIGITS training and set used in 4.1

Algorithm : baseline DTW augmented with an adaptive window constraint(4.1)

Approaches being compared: Removing silence utterances VS Removing silence utterance + downsampling VS baseline

Results:

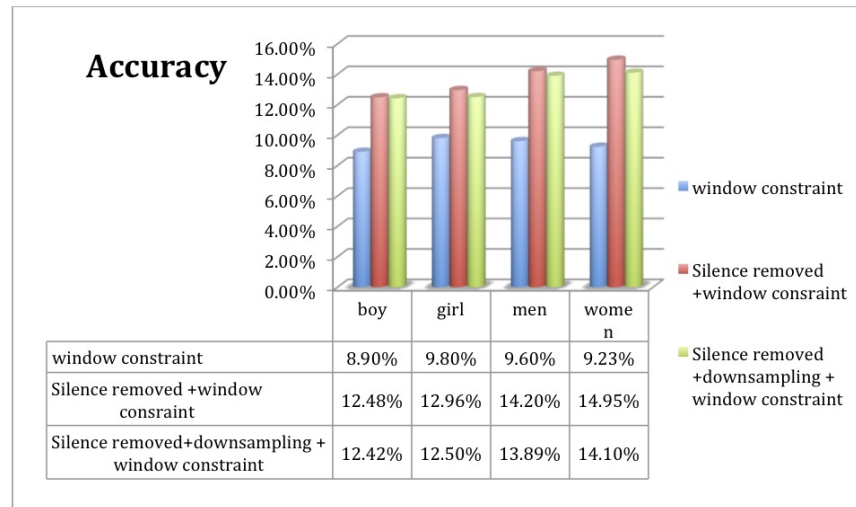


Figure 4.7

Observations:

Performing the two stage feature selection step that involves removing 'silence' utterances followed by downsampling allow DTW to still construct more optimal paths that are aligned along the main diagonal for similar patterns than using the entire 'raw' time series sequences. This procedure results in a 4% increase in accuracy on average. Furthermore, the loss of local information through downsampling the non-silence regions leads to a minimal decrease in the accuracy of the algorithm in comparison to using the entire non silence regions for pattern matching. This supports the claim that the classes are differentiated mainly by their global shape.

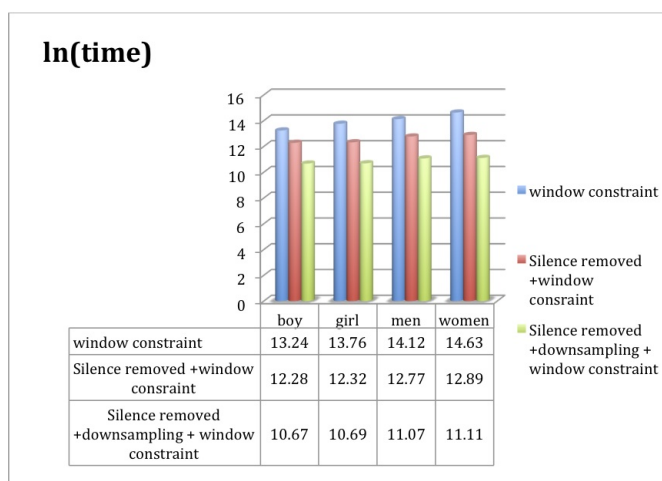


Figure 4.8: Integrating downsampling decreases the ln(run time)

Augmenting the down sampling procedure to the feature selection process leads to a further decrease of 1.5 in the $\ln(\text{run time})$ of the DTW algorithm in comparison to just removing silence regions as a preprocessing step. This is expected since in the first stage of the preprocessing phase, redundant features are dropped which reduces the dimensionality(i.e length) of the sequences. The length of the sequences is reduced even further through downsampling the the output sequences of stage 1. Since the computational cost of DTW is directly dependent on the length of the sequences, thus decrements in dimensionality leads to a decrease in the computational cost.

4.2 Domain Dependent Feature extraction

From the analysis conducted so far, it can be concluded that heuristically selecting only significant attributes from the time series sequences does **improve** both the accuracy and the speed of the DTW. However, from the observation of the experimental results gathered so far, it is quite clear that the accuracy of the algorithm is very low. So far, I have investigated the effect on using ‘raw’ values of the time series sequences on the performance of the DTW. In this section, I investigate the contribution of using the window constraint and the contribution of using domain dependent features on the performance of the DTW algorithm. There are two motivations behind conducting this analysis:

- The primary motivation is to improve the speed of the DTW algorithm without degrading the accuracy. Choosing an appropriate functional mapping, can help map the data to a lower dimensional feature space that can capture the intrinsic qualities of the data. Thus constructing appropriate functional mappings can achieve both dimensionality reduction and higher accuracy.
- The other motivation is to investigate to what degree is the low accuracy error credited to not using domain dependent features and to using a rigid window constraint has on the low accuracy(The features that we have considered so far are the raw values indexed by time). Understanding the underlying factors that that influence the performance of the algorithm can provide insights on what aspect of the algorithm needs to be changed to gain better performance.

4.2.1 Mel Cepstrum Cepstral Coefficients

The primary data set that I am working with is the TIGITS corpus which is composed of speech utterances. For speech, the most commonly used features are the MFCC features-mel cepstrum cepstral coefficients. This feature representation is based on the idea of the cepstrum. For human speech, a

speech waveform is created when a glottal source waveform of a particular frequency is passed through the vocal tract which because of its shape has a particular filtering characteristic. The exact position of the vocal tract is in fact the key attribute in providing useful information about phones(units of sounds). Cepstrum provides a useful way to separate the information of the vocal tract from the glottal source.

An outline of the MFCC feature extraction is given below:

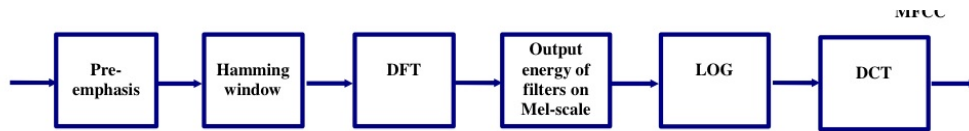


Figure 4.9: MFCC feature extraction

- i Pre-emphasis: boosts the energy of the signal at high frequencies to improve phone detection
- ii Windowing: partitions the time series sequence into frames using a hamming window
- iii DFT: extracts spectral information at different frequency bands
- iv Mel scale : transforming to mel scale improves recognition performance by allowing the model to take into account the property of human hearing
- v Log : makes the feature less sensitive to variations in input such as power variations on the speakers mouth.
- vi Cepstrum : separate the information of the vocal tract from the glottal source. The first 12 cepstral values from spectrum of the log of the spectrum are used

The windowing process results in dimensionality reduction i.e the length of the time-series sequences is reduced. Each sequence is segmented into frames of length 20 to 30 ms. These frames are then mapped using the procedure above to MFCC feature vectors. Since the result sequence of vectors is much smaller than the length of the original sequence resulting in the size of the DTW cost matrix is much smaller than before which in turn lowers the time and computation cost incurred by the algorithm. The time complexity of DTW is now reduced from $O(n^2)$ to $O(u^2)$ where $u = \frac{n}{l}$ (l denotes the length of the frame).

The experiments conducted in section 4.1.1 and 4.1.2, have shown that the DTW algorithm performs very poorly in terms of accuracy on the TIDIGITS test data when it employs the narrow Sakoe-Chuba band to minimise the time complexity. The reason for this low accuracy was credited to the influence of one or a combination of the following factors : using a narrow window constraint, using raw attribute values and not using domain-dependent features.

Having already investigated the influence of using raw values(4.1), for this part of the project, I constructed the following 3 models in order to investigate the relative isolated impacts of the other two factors. The models were tested on the TIDIGITS data set, thus allowing the results to be compared with the results of the previous experiments so far :

- i Model 1 employs the MFCC feature extraction mapping as a preprocessing step. The extracted features are used by the valued-based DTW algorithm augmented with the adaptive Sakoe-Chuba band constraint described in 4.1.1 to cluster similar patterns. The performance of this model can be compared to the performance of the base line model to measure the relative impact on the accuracy and run-time of the DTW of replacing each numerical value associated with each time index with a domain dependent feature vector.
- ii Model 2 employs a two stage preprocessing step. The feature selection procedure discussed in 4.1.1 is first applied to remove redundant features followed by MFCC feature extraction that achieves further dimensionality reduction. In this model dimensionality reduction occurs at both stages of the pre-processing step. The downsampling method discussed in 4.1.2 was deemed not necessary as a feature selection step since the feature extraction phase allows further reduction in dimensionality without any loss of information. The sequence of vectors are then used by the DTW algorithm to find optimal warping along the main diagonal of the DTW cost matrix.

By comparing the results of this model with the results of model 1 and the model discussed in 4.1, the optimum preprocessing strategy can be determined.

- iii Model 3 is identical to the version 2 with the exception that this version does not employ the window constraint. The main purpose of using this model is to check the relative impact of using window constraints. The difference in the performance between using model 2 and model 3 can be used to check to what degree is employing such a rigid window constraint affect the accuracy and run-time of the algorithm.

Experimental setup:

Dataset : The TIDIGITS training and test set (Chapter 2, 4.1.1)

RESULTS:

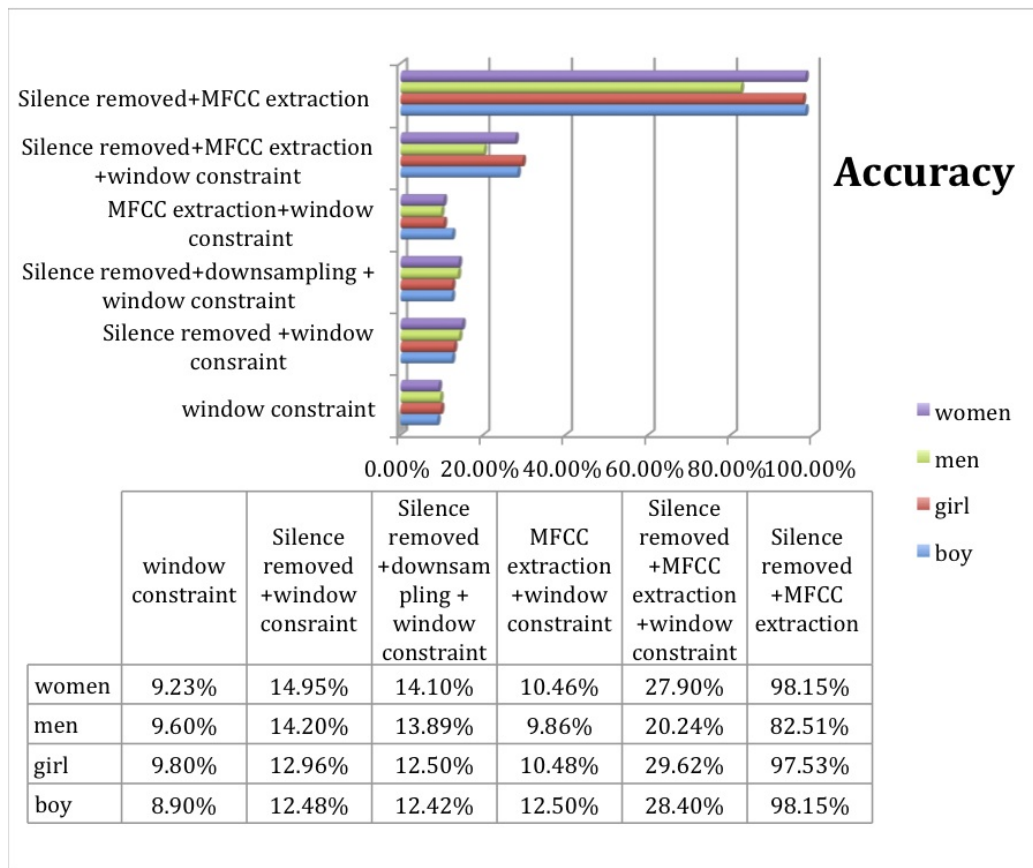


Figure 4.10: Accuracy achieved by all models

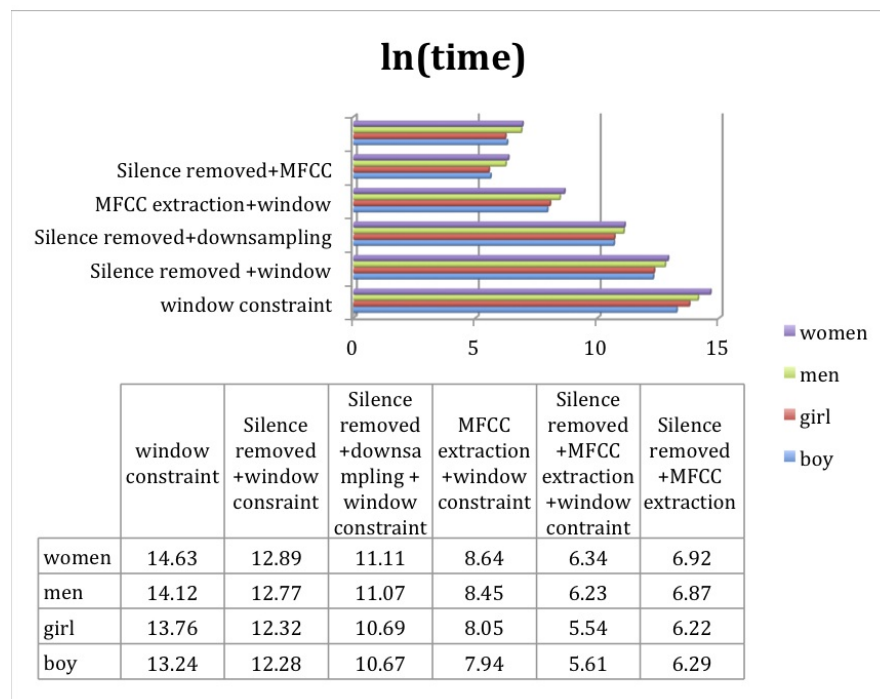


Figure 4.11: The ln(run time) incurred by all models

Observations:

- Making DTW domain-dependent has little significance on the accuracy when constraints are employed to minimise the time complexity.
 - In comparison to the base-line model, the accuracy of the window-constrained DTW only increases by 1.3% on average across all 4 categories.
 - The run-time on the other hand has improved considerably. In comparison to the baseline model, the average $\ln(\text{run time})$ has decreased by 5.7. This is obvious since the acoustic signal is mapped to smaller sequence of frames.
- Removing redundant features have greater relative impact on the accuracy than employing domain dependent MFCC features. This is evident if we compare the results of using model 1 with the model discussed in 4.1.1. The presence of silence regions force the optimal warping paths between patterns of the same lexical identity to lie outside the regions in the cost matrix bounded by the Sakoe-Chuba band. This forces the DTW to find an **approximate** optimal path with in the allowed regions which in turn leads to an increase in the error rate.
- Combining attribute/feature selection with MFCC feature extraction as a preprocessing step achieves greater improvement in accuracy and speed than using either of these approaches alone. In comparison to just using MFCC feature extraction as a preprocessing step, the accuracy has been boosted up by 15.17% on average while the $\ln(\text{time})$ have been reduced by 2.36. Similarly, in comparison to just using feature selection as a preprocessing step, the accuracy has increased by 12.9% on average while the $\ln(\text{time})$ have been reduced by 6.5.
- From the above observation alone, we can deduce two facts for this data set, one of which is not that obvious: removing redundant features have a greater relative impact on improving the performance of a constrained DTW than employing domain dependent features and the second fact which is quite obvious is the strong dependency between the algorithm's accuracy and the size of the window constraint. It can be concluded that the use of the rigid window constraint is the main contributing factor for achieving small accuracy rates.

Since the main goal is to improve **both** the accuracy and speed of DTW in handling sequences of high-dimensionality i.e long lengths, removal of silence segments provides an ideal mechanism to improve **both** the time complexity and the accuracy of the algorithm. Dropping the window constraint although will lead to considerable increase in the accuracy by will result in longer run-times. This is not ideal when working on large high dimensional datasets.

- Model 3 achieves almost near perfect accuracy. Dropping the window constraint improves the accuracy by 67.15% on average over model 2. In other words 67.15% of the time on average, the optimum warping path lie outside the regions bounded by the Sakoe-Chuba band constraints, This confirms that patterns belonging to the same lexical identity can have an overly temporal askew between them as result of the different contexts in which the words are spoken and/or as a result of different speakers speaking the same word.
- The run time of model 3 is lower than the run time of all models with the exception of model 2. Model 3 therefore provides the best balance in the fulfilling the two conflicting objectives of high accuracy and high speed that any of the other investigated models.

Conclusion

To summarise, to improve the performance of the DTW algorithm:

- In 4.1, I have investigated ways to remove redundant features by conducting exploratory data analysis.
- In 4.2, I introduced domain dependent feature extraction methods and investigated the influence of the use of such features on the performance of DTW
- I have investigated the investigated the relative isolated impacts of using raw values, employing a rigid window constraint and using domain dependent features on the performance of the DTW algorithm
- I have observed that although the DTW algorithm is domain independent, augmenting the DTW with a domain dependent preprocessing technique can greatly improve its performance in terms of **both** accuracy and speed with out the need of any global constraints. For the TIDIGITS data set, employing the preprocessing steps of 'silence' removal followed by MFCC feature extraction allows DTW to improve not only its accuracy but also speed even without the use of global window constraints.

Chapter 5

Improving DTW

So far, we have investigated methodologies that improve both the speed and accuracy of the DTW algorithm by integrating meta data (i.e knowledge of the domain) in the preprocessing stage. The problem with such methodologies is that the same algorithm cannot be extended across multiple domains: the MFCC feature extraction discussed in the previous chapter is only applicable to time series sequences that correspond to speech utterances. To develop a framework that can be extended across multiple domains, it is necessary to use features that are entirely data driven. In the first half of this chapter, I investigate in detail a recently proposed data driven feature extraction methodology [9] that is aimed to improve the accuracy of the DTW across multiple domains. In the second half of this chapter, I investigate alternative measures to using window constraints that can improve the performance of the algorithm in terms of **both** time and accuracy across different time series domains.

5.1 Domain-independent feature extraction

Ideally, we require features that reflect information about the structure of the data. This allows the DTW to build a complete picture of the data point in relation to the rest of the sequence and hence achieve optimal alignments that are close to the diagonal for similar sequences. The fundamental problem of baseline (value-based) DTW is that the ‘raw’ numerical value associated with each point in the time series sequence is not a complete picture of the data point in relation to the rest of the sequence. The context such as the position of the points in relation to their neighbours is ignored. To fix this issue, an alternative form of DTW known as *derivative* DTW is proposed but it too fails to achieve better performance across all domains as it ignores to take into account the common sub-patterns between two sequences (mainly global trends).

To address these drawbacks, recent works have been conducted to extract good feature extraction methods that are entirely data-driven. One particular approach that has been seen to achieve good accuracies across multiple domains is the method proposed Xie and Wiltgen in their paper [9]. The authors highlight a domain-independent feature extraction process where each point in the time series sequence is replaced by a 4 dimensional vector. This 4-d vector attempts to provide a complete picture of a point in the relation to the rest of the sequence. The first two features in this vector hold information of the local trends around a point while the last two features reflect information about the global trends. From experiments conducted on the UCR data sets, they have observed that embedding DTW with this feature extraction process yields greater accuracy across all datasets.

Definition of local feature given in [9] is as follows:

$$f_{\text{local}}(r_i) = (r_i - r_{i-1}, r_i - r_{i+1})$$

The first feature reflects the difference between the values of the current index and the previous index while the second feature corresponds to the difference between the value of the current index and the succeeding index.

The extraction of global features however, is constrained by two factors:

- the features must reflect information about global trends
- the features must be in the same scaling order as the local features. Being in the same scale allows them to be combined with local features.

In [9], the authors used the following method to extract global features from the time series sequence:

$$f_{\text{global}}(r_i) = (r_i - \sum_{k=1}^{i-1} \frac{r_k}{i-1}, r_i - \sum_{k=i+1}^M \frac{r_k}{M-i})$$

The first feature represents the deviation of the value at time i from the mean of the values of the sequence that has been seen so far while the second feature represents the deviation of the value at time i from the mean of the values that is yet to be seen. This formulation allows the detection of significant ‘drops’ or ‘rises’ in the series.

Note : The local and global features have no definition for the first and last points in a sequence and to keep the terminology clear, when I refer to the dimension of the time series, I mean the length of the time series.

One of the drawbacks of using this feature extraction methodology is the absence of achieving dimensionality reduction. The length of the sequence of vectors is approximately the same as the dimensionality of the original sequence. The DTW algorithm combined with this feature extraction process

therefore suffers from the curse of dimensionality as before. Since minimising the time complexity is a major priority for this analysis, the DTW algorithm is subjected to the adaptive Sakoe-Chuba band window constraint discussed in 4.1.1 to minimise the run time.

Xie and Witgen [9] have already shown that augmenting this feature extraction methodology to the DTW algorithm improves its accuracy across different domains. However, in their analysis due to the availability of sufficient computing power, they didn't use any window constraints when performing their experiments. For problem scenarios where availability of computing power is limited and the speed of the DTW is considered an equal priority along with the accuracy, it will be interesting to investigate whether this methodology can allow DTW to achieve better performance in terms of accuracy over the baseline method.

To investigate the effect of introducing this prior feature selection step, I conducted the following 2 experiments:

Objective Compare the affect of using global and local features to using raw values on the performance of a **window constrained** DTW algorithm.

- Experiment 1

Datasets: TIDIGITS data set(4.1.1)

Setup Prior to extracting these domain independent features , I performed the feature selection step of removing segments of utterances that correspond to silence. When conducting experiments using MFCC feature vectors, removing redundancy allows the optimal warping paths between similar patterns to lie closer to the main diagonal. Using this feature selection step also has the advantage of dimensionality reduction.

By comparing the experimental results of this model with the baseline model and the model of 4.1, we can observe whether for this data set, removing redundant features is more significant to using features that capture information about the global and local trends. Also we be able to investigate whether using such feature allows a constrained DTW algorithm to achieve higher accuracies than using raw values.

RESULTS

A summary of the results are given below:

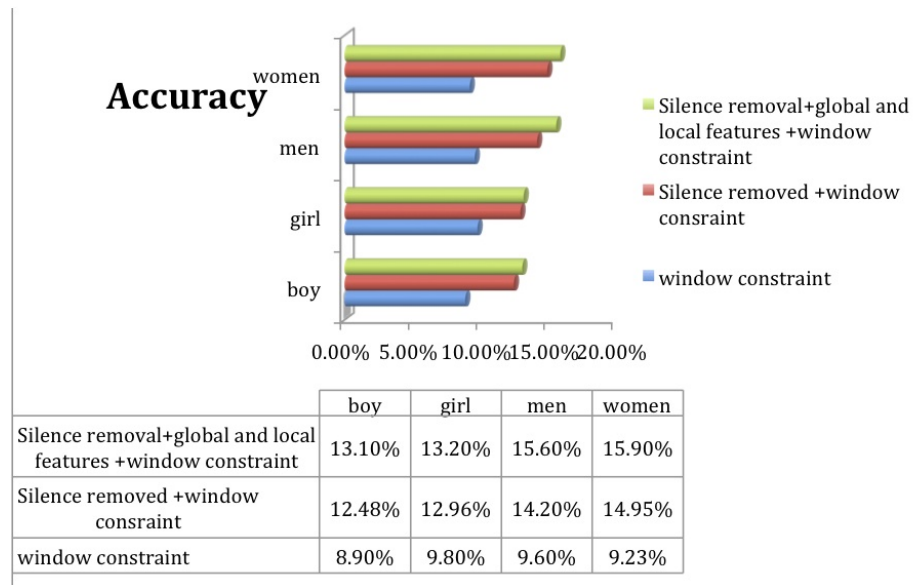


Figure 5.1

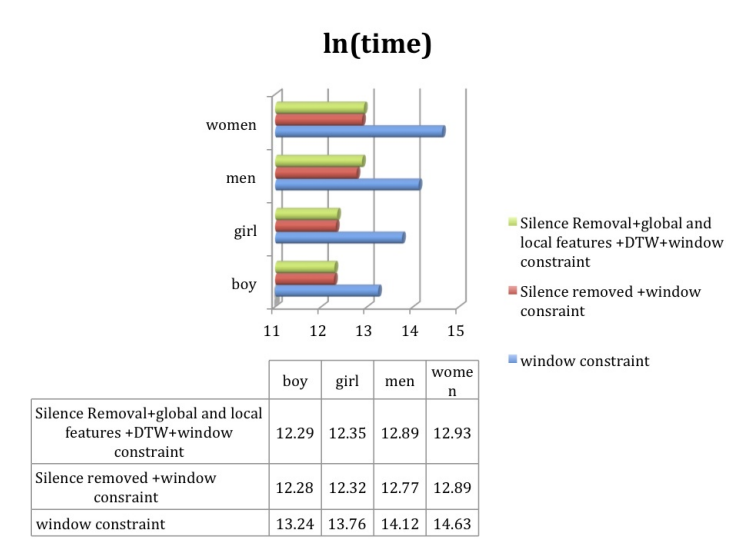


Figure 5.2: ln of the run time

Observations:

- Removing redundant features i.e removing regions of silence is a greater contributing factor in improving the performance of a window constrained DTW than applying a feature extraction process that integrates meta data(4.2.1) or that captures information about local and global trends.
- All 3 models achieve very low accuracies. As concluded from previous experiments, the low accuracy is primarily credited to the use of the rigid window constraint

- The computational cost incurred by the algorithm is higher than the version used for the model of 4.1.1 One possible explanation is that the cost of applying the euclidean metric on vectors > cost of applying the euclidean metric on points. Since the euclidean metric is applied mn times. The overall computational cost increases.

- Experiment 2

Datasets: UCR datasets: InlineSkate and Cinc_ECG_Torso

The results are as follows:

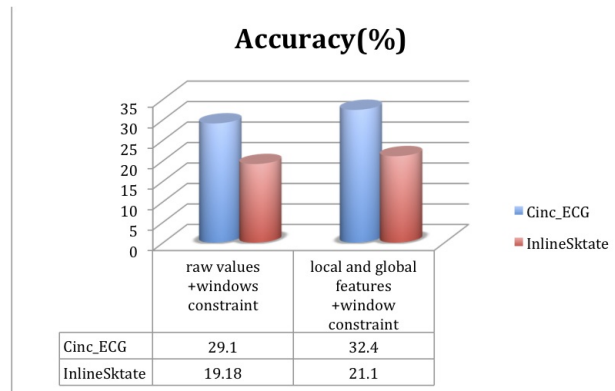


Figure 5.3: Using features that reflect information of trends improves the accuracy of the algorithm

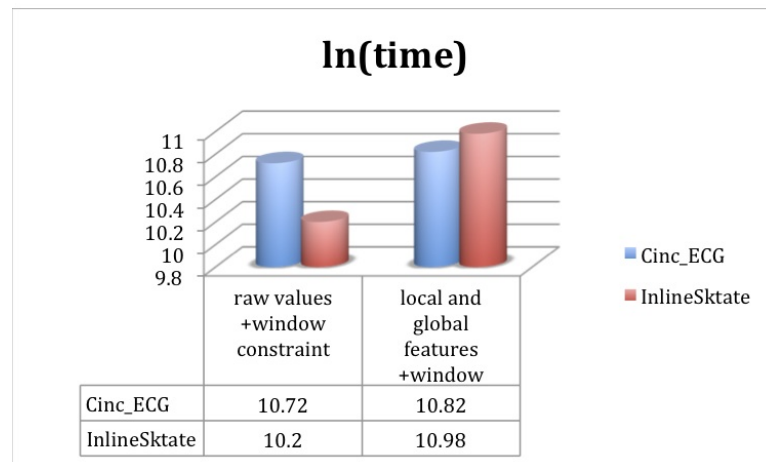


Figure 5.4: The computation time incurred

Observations

- The differences between performances of the two versions of DTW are consistent with the observations made in the previous experiment.
- In comparison to the base line method, there is only a minimum improvement in the accuracy of the window constrained DTW. For the

Cinc_ECG_Torso time series data set, using global and local features improves the accuracy by only 3.2% whereas for the InlineSkate data set, the accuracy improves by only 1.92%.

Conclusion:

The experiments conducted by Xie and Witgen[9] on the UCR datasets have shown that using their feature extraction methodology allow DTW to achieve much higher accuracies than using just 'raw' values . Optimal paths that closer to the diagonal region of the cost matrix have smaller distances than paths that are further away from the diagonal. The improved accuracy is credited to the construction of optimal paths that are closer to the diagonal than before for sequences belonging to the same class. However the results from their experiments do not provide any information on the degree of translation undergone by these warping paths. The results from my experiments provides this insight. Using the domain independent methodology only leads to a fractional increase in the accuracy of the DTW when it employs a window constraint. This shows that for similar patterns, the degree of translation undergone by the optimal warping paths is very small as very few ideal optimal paths enter the region defined by Sakoe-Chuba band.

The low accuracies of the DTW can be improved by increasing the width of the Sakoe-Chuba band. But increasing the width also leads to a reduction in speed. This provides the motivation to investigate alternative methods that can a better balance between the two conflicting goals of accuracy and speed. In the next section, I investigate a self-proposed method that is an alternative approach to using window constraints to speed up DTW. The new proposed methodology uses the data-driven feature extraction process that is discussed in the current section. The aim here to construct a domain independent framework that allows DTW to attain improvements in both speed and accuracy over the Sakoe-Chuba band window constrained DTW.

5.2 Extending DTW

The feature extraction methodology discussed in the previous section offers no advantage of dimensionality reduction. The time series sequence is mapped to sequence of vectors whose length is $\|X_n\| - 2$. (where $\|X_n\|$ denotes the length of the original time series sequence). The MFCC feature extraction process (4.2) on the other hand, does provide the advantage of dimensionality reduction. The time series sequence is first segmented into series of frames of length 20ms i.e 200 points. Through appropriate functional mapping, each frame is then mapped to a vector. Hence the time complexity of the DTW algorithm have been reduced from $O(n^2)$ to $O(u^2)$ where $u = \frac{n}{l}$ (l denotes the length of the frame).

Using the MFCC feature extraction method as motivation, I propose the following methodology:

- i Apply the feature extraction process of 5.1 to embed the information of local and global trends.
- ii Partition the sequence of vectors into frames of width m . The default value of m is set to 50. For speech utterances in the TIGITS data set, this is equivalent to having frames of size 5ms. Unlike the windowing process of MFCC extraction, the frames here correspond to sequence of vectors rather sequence of numerical values. This partitioning process reduces the length of the sequences by m times and hence decreases the time complexity of the DTW algorithm from $O(n^2)$ to $O(\frac{n}{m})^2$.
- iii Adapt the cost metric of the DTW algorithm to work on series of frames rather than series of vectors

The problem can now be shifted to finding an appropriate kernel that can be used to compute the similarity between frames composed of feature vectors. Ideally, we want a metric that takes into account the variation of speed and time when comparing two similar subsequences. To understand why we need the metric to be invariant to variations in speed and time, lets consider the following two signals:

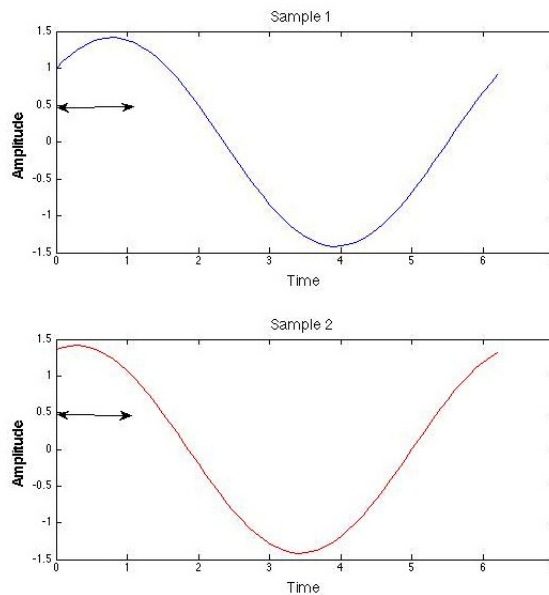


Figure 5.5: Two signals separated by translation

The signal denoted by the 'red' color is a 'slower' version of the signal denoted by the 'blue' color. Using a euclidean metric in this scenario is inappropriate. The euclidean metric in this context is identical to linear time warping where the two subsequences/frames will be matched based on a linear match of the

two temporal dimensions. In our context, we need a kernel that computes the similarity between two sub-sequences by warping the time axis. Intuitively speaking, the kernel must behave like a DTW algorithm that compares the global and local properties associated with a point in one frame with the global and local properties of all points in the second frame as illustrated by the figure below.

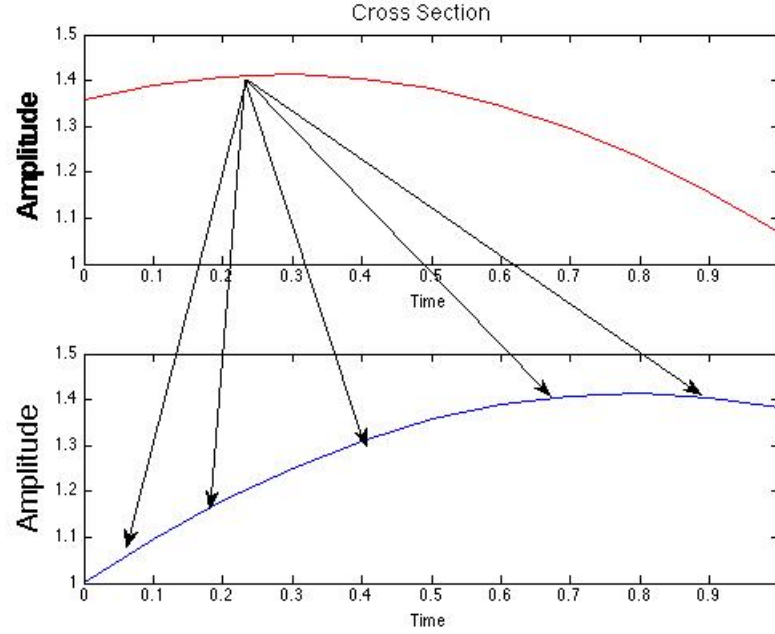


Figure 5.6: Two identical subsequences varying in time

The motivation behind my proposed kernel function comes from the polynomial kernel. Let x and z be two two-dimensional vectors and consider the simple polynomial kernel of degree 2 : $k(x, z) = (x^T z)^2$. This kernel can be expressed as :

$$\begin{aligned}
 k(x, z) &= (x^T z)^2 \\
 &= (x_1 z_1 + x_2 z_2)^2 \\
 &= x_1^2 z_1^2 + 2x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\
 &= (x_1^2, 2x_1 x_2, x_2^2)(z_1^2, 2z_1 z_2, z_2^2)^T \\
 &= \phi(x)^T \phi(z)
 \end{aligned}$$

The 2nd order polynomial kernel is equivalent to a corresponding feature mapping $\phi(x)$ that maps a two dimensional vector to $(x_1^2, 2x_1 x_2, x_2^2)$ where each attribute is monomial of order 2 . Generalising this notion to order M

then $k(x, z) = (x^T z)^M$ represents the sum of all monomials of order M. If we imagine x and z to be two images, then the polynomial kernel represents a particular **weighted** sum of all possible products of M pixels in the first image with M pixels in the second image.

Using this as motivation I propose the following kernel:

$$k(x, z) = \left\langle \sum_{i=1}^n x_i, \sum_{j=1}^n z_j \right\rangle$$

Here n denotes the length of the frame while x_i and z_j correspond to the individual 4-dimensional feature vectors that make up the frame. The above kernel corresponds to the dot product between the individual sums of the two frames. Although it may not look obvious, this construction actually allows the comparison between all feature vectors in the first frame with all feature vectors in the second frame as shown below:

$$\begin{aligned} k(x, z) &= \left\langle \sum_{i=1}^n x_i, \sum_{j=1}^n z_j \right\rangle \\ &= \left\langle (x_1 + x_2 + x_3 + \dots), (z_1 + z_2 + z_3 + \dots) \right\rangle \\ &= \left\langle x_1, z_1 \right\rangle + \left\langle x_1, z_2 \right\rangle + \left\langle x_1, z_3 \right\rangle + \dots + \left\langle x_2, z_1 \right\rangle + \left\langle x_2, z_2 \right\rangle + \dots \end{aligned}$$

From above expression, we can see that the proposed kernel corresponds to a sum of all possible dot products of pairs belonging to the set $\{(x_i z_j) | x_i \in \text{seq1}, z_j \in \text{seq2}\}$. It is easy to check that this proposed kernel is in fact a valid kernel function:

- $K(x, z) = K(z, x) \Rightarrow$ the function is symmetric.
- The kernel can be written as a scalar product in feature space: $K(x, z) = \phi(x)^T \phi(z)$ where the feature mapping corresponds to a finite summation of vectors $\phi(y) = \sum_{i=1}^n y_i$.

Augmenting the kernel to the DTW algorithm allows DTW to work on long time sequences without using a window constraint. To use this kernel as an appropriate cost function in the DTW algorithm, we need a functional mapping that:

1. constraints the codomain to be in the range from 0 to ∞ .
2. ensures larger values given by the function signify great degree of dissimilarity and smaller values signify a high degree of similitude.

An inspection of the kernel function shows the function represents the sum of dot products of all vectors in one frame with all vectors in the second frame. An ideal cost function that make use of dot products is the *arc-cosine*. Using an

appropriate substitution, I have thus constructed the following cost metric:

$$\theta = \frac{\langle X, Z \rangle}{|X||Z|}$$

where θ is the *arc-cosine* distance, $X = \sum_{i=1}^n x_i$ and $Z = \sum_{j=1}^n z_j$.

A formal outline of the entire methodology is given by the algorithm below:

Algorithm 4 Proposed DTW

```

1: procedure VALUE-BASED(seq1, seq2)    ▷ two sequences of feature vectors
2:   seq_1 ← segment(seq1, n)    ▷ Segment the sequences using a window of
   size n
3:   seq_2 ← segment(seq2, n)
4:   for i=1: to length(seq_1) do        ▷ Initialise the DTW cost matrix
5:     DTW(i, 0) = ∞
6:   end for
7:   for i=1 to length(seq_2) do
8:     DTW(0, i) = ∞
9:   end for
10:  for i=2 to length(seq_1) do
11:    for j=max(2, i-w) to min(length(seq_2), i+w) do
12:      DTW(i, j) =  $\theta = \frac{\langle X, Z \rangle}{|X||Z|} + \min\{ \text{DTW}(i-1, j) + \text{DTW}(i, j-1) + \text{DTW}(i-1, j-1) \}$ 
13:    end for                                ▷  $X = \sum_{i=1}^n x_i$  and  $Z = \sum_{j=1}^n z_j$ 
14:  end for
15:  return result =  $\frac{\text{DTW}(n, m)}{nm}$     ▷ n=length(seq1), m=length(seq2)
16: end procedure

```

5.2.1 Testing the methodology

The primary objective is to improve the performance of the DTW algorithm in problem domains where minimising time complexity has a high priority. To investigate whether the proposed changes does provide a better alternative to using the Sakoe-Chuba band window constraint, I have conducted the following experiments:

Experiment 1

Data set used : The TIDIGITS data set.

Model used : The model discussed in section 5.1: the framework consists of a two stage preprocessing step that involves feature selection process consisting of ‘silence’ removal followed by the domain independent feature extraction methodology proposed in [9]

Variables being compared: Sakoe-Chuba band window constraint VS the proposed methodology

RESULTS:

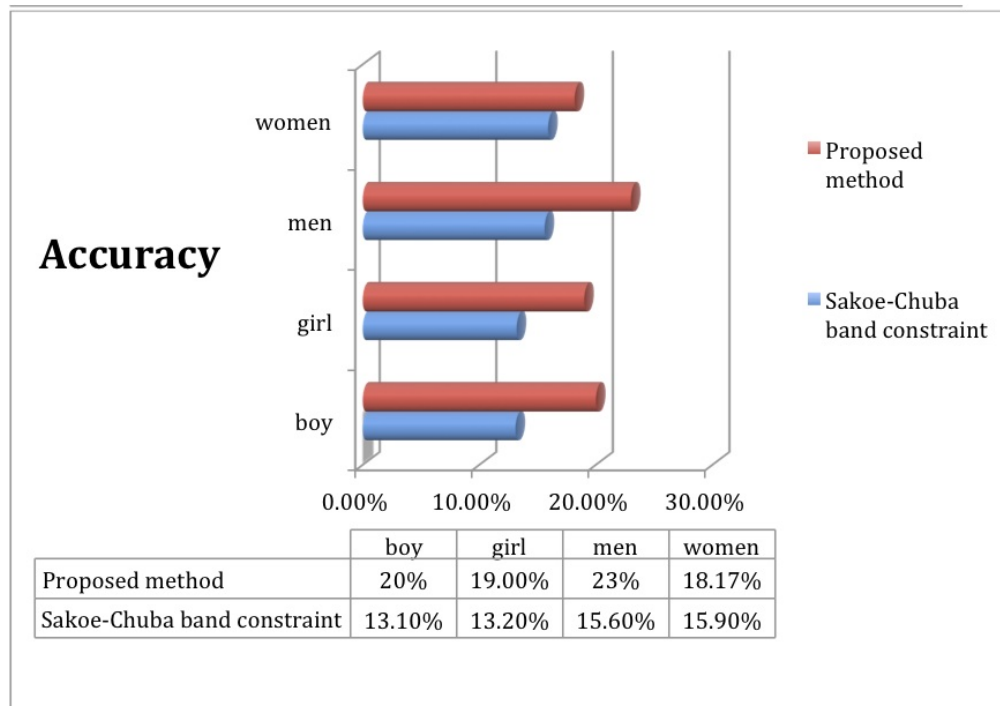


Figure 5.7: Accuracy

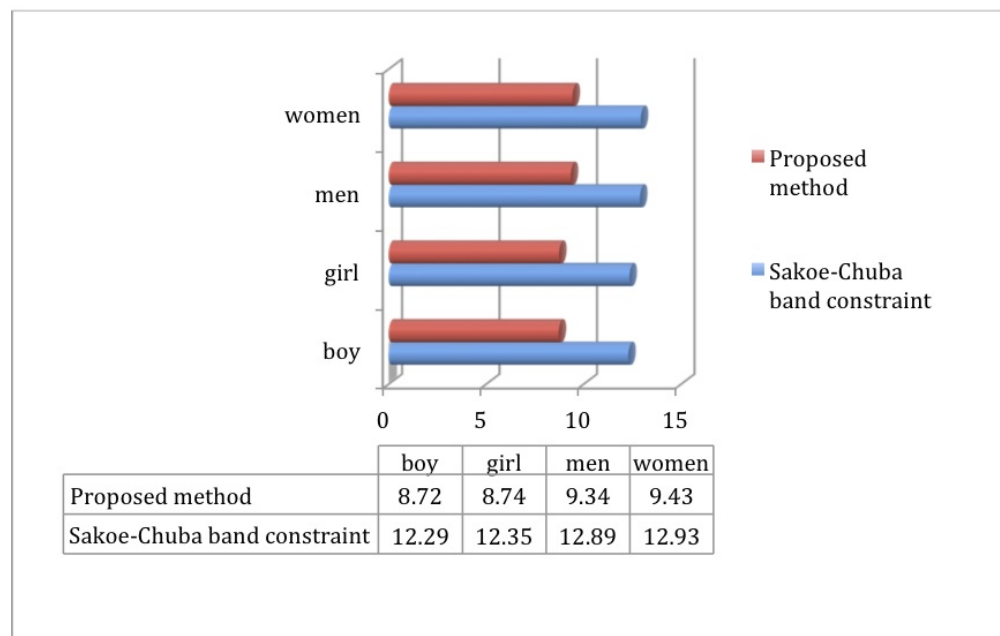


Figure 5.8: $\log_e(\text{run time})$

There are quite number of interesting observations that can made from figures

5.7 and 5.8.

- In comparison to employing the Sakoe-Chuba band window constraint, the alternative method allows DTW to improve its accuracy across all 4 categories by 6.54% on average.
- Equipped with the new changes, the run time of the algorithm has decreased exponentially by an **order** of 3.1 on average. The reduction of the time complexity is mainly due to the partitioning of the sequence into time slices of width 5 ms. The reduction in the length of the sequences by an order of 50 results in the shrinkage of the search space of DTW thus causing the algorithm to improve its speed.

The proposed methodology can also be adapted to use domain-dependent features. As I have stated earlier, the main motivation for constructing this framework is to provide better performance in terms of both accuracy and run-time for time series problem domains where the use of rigid window constraints is deemed necessary. In the previous chapter, we have seen that when the MFCC feature extraction is used as the only preprocessing step, to minimise the run-time, the use of the adaptive window constraint was deemed necessary. However from the experimental results, it can be seen enforcing such a rigid constraint results in a high error rate. To check that the new changes allow DTW to perform equally well when using domain dependent features, I have repeated the same experiment again but this time, as a preprocessing step I have just used the MFCC feature extraction.

A summary of the results are as follows:

Experiment 2

Data set used : The TIDIGITS test and training data.

Model : The model framework consists of single preprocessing step that involves the extraction of MFCC features

Variables being compared: employing window constraints vs the new proposed changes

Results

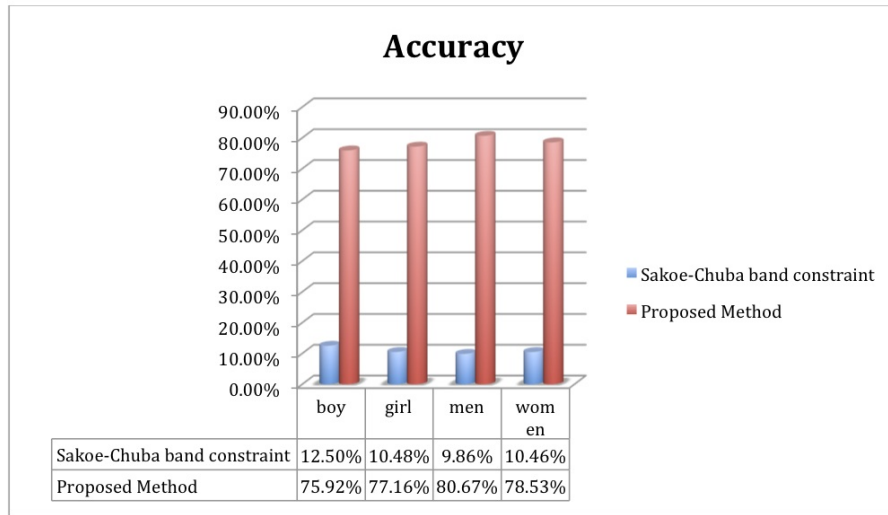
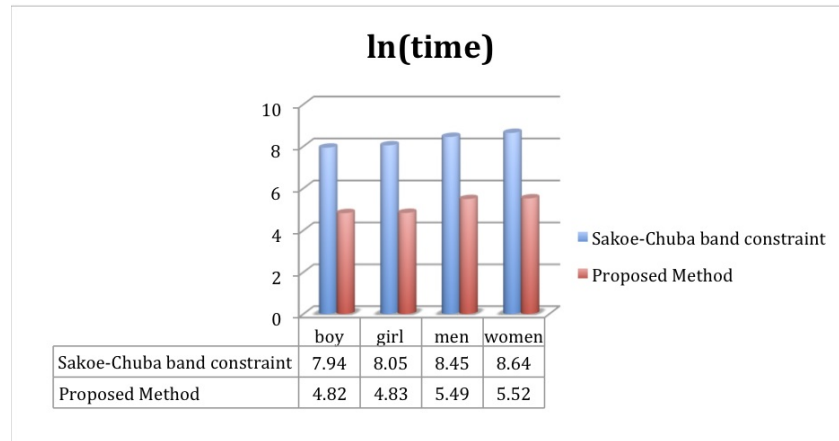


Figure 5.9: Accuracy

Figure 5.10: In of the run time: $\log_e(time)$

Observation The results are consistent with the findings in the previous experiment. The accuracy of the DTW algorithm has improved by over 60% on average and the average run time has decreased exponentially by an order of 3.12. Hence in comparison to the window constrained DTW, the new framework takes better advantage of employing domain dependent features.

However, since the tests so far has been conducted on the TIDIGITS test set, it is possible that this new approach is only tailored for this particular data set. Thus to confirm that the boost in the performance is not tailored for this particular time-series data set, I have the following experiments using the model of experiments on the UCR data sets: InlineSkate and CINC_ECG_TORSO.

Experiment 3

Data sets used : InlineSkate and CINC_ECG_TORSO

Setup :

Model used : The model discussed in section 5.1: the framework consists of a two stage preprocessing step that involves feature selection process consisting of ‘silence’ removal followed by the domain independent feature extraction methodology proposed in [9]

In the proposed approach, the width of the time slices has been kept fixed at a default value of 50 so far. In this experiment, I also investigate the influence of this parameter on the performance of the DTW. Decreasing its value reduces the size of the time slices which in principal should increase both accuracy and time-complexity . The core kernel used by the new algorithm is based on the function:

$$k(x,z) = < \sum_{i=1}^n x_i, \sum_{j=1}^n z_j >$$

$k(x,z)$ represents the sum of all possible dot-products. Using smaller subsequences allow the similarity measure to be dominated by the dot products of points whose local and global features are most alike. However, this suffers from the drawback of achieving lesser dimensionality reduction. Thus the time and computational complexity suffers.

RESULTS

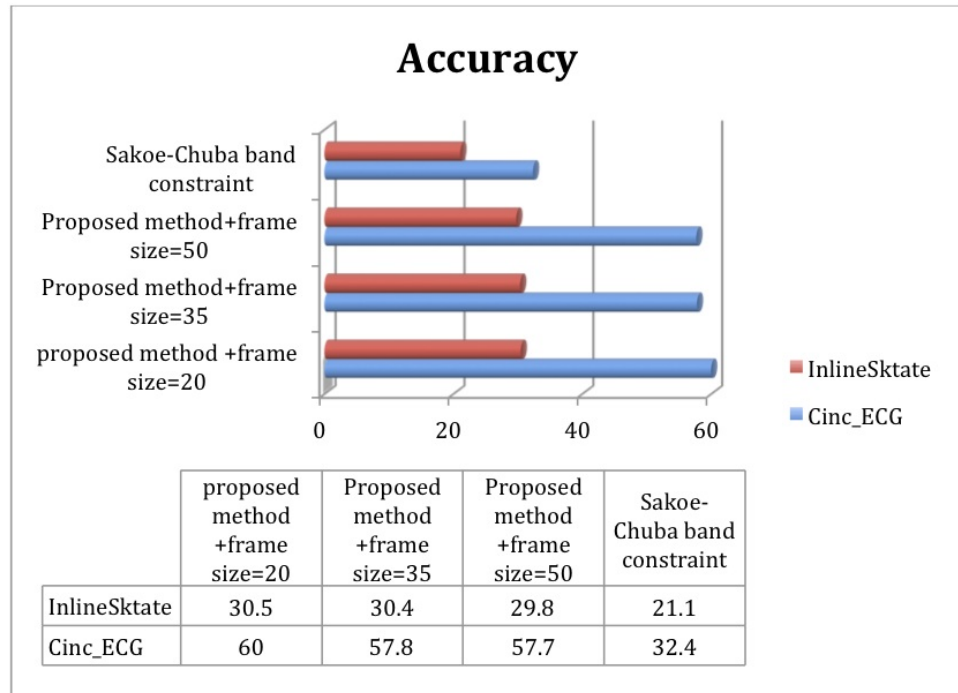


Figure 5.11: Accuracy

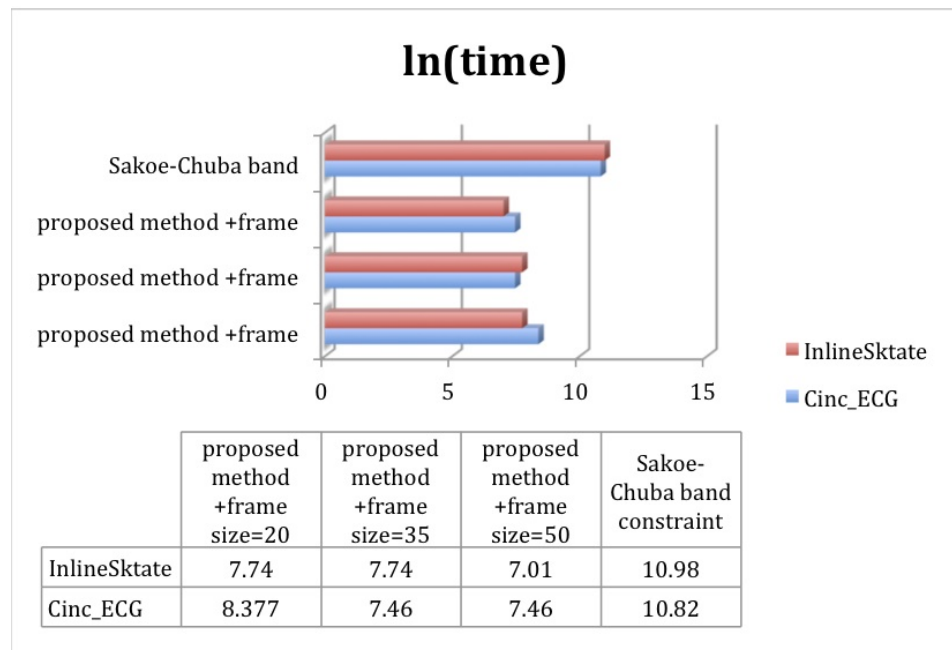


Figure 5.12: Run time in ln

Observation

- The proposed changes does provide a **better** alternative approach to using rigid constraints for problem domains where the time complexity is of high priority and the use of window constraints can not be avoided. The accuracy of the DTW algorithm under the new methodology is significantly higher then employing a window constrained DTW on sequences of extracted local and global feature vectors.
- Decreasing the size of the time slices only leads to a minimal increase in accuracy. Thus using the default value of 50 seems to be safe option as the algorithm better accuracy and speed than using the rigid Sakoe-Chuba band constraint .

Conclusion

- In chapter 3, we have seen that under the window constraint the time complexity of the algorithm decreases from $O(n^2)$ to $O(wn)$. From the experimental results, it can be observed that the new proposed changes allow DTW to achieve run times that are exponential lower than the run times achieved by the window constrained DTW. Thus it can be concluded that the time complexity of the proposed DTW variant is smaller that $O(wn)$.
- We have seen so far that increasing the speed of DTW negatively impacts the accuracy of the algorithm . The new methodology actually provides an exception. The use of the kernel function improves the accuracy of the DTW which implies that matching frames using the new cost function is

a better alternative than employing the euclidean distance to find local optimal warp path only through the constraint window. Combining this approach with the feature extraction method discussed in [9] results in the construction of a model that can applied for **different types** of time series data sets.

Chapter 6

Single Value Decomposition

High dimensional data vectors $\{x_n\}$ typically lie close to a non-linear manifold [23] whose intrinsic dimensionality is smaller than that of the input space as a result of strong correlations between the input variables. In data mining, to understand this intrinsic dimensionality of the data, the Single Value Decomposition(SVD) algorithm is widely used. SVD simplifies the data representation by showing only the number of important dimensions that captures the **variance** of the data. Intuitively speaking, SVD projects the high dimensional data vectors to an orthogonal subspace that maximises the variance of the data. Recent works[12] have shown that SVD can be applied to achieve dimensionality reduction in time sequences given that the sequences satisfy certain constraints. Applying SVD as a preprocessing step to such time series data sets can result in a significant reduction of the runtime of a classification/clustering algorithm. The focus of this chapter is to investigate compatible preprocessing methods that can be used alongside SVD to improve the accuracy of the 1 nearest neighbour classifier while minimising its run time.

6.1 Motivation

Unlike other data sets, clustering/classifying time series sequences by conventional distance metrics, such as the euclidean, may not result in high accuracy. The scope of such metrics is quite limited in the fact that they require sequences to share the same length and comparison of sequences is based on a linear match of the temporal dimensions of the two sequences. This represents a substantial drawback as the metrics fail to take into account that similar patterns may vary in terms of speed, length and scale. Therefore, this provides the motivation to look for preprocessing feature extraction techniques that can extract translation and scale invariant features that capture information about the intrinsic trends in the data.

However, recent works have shown that there exists time series domains where the use of conventional methods can still achieve accurate results. Korn in his paper [12] has shown that for time series sequences that share the same **speed** and **length**, the conventional methods can achieve good clustering/classification performance. If intra class sequences have the same speed i.e no time offsets then they will also share the same time localised trends(see figure 6.1). Applying SVD as a preprocessing step, results in the extraction of latent factors that represent the localised patterns in time. Through mapping the time series sequences into the latent space, we can therefore construct a simplified representation of the data which allows conventional methods such as the euclidean metric to cluster time sequences with lesser run time.

To see how SVD accomplishes this feat, lets consider the following toy example:

Let X be a matrix where rows correspond to customers, columns correspond to days and the values are the dollar amounts spent on phone each day.

X =	customer	wed	thurs	frid	sat	sun
	A	1	1	1	0	0
	B	2	2	2	0	0
	C	1	1	1	0	0
	D	5	5	5	0	0
	E	0	0	0	2	2
	F	0	0	0	3	3
	G	0	0	0	1	1

Observation

- There are only distinct time localised trends. From this we can infer that there are two groups of customers: one group makes calls only during week days while the other group makes calls only during weekends.

Using SVD to factorize the matrix gives:

$$X = U \times D \times V^T$$

$$X = \begin{pmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{pmatrix} \times \begin{pmatrix} 9.64 & 0 \\ 0 & 5.29 \end{pmatrix} \times \begin{pmatrix} 0.58 & 0 \\ 0.58 & 0 \\ 0.58 & 0 \\ 0 & 0.71 \\ 0 & 0.71 \end{pmatrix}^T$$

Note: The columns in the orthogonal matrix V that are the eigenvectors of the zero singular values in the diagonal matrix have been omitted. Omitting these column vectors results in no loss of information.

Key observations

- The rank of the matrix X is 2. This shows that there are effectively two groups of customers: weekday(business) and weekend(residential) callers.
- The U matrix can be thought of as a customer to pattern similarity matrix. The first column vector of U corresponds to the weekday customers while the second column vector represents the weekend customers
- The V matrix can be thought of as day to pattern similarity matrix. In the case of days, there are two patterns: the weekday pattern i.e. {Wed,Thurs,Frid} and the weekend pattern {Sat,Sun}

For SVD to be applied successfully across all time series datasets, there are two fundamental issues that must be addressed:

1. Time complexity: The time complexity of SVD is $O(D^3)$ where D represents the dimensionality of the data. For domains where the dimensionality of the data is really high, applying SVD as a preprocessing step increases the run time of a clustering/classification algorithm.
2. Variable dimensionality: SVD cannot be directly applied to datasets where the individual data points do not share the same dimensionality. This issue is specially seen in time series data sets such as speech. The acoustics samples in such data sets vary in length.

To address the above issues and the drawbacks associated with performing nearest neighbours classification on time series sequences, in the following three sections, I investigate :

- i methods to improve the time complexity of SVD in handling high dimensional sequences when the size of the data set is very small.
- ii preprocessing methods that can be used along side the SVD feature extraction scheme to boost the accuracy of the classifier
- iii techniques to adapt SVD in handling time series sequences of variable length

6.2 Improving Time Complexity

For data sets where N (the number of samples) $\ll D$ (dimensionality of the data), Bishop [23] offers the following solution that reduces the time complexity

of computing SVD from $O(D^3)$ to $O(N^3)$:

Let X be the constructed D by N data matrix where D is the number dimensions and N is the number of samples and $D \ll N$. By factorizing X , we get $X = U \times D \times V^T$. To achieve dimensionality reduction, we need to consider only the subset of columns vectors of V that are associated with the non-zero singular values. Since $N \ll D$, there will at most $N-1$ of these singular values. As stated earlier, the columns of the V are the eigenvectors of the covariance matrix XX^T .

The eigen-decomposition of the covariance matrix is $XX^T u_i = \lambda_i u_i$. XX^T is D by D matrix and the computational complexity of computing the eigenvectors is $O(D^3)$.

Now if we multiply both sides by X^T we get :

$$(X^T X) X^T u_i = \lambda_i X^T u_i$$

Setting $v_i = X^T u_i$ gives us the eigenvectors of $X^T X$.

From the above expression, it can be observed that the eigenvectors of $X^T X$ and XX^T share the **same** eigenvalues. Using this insight, we can thus solve the eigenvector problem in spaces of lower dimensionality with computational cost $O(N^3)$ instead of $O(D^3)$. The required eigenvectors of the covariance matrix can then be computed by the using the following expression:

$$u_i = \frac{1}{\lambda_i^{(1/2)}} X v_i$$

To verify the above approach, I have conducted the following experiment :

Objective : The experiment is designed to verify whether applying SVD as a preprocessing step can improve the run time of 1 nearest neighbour classifier on time series data sets, without affecting its accuracy.

Data sets used : InLineSkate and Cinc_ECG_TORSO.

Unlike the speech corpus, the intra class variance of the time series sequences in the UCR data sets are much lower. This is primarily due to the fact that sequences of the same class can be described by the same time-localised trends. Figure 6.1 shows examples of two sequences belonging to class '1' in the Cinc_ECG_TORSO data set. Apart from having the same shape, the two sequences also possess the same speed i.e they have no time offset. From figure 6.1, it can be seen that at around $t=600$, both patterns undergo a dip followed by a sharp peak. The fact that all sequences in the data set share the same length and intra class sequences have no time offset allow classification algorithms to treat the problem as a normal classification problem. This also provides the context to apply SVD directly to achieve dimensionality reduction. For

this experiment, SVD has been applied to extract all the eigenvectors of the covariance matrix that corresponds to non-zero singular values. Since the number of samples \ll the length of the sequences, the size of the latent space will be smaller than the original input space leading to dimensionality reduction without any loss of information.

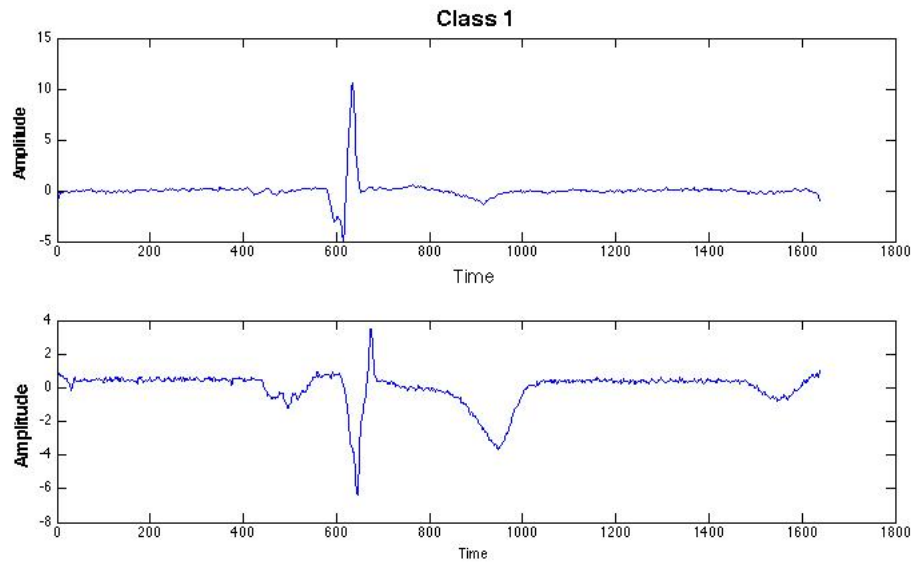


Figure 6.1: Time series sequences corresponding to class '1' in the Cinc_TORSO_ECG data set

Results:

	raw features	latent features
Cinc_ECG_TORSO	89.71	89.71
InlineSkate	34.18	34.18

Table 6.1: Accuracy

	raw features	latent features
Cinc_ECG_TORSO	0.24	0.72
InlineSkate	0.21	0.92

Table 6.2: Run times in seconds

Observations

- The accuracy of the 1 nearest classifier in both cases is consistent with the 1NN error rate given for each of the data sets in the UCR data source webpage.
- Applying SVD as a preprocessing step has no effect on the accuracy on the algorithm but reduces the run time of the classifier. Thus using Bishop's[23] formulation, we can use SVD to reduce the time complexity of clustering/classification algorithms for high dimensional time series data sets that satisfy the constraint identified by Korn[12].

Chapter 7

Improving 1 nearest neighbour classifier

In the last chapter, we have seen that the 1 nearest neighbour classifier using single value decomposition achieves good performance in both accuracy and run time in classifying sequences belonging to the Cinc_ECG_TORSO. The Cinc_ECG_TORSO is a rare example of a time series data set where there is no translation offset between sequences of the same class and intra class sequences share the same time localised local and global trends(see figure 6.1). This allows sequences to be classified/clustered based only on a linear match of their temporal dimensions.

For most time series data sets however, clustering/classifying sequences based only on linear matches of the temporal dimensions of sequences presents a limitation. The intra class variances in most time series datasets will be much higher as sequences of the same class may vary in size, shape and speed. The InlineSkate dataset is a prime example of such a dataset. Figure 6.2 shows examples of two instances of class 2 in the InlineSkate dataset. The two instances of class '2' share a global shape but possess different time localised trends: in the period between $t = 400$ to 600 , the first sequence is experiencing an upward trend while the second sequence is seen to experience a downward trend. Performing comparison by conducting only a linear match of the temporal dimensions is inappropriate in such cases as they increase the degree of dissimilarity between similar patterns. This creates the motivation to investigate feature extraction methodologies that minimise the intra class variance of time series sequences by mapping the data to a feature space that captures information about common their attributes such as global shape, trends etc. Through the construction of a such discrete feature set, the time series classification problem can then be converted to a general classification problem.

In the following chapter, I will be concentrating on constructing feature extrac-

tion techniques that capture information about the **global shape** of time series sequences. In the first half of this chapter, I will be exploring wavelet-based feature extraction techniques and will subsequently look into how they can be used alongside SVD as preprocessing step to improve the accuracy of the 1nearest neighbour classifier.

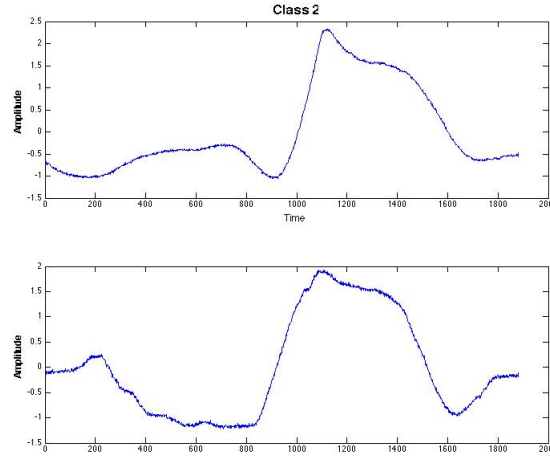


Figure 7.1: Time series sequences corresponding to class ‘2’ in the InlineSkate data set

7.1 Wavelet-based Feature Extraction

The inspiration for the wavelet transform came from the idea of multiresolution analysis. A multiresolution analysis decomposes a signal into a smoothed version of the original signal and a set of detail information at different scales. This type of decomposition is most easily understood by thinking of a picture (can be thought of as a two dimensional signal) and removing from the picture information that distinguishes the sharpest edges, leaving a new image that is slightly blurred. This blurred version of the original picture is a rendering at a slightly coarser scale. We then recursively repeat the procedure. The wavelet transform specifies such a multiresolution decomposition, with the wavelet functions defining the bandpass filter that determines the detail information. and associated with each wavelet is a smoothing function, which defines the complementary lowpass filter.

Mathematically, we can motivate the definition of the wavelet transform as follows:

Let $L^2(R)$ be the set of all functions with finite energy. Any discrete function(signal) $f \in L^2(R)$, can be written as a linear combination of translations of the scaling function $\phi(st)$ as shown below:

$f(t) = \sum_{n=0}^N \alpha_n \phi(st - n)$ where $\phi(st)$ is defined as :

$$\phi(st) = \begin{cases} 1 & \text{if } 0 \leq st < 1 \\ 0 & \text{otherwise} \end{cases}$$

Under this representation, the following facts hold.

- i The scaling function is orthogonal to its integer translates.
- ii As we increase the scale, the support of the function decreases.
- iii The subspaces spanned by the scaling function at low scales are nested within those spanned at higher scales. For example if restrict s to powers of 2 then: $\phi_{-1}(t) = \phi(2^{-1}t) = \phi_0(t) + \phi_0(t - 1)$.

Before proceeding any further, it is necessary to define the concept of the wavelet. A wavelet is a smooth and quickly oscillating function with good localisation in both frequency and time. To perform wavelet transformation the Haar function is commonly chosen as the mother wavelet ψ . At the any scale s , the function $\psi(st)$ is orthogonal to the scalar function $\phi(st)$ but can be expressed in terms of $\phi(s't)$ where $s' > s$. Using this knowledge combined with (iii), the wavelet transformation can be applied to decompose a finite signal by projecting f onto two orthogonal subspaces W_1 and V_1 of $L^2(R)$ where $L^2(R) = V_1 \oplus W_1$. If $f(t) = \sum_{n=0}^N \alpha_n \phi(st - n)$ then W_1 is spanned by the translations of Haar function $(s't)$ V_1 is spanned by the translations of scaling function $\phi(s't)$ where s' is.

The process is recursive. After removing the first set of detail information from f we are left with a slightly smoothed version of f . We iteratively remove detail information by applying the transform on the smoothed versions at each scale to progressively extract coarser details of f . We stop the process once we have enough detail information or a smooth enough version to do the analysis we desire. The details of f at any scale m is a projection of f onto the subspace W_m . The projection is represented by the map $Q_m : L^2(R) \rightarrow W_m$ where $Q_m f = \sum_{n=1}^K \psi_{Mn}$. Thus P_m is spanned by $\{\phi_{Mn}\}$. Hence the subspace W_m at different scale are spanned by dilations and translations of the mother wavelet.

Note :To ensure that $\{\psi_{Mn}\}$ forms an orthogonal basis, the scales are restricted to powers of 2.

Furthermore there exists another operator P_m that maps f to its approximation at scale m i.e $P_m : L^2(R) \rightarrow V_m \subseteq L^2(R)$. The functional space $L^2(R)$ is therefore

Therefore, the signal f can be now be expressed as :

$$f(t) = \sum_{n=0}^N \alpha_n \phi(t - n) = P_m f + \sum_{m=1} Q_m f$$

The broad trend is preserved in the approximation part while the localised changes are kept in the detail part, The original signal can fully be reconstructed
Mathematical definition:

Let $L^2(R)$ be the set of all functions with finite energy

The details of f at any scale \mathbf{m} is a projection of f onto the subspace W_m .
The projection can be represented by the map $Q_m : L^2(R) \rightarrow W_m$. Furthermore there exists another operator P_M that maps f to its approximation at scale m i.e $P_M : L^2(R) \rightarrow V_M \subseteq L^2(R)$

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