A Wavelet-Based Anytime Algorithm for K-Means Clustering of Time Series

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ABSTRACT

The emergence of the field of data mining in the last decade has sparked an increasing interest in clustering of time series. Although there has been much research on clustering in general, most classic machine learning and data mining algorithms do not work well for time series due to their unique structure. In particular, the high dimensionality, very high feature correlation, and the (typically) large amount of noise that characterize time series data present a difficult challenge. In this work we address these challenges by introducing a novel anytime version of k-Means clustering algorithm for time series. The algorithm works by leveraging off the multi-resolution property of wavelets. In particular, an initial clustering is performed with a very coarse resolution representation of the data. The results obtained from this "quick and dirty" clustering are used to initialize a clustering at a slightly finer level of approximation. This process is repeated until the clustering results stabilize or until the "approximation" is the raw data. In addition to casting k-Means as an anytime algorithm, our approach has two other very unintuitive properties. The quality of the clustering is often better than the batch algorithm, and even if the algorithm is run to completion, the time taken is typically much less than the time taken by the original algorithm. We explain, and empirically demonstrate these surprising and desirable properties with comprehensive experiments on several publicly available real data sets.

Keywords
Time Series, Data Mining, Clustering, Anytime Algorithms

1. INTRODUCTION

The emergence of the field of data mining in the last decade has sparked an increase of interest in clustering of time series [12, 16, 20, 21, 22, 33]. Such clustering is useful in its own right as a method to summarize and visualize massive datasets [34]. In addition, clustering is often used as a subroutine in other data mining algorithms such as similarity search [26, 30], classification [22] and the discovery of association rules [9]. Applications of these algorithms cover a wide range of activities found in finance, meteorology, industry, medicine etc.

Although there has been much research on clustering in general [5], the unique structure of time series means that most classic machine learning and data mining algorithms do not work well for time series. In particular, the high dimensionality, very high feature correlation, and the (typically) large amount of noise that characterize time series data present a difficult challenge [21].

In this work we address these challenges by introducing a novel anytime version of the popular k-Means clustering algorithm [15, 27] for time series. Anytime algorithms are algorithms that trade execution time for quality of results [19]. Their utility for data mining has been documented at length elsewhere [5, 31].

The algorithm works by leveraging off the multi-resolution property of wavelets [11]. In particular, an initial clustering is performed with a very coarse representation of the data. The results obtained from this "quick and dirty" clustering are used to initialize a clustering at a finer level of approximation. This process is repeated until the clustering results

stabilize or until the "approximation" *is* the original "raw" data. The clustering is said to stabilize when the objects do not change membership from the last iteration, or when the change of membership does not improve the clustering results. Our approach allows the user to interrupt and terminate the process at any level. In addition to casting the k-Means algorithm as an anytime algorithm, our approach has two other very unintuitive properties. The quality of the clustering is often better than the batch algorithm, and even if the algorithm is run to completion, the time taken is typically much less than the time taken by the batch algorithm. We explain, and empirically demonstrate these surprising and desirable properties with comprehensive experiments on several publicly available real data sets.

The rest of this paper is organized as follows. In Section 2 we review related work, and introduce the necessary background on the wavelet transform and k-Means clustering. In Section 3, we introduce our algorithm. Section 4 contains a comprehensive comparison of our algorithm to classic k-Means on real datasets. In Section 5 we summarize our findings and offer suggestions for future work.

2. BACKGROUND AND RELATED WORK

Since our work draws on the confluence of clustering, wavelets and anytime algorithms, we provide the necessary background on these areas in this section.

2.1 Background on Clustering

One of the most widely used clustering approaches is hierarchical clustering, due to the great visualization power it offers [22]. Hierarchical clustering produces a nested hierarchy of similar groups of objects, according to a pairwise distance matrix of the objects. One of the advantages of this method is its generality, since the user does not need to provide any parameters such as the number of clusters. However, its application is limited to only small datasets, due to its quadratic (or higher order) computational complexity.

A faster method to perform clustering is k-Means [5, 27]. The basic intuition behind k-Means (and a more general class of clustering algorithms known as iterative refinement algorithms) is shown in Table 1:

Algorithm *k-Means*	
1.	Decide on a value for *k*.
2.	Initialize the *k* cluster centers (randomly, if necessary).
3.	Decide the class memberships of the *N* objects by assigning them to the nearest cluster center.
4.	Re-estimate the *k* cluster centers, by assuming the memberships found above are correct.
5.	If none of the *N* objects changed membership in the last iteration, exit. Otherwise goto 3.

Table 1: An outline of the k-Means algorithm.

The *k-Means* algorithm for *N* objects has a complexity of O(*kNrD*) [27], with *k* the number of clusters specified by the user, *r* the number of iterations until convergence, and *D* the dimensionality of the points. The shortcomings of the algorithm are its tendency to favor spherical clusters, and the fact that the knowledge on the number of clusters, *k*, is required in advance. The latter limitation can be mitigated by placing the algorithm in a loop, and attempting all values of *k* within a large range. Various statistical tests can then be used to determine which value of *k* is most parsimonious. Since k-Means is essentiality a hill-climbing algorithm, it is guaranteed to converge on a local but not necessarily global optimum. In other words, the choices of the initial centers are critical to the quality of results. Nevertheless, in spite of these undesirable properties, for clustering large datasets of time-series, k-Means is preferable due to its faster running time.

In order to scale the various clustering methods to massive datasets, one can either reduce the number of objects, *N*, by sampling [5], or reduce the dimensionality of the objects [1, 6, 14, 25, 29, 35, 36, 22, 23]. In the case of time-series, the objective is to find a representation at a lower dimensionality that preserves the original information and describes the original shape of the time-series data as closely as possible. Many approaches have been suggested in the literature, including the Discrete Fourier Transform (DFT) [1, 14], Singular Value Decomposition [25], Adaptive Piecewise Constant Approximation [23], Piecewise Aggregate Approximation (PAA) [7, 36], Piecewise Linear Approximation [22] and the Discrete Wavelet

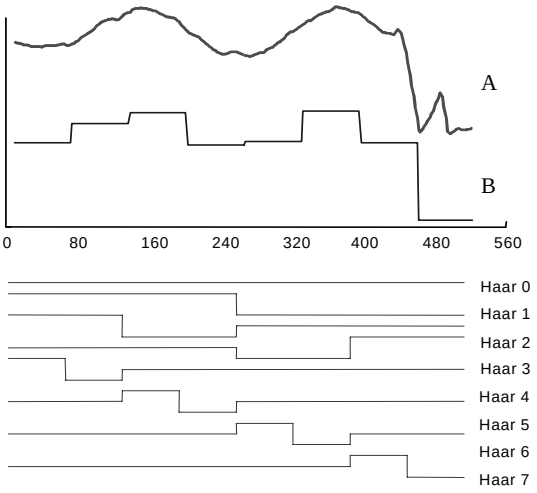

Figure 1: The Haar Wavelet representation can be visualized as an attempt to approximate a time series with a linear combination of basis functions. In this case, time series A is transformed to B by Haar wavelet decomposition, and the dimensionality is reduced from 512 to 8.

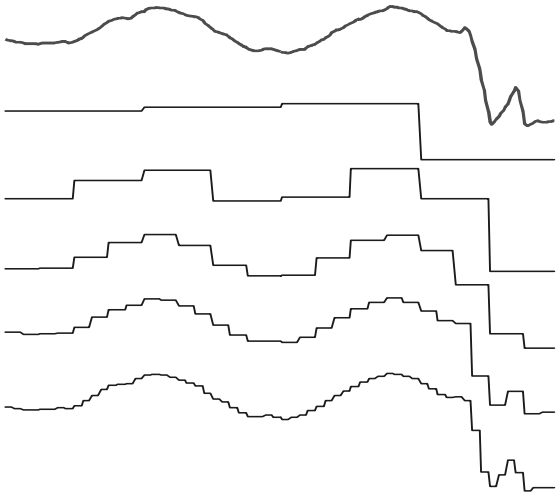

Figure 2: The Haar Wavelet can represent data at different levels of resolution. Above we see a raw time series, with increasingly finer wavelet approximations below.

Transform (DWT) [6, 29]. While all these approaches have shared the ability to produce a high quality reduced-dimensionality approximation of time series, wavelets are unique in that their representation of data is intrinsically multi-resolution. This property is critical to our proposed algorithm and will be discussed in detail in the next section.

Although we choose the Haar wavelet for this work, the algorithm can generally utilize any wavelet basis. The preference for the Haar wavelet is mainly based on its simplicity and its wide usage in the data mining community.

2.2 Background on Wavelets

Wavelets are mathematical functions that represent data or other functions in terms of the averages and differences of a prototype function, called the analyzing or mother wavelet [11]. In this sense, they are similar to the Fourier transform. One fundamental difference is that wavelets are localized in time. In other words, some of the wavelet coefficients represent small, local subsections of the data being studied, as opposed to Fourier coefficients, which always represent global contributions to the data. This property is very useful for multi-resolution analysis of data. The first few coefficients contain an overall, coarse approximation of the data; additional coefficients can be perceived as "zooming-in" to areas of high detail. Figure 1 and 2 illustrate this idea.

The Haar Wavelet decomposition works by averaging two adjacent values on the time series function at a given resolution to form a smoothed, lower-dimensional signal, and the resulting coefficients are simply the differences between the values and their averages [6]. The coefficients can also be computed by averaging the differences between each pair of adjacent values. The coefficients are crucial for reconstructing the original sequence, as they store the detailed information lost in the smoothed signal. For example, suppose we have a time series data T = (2 8 1 5 9 7 2 6). Table 2 shows the decomposition at different resolutions. As a result, the Haar wavelet decomposition is the collection of the coefficients at all resolutions, with the overall average being its first component: (5 –1 1 2 –3 –2 1 –2). It is clear to see that the decomposition is completely reversible and the original sequence can be reconstructed from the coefficients. For example, to get the signal of the second level, we compute $5 \pm (-1) = (4, 6)$.

Resolution	Averages	Differences (coefficients)
8	(2 8 1 5 9 7 2 6)	
4	(5 3 8 4)	(-3 –2 1 –2)
2	(4 6)	(1 2)
1	5	-1

Table 2. Haar Wavelet Decomposition on time series (2 8 1 5 9 7 2 6)

Recently there has been an explosion of interest in using wavelets for time series data mining. Researchers have introduced several non-Euclidean, wavelet-based distance measures [20, 33]. Chan and Fu [6] have demonstrated that Euclidean distance indexing with wavelets is competitive to Fourier-based techniques [14].

2.3 Background on Anytime Algorithms

Anytime algorithms are algorithms that trade execution time for quality of results [19]. In particular, an anytime algorithm always has a best-so-far answer available, and the quality of the answer improves with execution time. The user may examine this answer at any time, and choose to terminate the algorithm, temporarily suspend the algorithm, or allow the algorithm to run to completion.

The usefulness of anytime algorithms for data mining has been extensively documented [5, 31]. Suppose a batch version of an algorithm takes a week to run (not an implausible scenario in data mining massive data sets). It would be highly desirable to implement the algorithm as an anytime algorithm. This would allow a user to examine the best current answer after an hour or so as a "sanity check" of all assumptions and parameters. As a simple example, suppose the user had accidentally set the value of K to 50 instead of the desired value of 5. Using a batch algorithm the mistake would not be noted for a week, whereas using an anytime algorithm the mistake could be noted early on and the algorithm restarted with little cost.

The motivating example above could have been eliminated by user diligence! More generally, however, data mining algorithms do require the user to make choices of several parameters, and an anytime implementation of *k-Means* would allow the user to interact with the entire data mining process in a more efficient way.

2.4 Related Work

Bradley et. al. [5] suggest a generic technique for scaling the *k-Means* clustering algorithms to large databases by attempting to identify regions of the data that are compressible, that must be retained in main memory, and regions that may be discarded. However, the generality of the method contrasts with our algorithm's explicit exploitation of the structure of the data type of interest.

Our work is more similar in spirit to the dynamic time warping similarity search technique introduced by Chu et. al. [7]. The authors speed up linear search by examining the time series at increasingly finer levels of approximation.

3. OUR APPROACH – THE I-kMEANS ALGORITHM

As noted in Section 2.1, the complexity of the k-Means algorithm is *O(kNrD)*, where *D* is the dimensionality of data points (or the length of a sequence, as in the case of time-series). For a dataset consisting of long time-series, the *D* factor can burden the clustering task significantly. This overhead can be alleviated by reducing the data dimensionality.

Another major drawback of the k-Means algorithm derives from the fact that the clustering quality is greatly dependant on the choice of initial centers (i.e., line 2 of Table 1). As mentioned earlier, the k-Means algorithm guarantees local, but not necessarily global optimization. Poor choices of the initial centers, therefore, can degrade the quality of clustering solution and result in longer execution time (See [15] for an excellent discussion of this issue). Our algorithm addresses these two problems associated with k-Means, in addition to offering the capability of an anytime algorithm, which allows the user to interrupt and terminate the program at any stage.

We propose using the wavelet decomposition to perform clustering at increasingly finer levels of the decomposition, while displaying the gradually refined clustering results periodically to the user.

We compute the Haar Wavelet decomposition for all time-series data in the database. The complexity of this transformation is linear to the dimensionality of each object; therefore, the running time is reasonable even for large databases. The process of decomposition can be performed off-line, and the time series data can be stored in the Haar decomposition format, which takes the same amount of space as the original sequence. One important property of the decomposition is that it is a lossless transformation, since the original sequence can always be reconstructed from the decomposition.

Once we compute the Haar decomposition, we perform the k-Means clustering algorithm, starting at the second level (each object at level i has $2^{(i-1)}$ dimensions) and gradually progress to finer levels. Since the Haar decomposition is completely reversible, we can reconstruct the approximation data from the coefficients at any level and perform clustering on these data. We call the new clustering algorithm ***I-kMeans***, where *I* stands for "interactive." Figure 3 illustrates this idea.

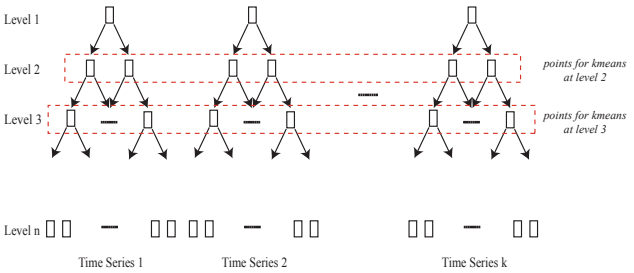

Figure 3. k-Means is performed on each level on the reconstructed data from the Haar wavelet decomposition, starting with the second level.

The intuition behind this algorithm originates from the observation that the general shape of a time series sequence can often be approximately captured at a lower resolution. As shown in Figure 2, the shape of the time series is well preserved, even at very coarse approximations. Because of this desirable feature of wavelets, clustering results typically stabilize at a low resolution, thus saving time by eliminating the need to run at full resolution (the raw data). The pseudo-code of the algorithm is provided in Table 3.

The algorithm achieves the speed-up by doing the vast majority of reassignments (Line 3 in Table 1), at the lower resolutions, where the costs of distance calculations are considerably lower. As we gradually progress to finer resolutions, we already start with good initial centers (the choices of initial centers will be discussed later in this section). Therefore, the number of iterations r until convergence will typically be much lower.

The I-kMeans algorithm allows the user to monitor the quality of clustering results as the program executes. The user can interrupt the program at any level, or wait until the execution terminates once the clustering results stabilize. One surprising and highly desirable finding from the experimental results (as shown in the next section), is that even if the program is run to completion (until the last level, with full resolution), the total execution time is generally less than that of clustering on raw data.

Algorithm I-*k*Means	
1.	Decide on a value for *k*.
2.	Initialize the *k* cluster centers (randomly, if necessary).
3.	Run the *k*-Means algorithm on the $level_i$ representation of the data
4.	Use final centers from $level_i$ as initial centers for $level_{i+1}$. This is achieved by projecting the k centers returned by *k*-Means algorithm for the 2^i space in the 2^{i+1} space.
5.	If none of the *N* objects changed membership in the last iteration, exit. Otherwise goto 3.

Table 3: An outline of the I-kMeans algorithm.

As mentioned earlier, on every level except for the starting level (i.e. level 2), which uses random initial centers, the initial centers are selected based on the final centers from the previous level. More specifically, the final centers computed at the end of level i will be used as the initial centers on level $i+1$. Since the length of the data reconstructed from the Haar decomposition doubles as we progress to the next level, we project the centers computed at the end of level i onto level $i+1$ by doubling each coordinate of the centers. This way, they match the dimensionality of the points on level $i+1$. For example, if one of the final centers at the end of level 2 is (0.5, 1.2), then the initial center used for this cluster on level 3 is (0.5, 0.5, 1.2, 1.2). This

approach resolves the dilemma associated with the choice of initial centers, which is crucial to the quality of clustering results [15]. It also contributes to the fact that our algorithm often produces better clustering results than the k-Means algorithm.

4. EXPERIMENTAL EVALUATION

To show that our approach is superior to the k-Means algorithm for clustering time series, we performed a series of experiments on publicly available real datasets. For completeness, we ran the I-kMeans algorithm for all levels of approximation, and recorded the cumulative execution time and clustering accuracy at each level. In reality, however, the algorithm stabilizes in early stages and can automatically terminate much sooner. We compare the results with that of k-Means on the original data. Since both algorithms start with random initial centers, we execute each algorithm 100 times with different centers. However, for consistency we ensure that for each execution, both algorithms are seeded with the same set of initial centers. After each execution, we compute the error (more details will be provided in Section 4.2) and the execution time on the clustering results. We compute and report the averages at the end of each experiment. We believe that by taking the average, we achieve better objectiveness than taking the best (minimum), since in reality, we would not have the knowledge of the correct clustering results, or the "oracle," to compare against our results (as the case with one of our test datasets).

4.1 Datasets and Methodology

We tested on two publicly available, real datasets. The dataset cardinalities range from 1,000 to 8,000. The length of each time series has been set to 512 on one dataset, and 1024 on the other. Each time series is z-normalized to have mean value of 0 and standard deviation of 1.

• **JPL:** This dataset consists of readings from various inertial sensors from Space Shuttle mission STS-57. The data is particularly appropriate for our experiments since the use of redundant backup sensors means that some of the data is very highly correlated. In addition, even sensors that measure orthogonal features (i.e. the X and Y axis) may become temporarily correlated during a particular maneuver; for example, a "roll reversal" [13]. Thus, the data has an interesting mixture of dense and sparse clusters. To generate datasets of increasingly larger cardinalities, we extracted time series of length 512, at random starting points of each sequence from the original data pool.

• **Heterogeneous:** This dataset is generated from a mixture of 10 real time series data from the UCR Time Series Data Mining Archive [24]. Figure 4 shows how the data is generated, and figure 5 shows the 10 time-series we use as seeds. We produced variations of the original patterns by adding small time warping (2-3% of the series length), and interpolated Gaussian noise. Gaussian noisy peaks are interpolated using splines to create smooth random variations.

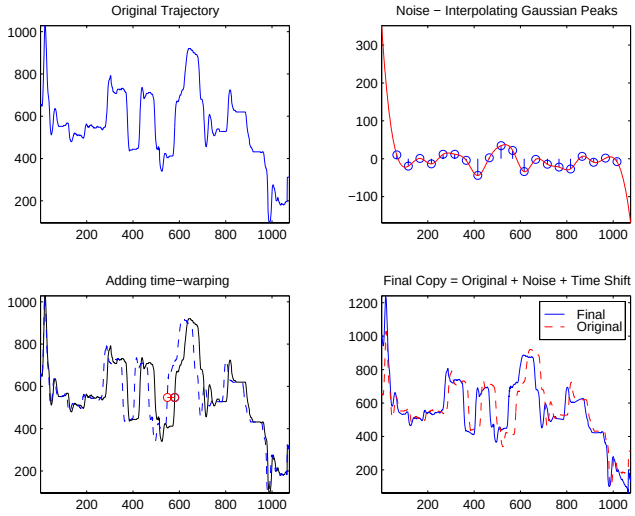

Figure 4: Generation of variations on the heterogeneous data. We produced variations of the original patterns by adding small time warping (2-3% of the series length), and interpolated Gaussian noise. Gaussian noisy peaks are interpolated using splines to create smooth random variations.

In the Heterogeneous dataset, we know that the number of clusters (*k*) is 10. However, for the JPL dataset, we lack this information. Finding k is an open problem for the k-Means algorithm and is out of scope of this paper. To determine the optimal *k* for k-Means, we attempt different values of *k*, ranging from 2 to 8. Nonetheless, our algorithm out-performs the k-Means algorithm regardless of *k*. In this paper we only show the results with *k* equals to 5. Figure 6 shows that our algorithm produces the same results as does the hierarchical clustering algorithm, which is generally more costly.

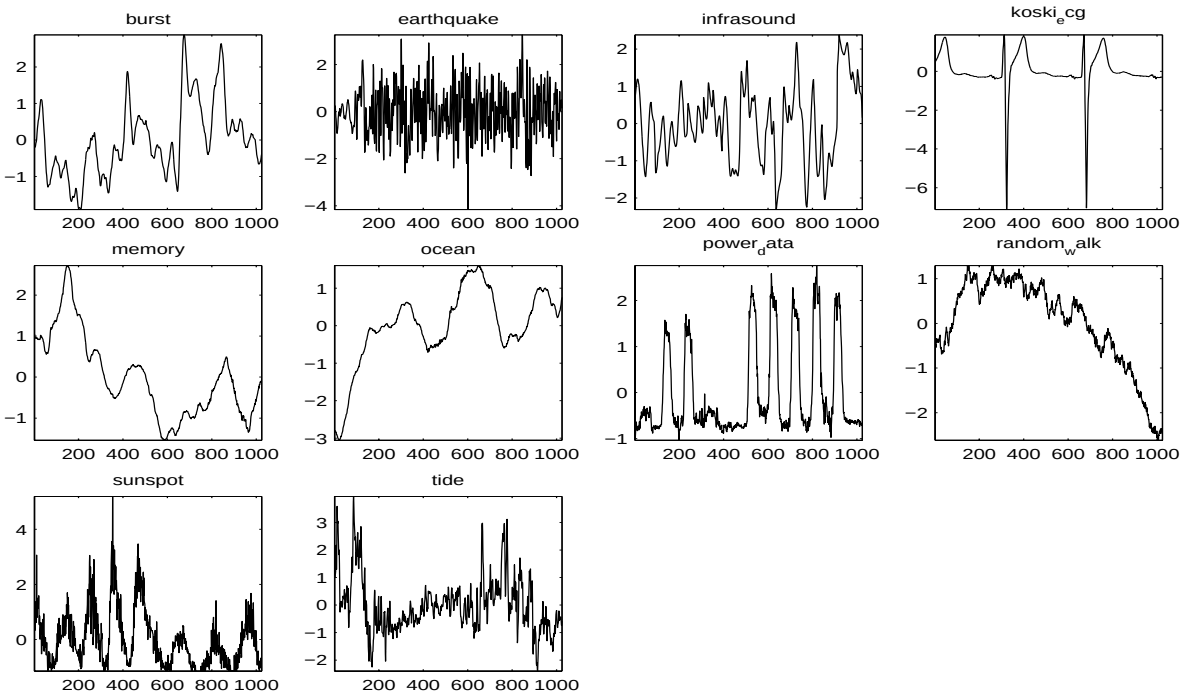

Figure 5: Real time series data from UCR Time Series Data Mining Archive. We use these time series as seeds to create our Heterogeneous dataset.

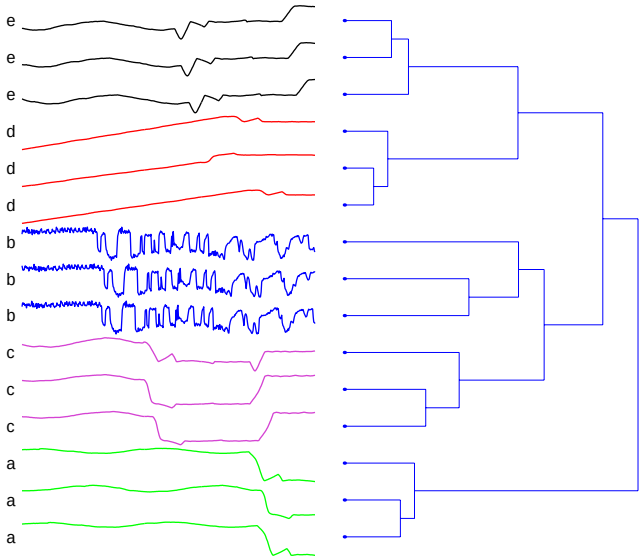

Figure 6: On the left-hand side, we show three instances from each cluster discovered by the I-kMeans algorithm. We can visually verify that our algorithm produces intuitive results. On the right-hand side, we show that hierarchical clustering (using average linkage) discovers the exact same clusters. However, hierarchical clustering is more costly than our algorithm.

4.2 Error of Clustering Results

In this section we compare the clustering quality for the I-kMeans and the classic k-Means algorithm.

Since we generated the heterogeneous datasets from a set of given time series data, we have the knowledge of correct clustering results in advance. In this case, we can simply compute the clustering error by summing up the number of incorrectly classified objects for each cluster *c* and then dividing by the dataset cardinality.

$$\text{clustering error} = \frac{\sum_{c=1}^{k} misclassified_c}{|data|} \qquad (1)$$

The error is computed at the end of each level. The label of each final cluster is assigned according to the majority of objects that originally belonged to the same cluster. For example, if a final cluster consists of 490 objects from cluster A and 10 objects from cluster B, the latter objects are going to be considered misclassified. However, we would like to

emphasize that in reality, the correct clustering results would not be available in advance. The incorporation of such known results in our error calculation merely serves the purpose of demonstrating the quality of both algorithms.

For the JPL dataset, we do not have prior knowledge of correct clustering results (which conforms more closely to real-life cases). Lacking this information, we cannot use the above formula to determine the error.

Since the k-Means algorithm seeks to optimize the objective function by minimizing the sum of squared intra-cluster errors, we evaluate the quality of clustering by using the objective functions. However, since the I-kMeans algorithm involves data with smaller dimensionality except for the last level, we have to compute the objective functions on the raw data, in order to compare with the k-Means algorithm. We show that the objective functions obtained from the I-kMeans algorithm are better than those from the k-Means algorithm. The results are consistent with the work of [8], in which the authors show that dimensionality reduction reduces the chances of the algorithm being trapped in a local minimum. Furthermore, even with the additional step of computing the objective functions from the original data, the I-kMeans algorithm still takes less time to execute than the k-Means algorithm.

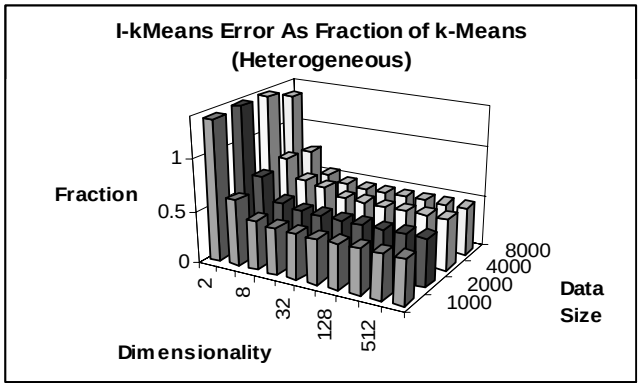

Figure 7: Error of I-kMeans algorithm on the Heterogeneous dataset, presented as fraction of the error from the k-Means algorithm. Our algorithm results in smaller error than the k-Means after the second stage (i.e. 4 dimensions), and stabilizes typically after the third stage (i.e. 8 dimensions).

In figures 7 and 8, we show the errors/objective functions from the I-kMeans algorithm as a fraction of those obtained from the k-Means algorithm. As we can see from the plots, our algorithm stabilizes at early stages and consistently results in smaller error than the classis k-Means algorithm.

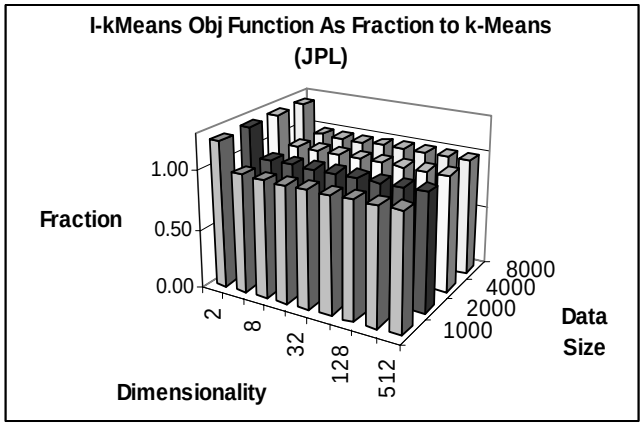

Figure 8: Objective functions of I-kMeans algorithm on the JPL dataset, presented as fraction of error from the k-Means algorithm. Again, our algorithm results in smaller objective functions (i.e. better clustering results) than the k-Means, and stabilizes typically after the second stage (i.e. 4 dimensions).

4.3 Running Time

In figures 9 and 10, we present the cumulative running time for each level on the I-kMeans algorithm as a fraction to the k-Means algorithm. The cumulative running time for any level i is the total running time from the starting level (level 2) to level i. In most cases, even if the I-kMeans algorithm is run to completion, the total running time is still less than that of the k-Means algorithm. We attribute this improvement to the good choices of initial centers for successive levels after the starting level, since they result in very few iterations until convergence. Nevertheless, we have already shown in the previous section that the I-kMeans algorithm finds the best result in relatively early stage and does not need to run through all levels.

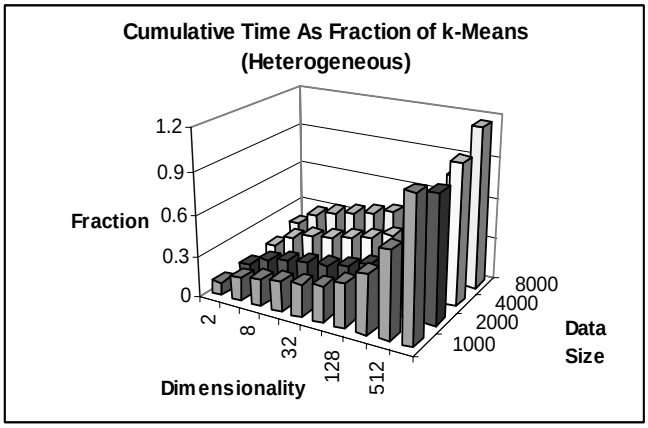

Figure 9: Cumulative running time for the Heterogeneous dataset. Our algorithm typically cuts the running time by half as it does not need to run through all levels to retrieve the best results.

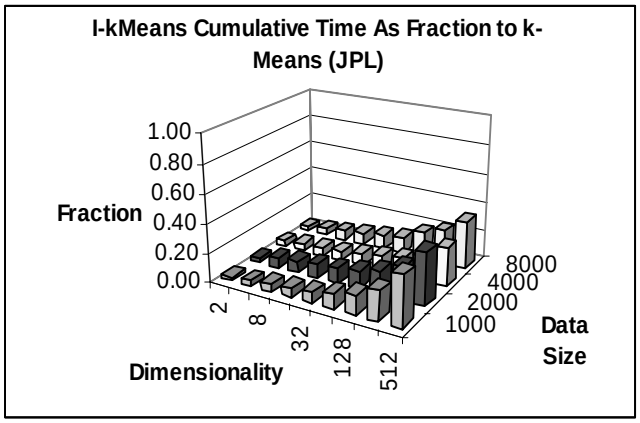

Figure 10: Cumulative running time for the JPL dataset. Our algorithm typically takes only 30% of time. Even if it is run to completion, the cumulative running time is still 50% less than that of the k-Means algorithm!

4.4 I-kMeans Algorithm vs. k-Means Algorithm

In this section (Fig. 11 and 12), rather than showing the error/objective function on each level, as in Section 4.2, we present only the error/objective function returned by the I-kMeans algorithm when it stabilizes or, in the case of JPL dataset, outperforms the k-Means algorithm in terms of the objective function. We also present the time taken for the I-kMeans algorithm to stabilize. We compare the results to those of the k-Means algorithm. From the figures we can observe that our algorithm achieves better clustering accuracy at significantly faster response time.

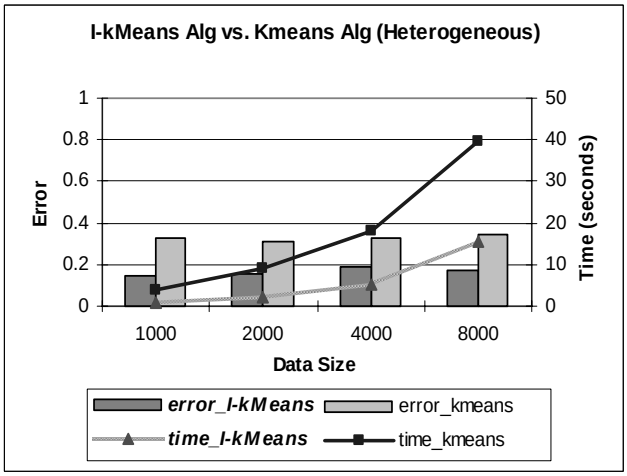

Figure 11: The I-kMeans algorithm is highly competitive with the k-Means algorithm. The errors and execution time are significantly smaller.

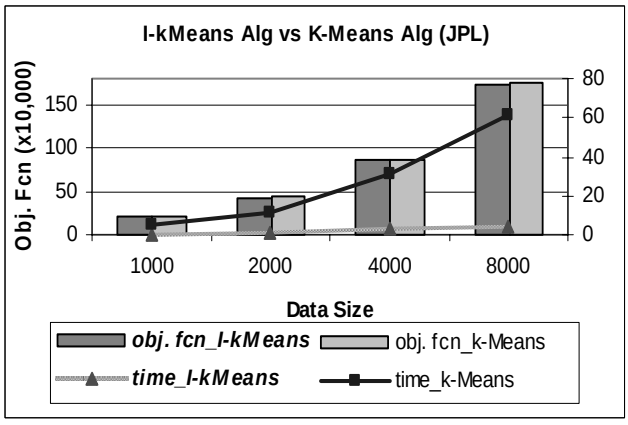

Figure 12: I-kMeans vs. k-Means algorithms in terms of objective function and running time for JPL dataset. Our algorithm outperforms the k-Means algorithm. The running time remains small for all data sizes because the algorithm terminates at very early stages.

Figure 13 shows the average level where the I-kMeans algorithm stabilizes or, in the case of JPL, outperforms the k-Means algorithm in terms of objective function. Since the length of the time series data is 1024 in the Heterogeneous dataset, there are 11 levels. Note that the JPL dataset has only 10 levels since the length of the time series data is only 512. We skip level 1, in which the data has only one dimension (the average of the time series) and is the same for all sequences, since the data has been normalized (zero mean). Each level i has $2^{(i-1)}$ dimensions. From the plot we can see that our algorithm generally stabilizes at levels 3-6 for the Heterogeneous dataset and at levels 2-4 for the JPL

dataset. In other words, the I-kMeans algorithm operates on data with a maximum dimensionality of 32 and 8, respectively, rather than 1024 and 512.

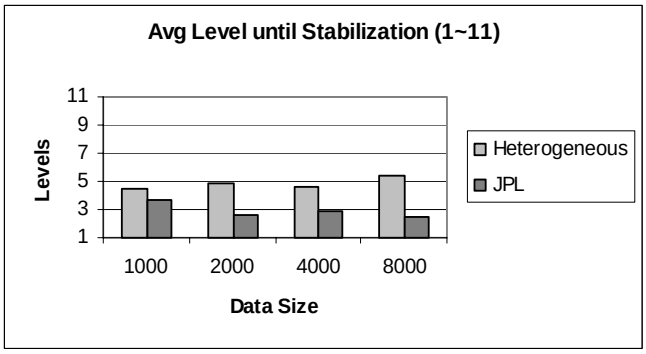

Figure 15: Average level until stabilization. The algorithm generally stabilizes between level 3 and level 6 for Heterogeneous dataset, and between level 2 and 4 for the JPL dataset. So it operates on data with a maximum dimensionality of 32 instead of 1024, and 8 instead of 512, respectively.

5. CONCLUSIONS AND FUTURE WORK

We have presented an approach to perform incremental clustering of time-series at various resolutions using the Haar wavelet transform. Using *k-Means* as our clustering algorithm, we reuse the final centers at the end of each resolution as the initial centers for the next level of resolution. This approach resolves the dilemma associated with the choices of initial centers for k-Means and significantly improves the execution time and clustering quality. Our experimental results indicate that this approach yields faster execution time than the traditional *k-Means* approach, in addition to improving the clustering quality of the algorithm. Since it conforms with the observation that time series data can be described with coarser resolutions while still preserving a general shape, the anytime algorithm stabilizes at very early stages, eliminating the needs to operate on high resolutions. In addition, the anytime algorithm allows the user to terminate the program at any stage.

In future work we plan to investigate the following:

- Extending our algorithm to other iterative refinement clustering techniques, especially the EM-algorithm.
- Extending our algorithm to other data types, for example, both histograms and images can be successfully represented with wavelets [11, 33].
- Examining the possibility of re-using the results (i.e. objective functions that determine the quality of clustering results) from the previous stages to eliminate the need to re-compute all the distances.
- Generalizing our approach to a broader class of algorithms and decompositions. For example, even though we have used the wavelet decomposition in this work, our algorithm can be easily generalized to Fourier coefficients as well.

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