Closing the Loop on a Complete Linkage Hierarchical Clustering Method

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Abstract: To develop a complete linkage hierarchical clustering method that 1) substantially improves upon the accuracy of the standard complete linkage method and 2) can be fully automated or used with minimal operator supervision, the assumptions underlying the standard complete linkage method are unwound, evaluating pairs of data points for linkage is decoupled from constructing cluster sets, and cluster sets are constructed *de novo*. These design choices make it possible to construct only the cluster sets that correspond to select, possibly non-contiguous levels of an $\frac{n\cdot(n-1)}{2}+1$-level hierarchical sequence. To construct meaningful cluster sets without constructing an entire hierarchical sequence, a means that uses distance graphs is used to find meaningful levels of such a hierarchical sequence. This paper presents an approach that mathematically captures the graphical relationships that are used to find meaningful levels and integrates the means into the new clustering method. The approach is inexpensive to implement. Consequently, the new clustering method is self-contained and incurs almost no extra cost to determine which cluster sets should be constructed and which should not. Empirical results from four experiments show that the approach does well at finding meaningful levels of hierarchical sequences.

1 INTRODUCTION

This paper presents the third part of a three-part research project and is a companion paper to Means for Finding Meaningful Levels of a Hierarchical Sequence *Prior* to Performing a Cluster Analysis (Olsen, 2014b). The goal of this project was to develop a general, simplistic, complete linkage hierarchical clustering method that 1) substantially improves upon the accuracy of the standard complete linkage method and 2) can be fully automated or used with minimal operator supervision. It was motivated by the need to bring machine learning, and complete linkage hierarchical clustering in particular, over from the "computational side of things ... to the system ID/model ID kind of thinking" (Gill, 2011) as part of closing the loop on cyber-physical systems.

For the first part of the project, a new, complete linkage hierarchical clustering method was developed. *See* (Olsen, 2014a). The new clustering method is consonant with the model for a measured value that scientists and engineers commonly use[1], so it substantially improves upon the accuracy of the standard complete linkage method. Further, it can construct cluster sets for select, possibly non-contiguous levels of an $\frac{n\cdot(n-1)}{2}+1$-level hierarchical sequence. The new clustering method was designed with small-n, large-m data sets in mind, where n is the number of data points, m is the number of dimensions, and "large" means thousands and upwards (Murtagh, 2009).[2]

Because the computational power presently exists to apply hierarchical clustering methods to much larger data sets than when the standard complete linkage method was developed, the new clustering method unwinds the assumptions that underlie the standard complete linkage method. However, by unwinding these assumptions and letting the size of a

[1]The model for a measured value is measured value = true value + bias (accuracy) + random error (statistical uncertainty or precision) (Navidi, 2006). This model has substantially broader applicability than the taxonomic model that is the basis for the standard complete linkage method.

[2]These data sets are used by many cyber-physical systems and includes time series. For example, a typical automobile has about 500 sensors; a small, specialty brewery has about 600 sensors; and a small power plant has about 1100 sensors. The new clustering method may accommodate large-n, large-m data sets as well, and future work includes using multicore and/or heterogeneous processors to parallelize parts of the new clustering method, but large-n, large-m data sets are not the focus here.

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hierarchical sequence revert back from n levels to $\frac{n \cdot (n-1)}{2} + 1$ levels, the time complexity to construct cluster sets becomes O(n^4). This is large even for small-n, large-m data sets. Moreover, the *post hoc* heuristics for cutting dendrograms are not suitable for finding meaningful cluster sets[3] of an $\frac{n \cdot (n-1)}{2} + 1$-level hierarchical sequence.

Thus, with today's technology, the project went back more than 60 years to solve a problem that could not be solved then. For the second part of the project, a means was developed for finding meaningful levels of an $\frac{n \cdot (n-1)}{2} + 1$-level (complete linkage) hierarchical sequence *prior* to performing a cluster analysis. The means constructs a distance graph[4] and visually examines this graph for features that correlate with the meaningful levels. (Olsen, 2014b). By finding meaningful levels of such a hierarchical sequence *prior* to performing a cluster analysis, it is possible to know which cluster sets to construct and construct only these cluster sets.

9-Mote Test Bed C
proximity vector =

580.8	4	9
608.4	6	8
635.8	5	9
638.9	4	5
652.1	1	8
662.8	1	6
692.7	1	3
707.3	3	6
756.2	3	8
1224.2	2	7
1235.9	1	2
1251.4	2	3
1290.5	2	6
1299.9	2	8
1358.7	4	7
1391.8	2	4
1412.0	5	7
1417.2	2	5
1428.1	7	9
1437.0	3	7
1483.7	7	8
1485.5	2	9
...		
1938.6	1	9

d' = 1485.5
state matrix =

	1	2	3	4	5	6	7	8	9
1	1	1	1	0	0	1	0	1	0
2	1	1,2	1	2	2	1	2	1	2
3	1	1	1	0	0	1	2	1	0
4	0	2	0	2	2	0	2	0	2
5	0	2	0	2	2	0	2	0	2
6	1	1	1	0	0	1	0	1	0
7	0	2	2	2	2	0	2	2	2
8	1	1	1	0	0	1	2	1	0
9	0	2	0	2	2	0	2	0	2

d' = 1428.1
state matrix =

	1	2	3	4	5	6	7	8	9
1	1	1	1	0	0	1	0	1	0
2	1	1	1	2	2	1	2	1	0
3	1	1	1	0	0	1	0	1	0
4	0	2	0	2	2	0	2	0	2
5	0	2	0	2	2	0	2	0	2
6	1	1	1	0	0	1	0	1	0
7	0	2	0	2	2	0	2	0	2
8	1	1	1	0	0	1	0	1	0
9	0	0	0	2	2	0	2	0	2

Figure 1: Proximity vector and state matrices for a data set similar to that described in Subsection 5.2. The numbers in the state matrices highlight the different clusters and are for illustrative purposes only. How these data structures are used is fully described in (Olsen, 2014a).

[3] A "meaningful cluster set" refers to a cluster set that can have real world meaning. Under ideal circumstances, a "meaningful level" refers to a level of a hierarchical sequence at which a new configuration of clusters has finished forming. These definitions appear to be synonymous for $\frac{n \cdot (n-1)}{2} + 1$-level hierarchical sequences. The cluster set that is constructed for a meaningful level is a meaningful cluster set, so these terms are used interchangeably.

[4] Examples of distance graphs can be found in Fig. 2 and the experiments in Section 5.

This reduces the time complexity to construct cluster sets from $O(n^4)$ to $O(ln^2)$, where l is the number of meaningful levels. *These are the cluster sets that can have real world meaning.* It is notable that the means does not rely on dendrograms or *post hoc* heuristics to find meaningful cluster sets. The second part also looked at how increasing the dimensionality of the data points helps reveal inherent structure in noisy data, which is necessary for finding meaningful levels.

The third part of the project resolved how to mathematically capture the graphical relationships that underlie the above-described features and integrate the means into the new clustering method. By doing so, the new clustering method becomes self-contained and can be fully automated or used with minimal operator supervision.

2 CONSTRUCTING SELECT CLUSTER SETS

Let $X = \{x_1, x_2, ..., x_n\}$ be a data set that contains a finite number of data points n, where each data point has m dimensions. Further, suppose that each data point is a sequence of samples and that at any moment in time, with respect to each class or source, all the samples have the same true values and biases[5]. The INCLude (InterNodal Complete Linkage) hierarchical clustering method (Olsen, 2014a) is a complete linkage hierarchical clustering method that assumes only that the clusters are globular or compact, and preferably maximally complete subsets of data points. It uses interpoint distances instead of intercluster distances to construct clusters, allows clusters to overlap, and allows data points to migrate between clusters.

Unlike the standard complete linkage method, or the clique detection method described in (Peay, 1974) and (Peay, 1975), the new clustering method is *not* an updating method. Instead, as Fig. 1 shows, the new clustering method substitutes two data structures, a proximity vector for holding information about the distances between the data points and a state matrix for holding information about linkage, for the proximity matrix used by the standard complete linkage method. In particular, a proximity vector is a rank ordered list of ordered triples $(d_{i,j}, i, j)$ comprised of a distance $d_{i,j}$ between data points x_i and x_j, $i, j = 1, 2, ..., n, i \neq j$, and the indices of the respective data points. The ordered triples are sorted into rank or ascending order according to their distance elements,

[5] In real world terms, this is the same as calibrating the sensors.

and the row indices of the proximity vector are used to index the sorted ordered triples (the "rank order indices").

Next, the ordered triples are evaluated in ascending order for linkage. As the ordered triples are evaluated, threshold distance (index) d' increases implicitly from 0 to the maximum of all the distance elements. Threshold distance $d' \in R$ is a continuous variable that determines which pairs of data points in a data set are linked and which are not. Data points x_i and x_j, $i, j = 1,2,...,n, i \neq j$, are linked if the distance between them is less than or equal to threshold distance d', i.e., $d_{i,j} \leq d'$. From the linkage information that is stored in the state matrix and the degrees of the data points, a hierarchical sequence of cluster sets is constructible.

Because evaluating ordered triples for linkage is decoupled from cluster set construction, the linkage information in a state matrix can be updated without constructing cluster sets. Further, cluster sets are constructed *de novo*. In other words, the cluster set for each level of an $\frac{n\cdot(n-1)}{2}$+1-level hierarchical sequence is constructed independently of the cluster sets for the other levels. This scheme has at least two advantages. First, data points can migrate naturally as a part of cluster set construction. Second, it is possible to construct only the cluster sets that correspond to select, possibly non-contiguous levels of a hierarchical sequence. Consequently, it is possible to construct only the cluster sets for meaningful levels of a hierarchical sequence.

3 USING DISTANCE GRAPHS TO FIND MEANINGFUL LEVELS

To find meaningful levels of an $\frac{n\cdot(n-1)}{2}$ + 1-level hierarchical sequence, a distance graph is constructed and visually examined. For 2-norm distance measures such as Euclidean distance, using distance graphs is motivated by the realization that as $m \to \infty$, the variance $\sigma^2_{Z_m}$ of the random variable $Z_m = (\sum_{k=1}^m Y_k^2)^{\frac{1}{2}}$ converges to $\frac{\sum_{k=1}^m \sigma_k^4}{2(\sum_{k=1}^m \sigma_k^2+\sum_{k=1}^m \mu_k^2)} + \frac{\sum_{k=1}^m \sigma_k^2 \mu_k^2}{\sum_{k=1}^m \sigma_k^2+\sum_{k=1}^m \mu_k^2}$.[6] Y_k is a normally distributed random variable such that $Y_k \sim N(\mu_k, \sigma_k)$. Often, as the dimensionality of the data points increases and the 2-norm interclass distances become larger, the standard deviations of the 2-norm interclass distances, i.e., σ_{Z_m}, nonetheless remain relatively small or constant. *See* (Olsen, 2014b).

When this scenario holds, data points that belong to the same class link at about the same time *even at higher dimensionalities*. Classes of data points can be close together at lower dimensionalities. When they are, the magnitudes of many intraclass distances and interclass distances are about the same, so the two kinds of distances commingle. However, the classes of data points are farther apart at higher dimensionalities, so the intraclass distances and the interclass distances segregate into bands. Thus, higher dimensionalities can attenuate the effects of noise[7] that preclude finding meaningful levels of a hierarchical sequence at lower dimensionalities and distinguish between the classes. Moreover, this pattern repeats itself as clusters become larger from including more data points.

Consequently, as the dimensionality of the data points increases, the distance graphs for a data set can exhibit identifiable features that correlate with meaningful levels of the corresponding hierarchical sequences. *These levels are the levels at which multiple classes have finished linking to form new configurations of clusters.* In particular, assuming that the data set has inherent structure, a distance graph takes on a shape whereby sections of the graph run nearly parallel to one of the graph axes. Where there is very little or no linking activity, the sections run nearly vertically. Where there is significant activity, i.e., where new configurations of clusters are forming, the sections run nearly horizontally. Thus, portions of the graph that come after the lower-right corners and before the upper-left corners indicate where new configurations of clusters have finished forming. A distance graph can be visually examined *prior* to performing a cluster analysis. Since a distance graph is used to find meaningful levels of a hierarchical sequence *prior* to performing a cluster analysis, it is not a summary of the results obtained from the analysis. Instead, it enables a user to selectively construct only meaningful cluster sets, i.e., cluster sets where new configurations of clusters have finished forming.

Finding meaningful levels is remarkably easy: First, the differences (dissimilarities) between data points x_i and x_j, $i, j = 1,2,...,n, x_i \neq x_j$, are calculated. Then, using a p-norm, $p \in [1,\infty)$, the lengths or magnitudes of the vectors that contain these differences are calculated. Next, ordered triples $(d_{i,j}, i, j)$ are constructed from these distances and the indices of the respective data points, the ordered triples are sorted into rank or ascending order according to their distance elements, and rank order indices are assigned to the sorted ordered triples. The rank order indices and the ordered triples are used to construct a distance graph. The rank order indices and/or the distance el-

[6] An analog exists for 1-norm distance measures such as city block distance.

[7] Attenuating the effects of noise refers to reducing the effects of noise on cluster construction.

ements that correspond to where the lower-right corners appear in the graph are identified along the axes of the distance graph. These rank order indices and distance elements coincide with the meaningful levels and the respective threshold distances d' of the corresponding hierarchical sequence. Each different distance measure has its own distance graph and corresponding hierarchical sequence, and thus its own set of meaningful levels. As a visual tool, however, distance graphs are not well suited for automation.

4 INTEGRATING THE MEANS

Integrating the means for finding meaningful levels into the new clustering method is based on the same two assumptions that underlie the means when distance graphs are visually examined. First, the approach assumes that noise (random error) is the only random component in a measured value and that the noise that is embedded in each dimension (sample) of each data point is statistically independent.[8] Second, the approach assumes that the dissimilarities between the data points are non-negative values. This assumption is needed because p-norm distance measures do not distinguish between positive and negative correlation.

To mathematically capture the graphical relationships that underlie the above-described features of a distance graph, the rank order indices that coincide with the meaningful levels of the corresponding hierarchical sequence, or the distance elements that coincide with the respective threshold distances d', must be identifiable *without* visually examining the distance graph. In other words, this objective must be attainable by looking only at the rank order indices and the information that is contained within the ordered triples. As mentioned above, those portions of a distance graph that come after the lower-right corners and before the upper-left corners indicate where new configurations of clusters have finished forming. The approach focuses on the lower-right corners because, under ideal circumstances, these are the features that correspond to having evaluated every ordered triple whose distance element is less than threshold distance d'. As Fig. 2 shows, one way to mathematically capture these relationships compares 1) the tangent of the angle that the distance graph forms with the x-axis of

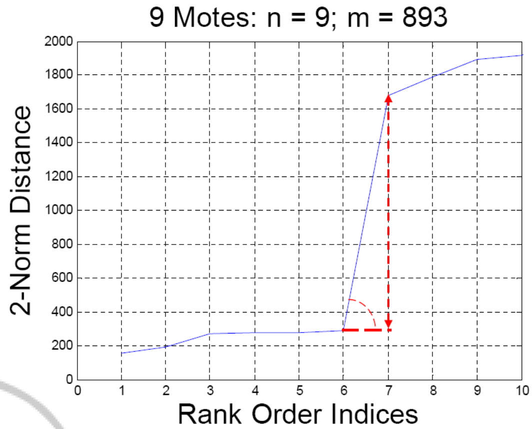


Figure 2: Lower left portion of the distance graph from the experiment in Subsection 5.2. The enlargement shows one of the angles used to find meaningful levels of the corresponding hierarchical sequence. The dashed arrow represents $DISTROI_{i+1} - DISTROI_i$. Here, $DISTROI_{i+1}$ is the distance element of the 7th ordered triple and $DISTROI_i$ is the distance element of the 6th ordered triple.

the graph at each rank order index i with 2) the difference between the distance elements of the $i+1th$ and ith ordered triples, $i = 1, 2, \ldots, \frac{n\cdot(n-1)}{2}$. The experiments in Section 5 show that the range of these angles typically is between 60 degrees and 90^- degrees, or nearly orthogonal under ideal circumstances.

Proximity vectors are well suited for finding these angles. With respect to a specific distance measure, a proximity vector is a permanent record of the interpoint distances between the data points in a data set. After each ordered triple is evaluated for linkage, a test is performed to determine whether the next level of the corresponding hierarchical sequence is meaningful. The ith level of a hierarchical sequence is *deemed* to be meaningful if the following test returns true:

$$DISTROI_{i+1} - DISTROI_i \geq tan(cutoffAngle) \cdot MAXDIST / MAXROI.$$

$DISTROI_{i+1}$ is the distance element of the $i+1th$ ordered triple, $DISTROI_i$ is the distance element of the ith ordered triple, $cutoffAngle$ is the minimum angle that the distance graph must form with the positive x-axis of the graph at the ith rank order index, $MAXDIST$ is the maximum distance element, and $MAXROI$ is $\frac{n\cdot(n-1)}{2}$ or the number of ordered triples. The normalization factor is on the right side of the equation to reduce the number of multiplications. Typically, a distance graph is constructed and examined before any of the ordered triples are evaluated for linkage. The test is performed after each ordered triple is evaluated. If the test returns true

[8] To make the proofs mathematically tractable, the work on finding meaningful levels also assumed that noise can be modeled as Gaussian random variables. When noise is uniformly distributed, the results are analogous to those when noise is normally distributed, indicating that the Gaussian random variable assumption is reasonable (Olsen, 2014b).

after the ith ordered triple is evaluated, the cluster set for the ith level of the hierarchical sequence is constructed. The first cluster set (all the data points are singletons) and the last cluster set (all the data points belong to the same cluster or stopping criteria have been met) are always constructed.

Two parameters need tuning. One is the dimensionality at which inherent structure in a data set has good definition (or as good as is practically possible). The other is $cutoffAngle$. These can be tuned online with minimal operator intervention or hardwired based on domain knowledge. Alternatively, it should be possible to learn them. The results for a data set can be characterized by the data set and the index $m(\angle cutoffAngle)$, where m is the dimensionality of the data points.

5 EMPIRICAL RESULTS

The remainder of this paper describes the empirical results from four experiments that were rerun to evaluate the above-described approach. The original experiments are part of the work described in (Olsen, 2014a) and (Olsen, 2014b). In all four experiments, the approach is used to find meaningful levels of hierarchical sequences. These results are compared with those obtained from visually examining the corresponding distance graphs. Defining false positives to mean meaningful levels that should not be constructed but are and false negatives to mean meaningful levels that should be constructed but are not, the third experiment also calculates the number of false positives and false negatives as the dimensionality of the data set is increased. The fourth experiment looks at the ranges over which $cutoffAngle$ can vary without incurring any false positives or false negatives.

Both the 2-norm distance measure (Euclidean distance) and the 1-norm distance measure (city block distance) are used to calculate the distances. $level$ is a variable that is used to refer to individual meaningful levels, and d' refers to the respective threshold distances d'. Before the means was integrated, the new clustering method was compared with the standard complete linkage method and a flat method in (Olsen, 2014a).

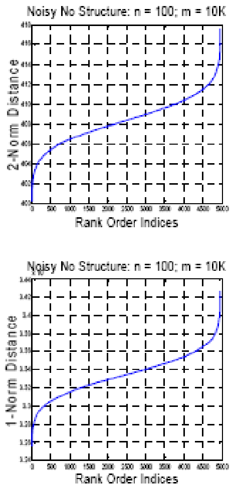
5.1 No Structure

A uniform distribution pseudo-random number generator is used to construct 100 data points having 10,000 dimensions each. Out of 4951 levels in total, the graphs in Fig. 3 suggest that the corresponding hierarchical sequences have no meaningful levels other than the end levels. The data for the 2-norm distance measure include 9 false positives at 10K($\angle$60), 9 false positives at 10K($\angle$65), 3 false positives at 10K($\angle$70), 3 false positives at 10K($\angle$75), 1 false positive at 10K($\angle$80), and no false positives at 10K($\angle$85). The data for the 1-norm distance measure include 6 false positives at 10K($\angle$60), 5 false positives at 10K($\angle$65), 5 false positives at 10K($\angle$70), 3 false positives at 10K($\angle$75), 1 false positive at 10K($\angle$80), and no false positives at 10K($\angle$85). The false positives come at either end of the hierarchical sequences for both distance measures.

5.2 Sampling Luminescence

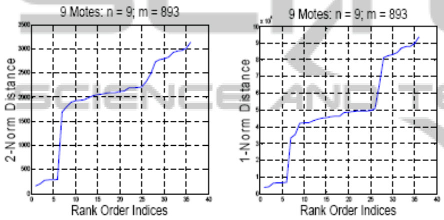
Nine Crossbow® MicaZ motes with MTS300CA sensor boards attached thereto are configured into a 1x1 meter grid and programmed to take light readings (lux) of an overhead light source every 1 second for 15 minutes. Canopies are placed over some of the motes during part or all of the experiment. Out of 37 levels in total, the graphs in Fig. 4 suggest that the corresponding hierarchical sequences have four meaningful levels. At $level$ = 6 (d' = 287.97 for the 2-norm distance measure and d' = 6723.20 for the 1-norm distance measure; m = 893), there are five non-overlapping clusters, one for motes that are always exposed to direct light (motes 2, 4, and 9), another for motes that are never exposed to direct light (motes 1, 6, and 8), and one for each of the motes that are exposed to direct light during different time intervals (motes 3, 5, and 7). At $level$ = 27 (d' = 2488.63 for the 2-norm distance measure and d' = 64,391.60 for the 1-norm distance measure; m = 893), there are two overlapping clusters, one for those motes that were exposed to direct light during part or all of the experiment (motes 2, 3, 4, 5, 7, and 9) and the other for those motes that were not exposed to direct light during part or all of the experiment (motes 1, 3, 5, 6, 7, and 8).

The meaningful levels of the hierarchical sequence for the 2-norm distance measure are identifiable from 893($\angle$60) to 893($\angle$70). At 893($\angle$65) and 893($\angle$70), the meaningful levels are identifiable without incurring any false positives or false negatives. The meaningful levels of the hierarchical sequence for the 1-norm distance measure are identifiable from 893($\angle$60) to 893($\angle$80). At 893($\angle$80), the meaningful levels are identifiable without incurring any false positives or false negatives.



Human Inspect.	60 degrees		65 degrees		70 degrees		75 degrees		80 degrees		85 degrees	
	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm
Start	Start	Start	Start	Start	Start	Start	Start	Start	Start	Start	Start	Start
	1		1									
	2		2		2		2					
	3	3	3	3	3	3	3	3		3		
	4		4		4		4		4			
	4930		4930									
	4935		4935									
		4941		4941		4941						
	4944	4944	4944	4944		4944						
		4945										
	4946		4946									
		4947		4947		4947		4947				
	4948		4948									
		4949		4949		4949		4949				
4950	4950	4950	4950	4950	4950	4950	4950	4950	4950	4950	4950	4950

Figure 3: Distance graphs for the structureless data set at m = 10,000 dimensions and levels identified as meaningful for 10K(∠60) to 10K(∠85).



Human Inspect.	60 degrees		65 degrees		70 degrees		75 degrees		80 degrees		85 degrees	
	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm
Start	Start	Start	Start	Start	Start	Start	Start	Start	Start	Start	Start	Start
6	6	6	6	6	6	6	6	6	6	6	6	
		8		8								
	26	26		26		26		26				
27	27	27	27	27	27	27		27		27		
36	36	36	36	36	36	36	36	36	36	36	36	36

Figure 4: Distance graphs for the nine motes data set at m = 893 dimensions and levels identified as meaningful for 893(∠60) to 893(∠85).

5.3 17-Point Geometric Pattern

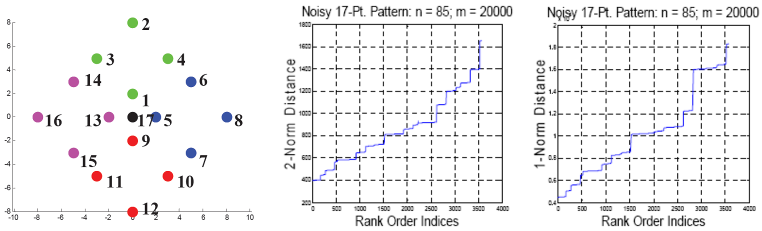
As shown in Fig. 5, a 17-point geometric pattern is constructed, and five copies of each point are used to construct a data set having 85 data points. The dimensionality of the data points is increased to 80,000 dimensions by increments of 10,000 dimensions, and noise ($N(0,2^2)$) is added to each dimension of each data point in each data set. The graphs in Fig. 5 suggest that the hierarchical sequence for the 2-norm distance measure has 19 meaningful levels while that for the 1-norm distance measure has 16 levels. These levels are provided in (Olsen, 2014a).

This experiment compares how many false positives and how many false negatives are incurred at different dimensionalities. As the table in Fig. 5 shows, except when $cutoffAngle$ equals 80 or 85 degrees, the number of false positives is greater than the number of false negatives. Most false positives are levels of the hierarchical sequences just to either side of the meaningful levels. More false positives occur at lower dimensionalities, most likely due to noise, and at lower $cutoffAngle$s, because the criterion for constructing cluster sets is less stringent. If they occur, false negatives tend to occur at very high $cutoffAngle$s or at lower dimensionalities, where the definition of the meaningful levels is not as good as it is at higher dimensionalities. From 70K(∠75) to 80K(∠85), there are no false positives or false negatives.

5.4 Health Monitoring

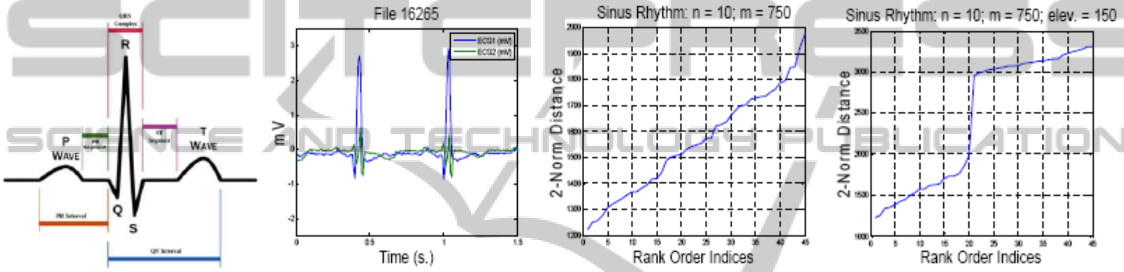
The data used in this experiment come from file 16265 of the MIT-BIH PhysioNet Normal Sinus Rhythm database (Goldberger et al., 2000). This file contains ECG readings collected at 128 hertz. The P,Q,R,S,T interval of each heart beat, as illustrated by the left-most graphs in Fig. 6, describes how a heart pumps blood to other parts of a body. Here, 25 samples per beat that include the Q,R,S complex and at least the left side of the ST element are extracted from the first 300 consecutive beats of the file, and the data set is divided into 10 segments (approx. 25 seconds each). The third graph in Fig. 6 shows that this data set has almost no inherent structure.

An elevated ST element is simulated by adding a constant c_{elevST} equal to 80, 100, or 150 mV to samples 11-22 of the excerpts in the last 1, 2, 3, 4, or 5 segments. This experiment looks at how early



Dimensions m	60 degrees		65 degrees		70 degrees		75 degrees		80 degrees		85 degrees	
	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm	2-norm	1-norm
20,000	32+/0-	28+/1-	21+/0-	18+/1-	10+/0-	11+/1-	4+/1-	6+/1-	0+/1-	3+/2-	0+/2-	0+/2-
30,000	13+/1-	14+/0-	7+/1-	6+/0-	5+/1-	2+/0-	2+/1-	1+/0-	0+/1-	0+/0-	0+/1-	0+/1-
40.,000	16+/0-	16+/0-	10+/0-	13+/0-	4+/0-	10+/0-	0+/0-	4+/0-	0+/0-	1+/0-	0+/1-	0+/1-
50,000	17+/0-	16+/0-	11+/0-	11+/0-	4+/0-	7+/0-	1+/0-	3+/0-	1+/0-	1+/0-	0+/1-	0+/1-
60,000	12+/0-	12+/0-	8+/0-	10+/0-	3+/0-	6+/0-	1+/0-	1+/0-	0+/0-	0+/0-	0+/1-	0+/1-
70,000	6+/0-	9+/0-	2+/0-	4+/0-	0+/0-	1+/0-	0+/0-	0+/0-	0+/0-	0+/0-	0+/0-	0+/0-
80.000	7+/0-	12+/0-	2+/0-	6+/0-	1+/0-	3+/0-	0+/0-	0+/0-	0+/0-	0+/0-	0+/0-	0+/0-

Figure 5: 17-point geometric pattern, distance graphs for the 17-point geometric pattern data set at m = 20,000 dimensions, and false positives (+) and false negatives (-) for 20K(∠60) to 80K(∠85).



		1 Segment	2 Segments	3 Segments	4 Segments	5 Segments
m = 250	2-Norm	None	None	None	None	None
elev. = 80 mV	1-Norm	70-80	65-80	70-80	70-80	70-80
m = 250	2-Norm	None	None	None	None	None
elev. = 100 mV	1-Norm	65-85	65-85	65-85	65-85	65-85
m = 250	2-Norm	60-85	65-85	60-85	60-85	60-85
elev. = 150 mV	1-Norm	60-85	60-85	60-85	60-85	60-85
m = 500	2-Norm	None	65	65	None	None
elev. = 80 mV	1-Norm	70-85	60-85	60-85	65-85	50-85
m = 500	2-Norm	None	70-75	70-80	65-80	70
elev. = 100 mV	1-Norm	70-85	55-85	60-85	60-85	50-85
m = 500	2-Norm	65-85	60-85	55-85	60-85	70-85
elev. = 150 mV	1-Norm	65-85	50-85	50-85	55-85	40-85
m = 750	2-Norm	None	70	60-65	50-65	None
elev. = 80 mV	1-Norm	70-85	60-85	65-85	65-85	65-85
m = 750	2-Norm	70	70-80	60-80	45-80	70
elev. = 100 mV	1-Norm	70-85	55-85	60-85	60-85	60-85
m = 750	2-Norm	65-85	55-85	50-85	40-85	65-85
elev. = 150 mV	1-Norm	60-85	45-85	50-85	50-85	50-85

Figure 6: ECG, distance graphs for m = 750 dimensions, and ranges over which $cutoffAngle$ can vary without incurring any false positives or false negatives. The data used in this experiment come from file 16265 of the MIT-BIH Normal Sinus Rhythm database.

an elevated ST element is detectable without incurring any false positives or false negatives. Increasing c_{elevST} or increasing the dimensionality of the segments increases the ranges of $cutoffAngle$ over which an event is detectable. Increasing c_{elevST} adds structure to the data sets and has the biggest impact on the ranges over which an event is detectable. Increasing the dimensionality of the segments does not add structure to the data sets, and the law of diminishing returns eventually sets in. The widest ranges of detection are where both c_{elevST} and m are large. The number of segments to which c_{elevST} is added does not show a clear trend. This is consistent with the view that increasing or decreasing the number of segments should not have an effect on the ranges. For this experiment, the ranges for the 1-norm distance measure tend to be wider than those for the 2-norm distance measure.

6 CONCLUSION

To develop a complete linkage hierarchical clustering method that 1) substantially improves upon the accuracy of the standard complete linkage method and 2) can be fully automated or used with minimal operator supervision, the assumptions underlying the standard complete linkage method are unwound. The new clustering method substitutes two data structures, a proximity vector and a state matrix, for the proximity matrix used by the standard complete linkage method. Consequently, evaluating pairs of data points for linkage is decoupled from constructing cluster sets. Further, cluster sets are constructed *de novo*. These design choices make it possible to construct only the cluster sets that correspond to select, possibly non-contiguous levels of an $\frac{n\cdot(n-1)}{2}$ + 1-level hierarchical sequence. To construct meaningful cluster sets without constructing an entire hierarchical sequence, a means that uses distance graphs is used to find meaningful levels of such a hierarchical sequence.

This paper presents an approach that mathematically captures the graphical relationships that are used to find meaningful levels and integrates the means into the new clustering method. The test that determines which cluster sets are meaningful is easy to calculate and uses the same data that are used by the new clustering method. Consequently, the new clustering method is self-contained and incurs almost no extra cost to administer the test after each ordered triple is evaluated. Moreover, the approach is adaptable and broadly applicable because it does not rely on predetermined parameters. Future work includes trying the new clustering method at a beta site and making enhancements to the cluster set construction module.

The empirical results from four experiments show that the approach does well at finding meaningful levels of hierarchical sequences. Most false positives are levels just to either side of the meaningful levels. The results also show that it is possible to identify meaningful levels of a hierarchical sequence without incurring any false positives or false negatives.

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