A Novel Algorithm for Meta Similarity Clusters Using Minimum Spanning Tree

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Summary
The minimum spanning tree clustering algorithm is capable of detecting clusters with irregular boundaries. In this paper we propose two minimum spanning trees based clustering algorithm. The first algorithm produces k clusters with center and guaranteed intra-cluster similarity. The second algorithm is proposed to create a dendrogram using the k clusters as objects with guaranteed inter-cluster similarity. The first algorithm uses divisive approach, where as the second algorithm uses agglomerative approach. In this paper we used both the approaches to find Meta similarity clusters.

Key Words:
Euclidean minimum spanning tree, Subtree, Clustering, Eccentricity, Center, Hierarchical clustering, Dendrogram, Subtree.

1. Introduction

Given a connected, undirected graph $G = (V, E)$, where V is the set if nodes, E is the set of edges between pairs of nodes, and a weight $w (u , v)$ specifying weight of the edge (u, v) for each edge $(u, v) \in E$. A spanning tree is an acyclic subgraph of a graph G, which contains all vertices from G. The Minimum Spanning Tree (**MST**) of a weighted graph is minimum weight spanning tree of that graph. Several well established **MST** algorithms exist to solve minimum spanning tree problem [17], [12], [13]. The cost of constructing a minimum spanning tree is $O (m \log n)$, where m is the number of edges in the graph and n is the number of vertices. More efficient algorithm for constructing **MST**s have also been extensively researched [11], [4], [7]. These algorithms promise close to linear time complexity under different assumptions. A Euclidean minimum spanning tree (**EMST**) is a spanning tree of a set of n points in a metric space (**E**^{n}), where the length of an edge is the Euclidean distance between a pair of points in the point set.

The hierarchical clustering approaches are related to graph theoretic clustering. Clustering algorithms using minimal spanning tree takes the advantage of **MST**. The **MST** ignores many possible connections between the data patterns, so the cost of clustering can be decreased. The **MST** based clustering algorithm is known to be capable of detecting clusters with various shapes and size [20]. Unlike traditional clustering algorithms, the **MST** clustering algorithm does not assume a spherical shapes structure of the underlying data. The **EMST** clustering algorithm [16], [20] uses the Euclidean minimum spanning tree of a graph to produce the structure of point clusters in the *n*-dimensional Euclidean space. Clusters are detected to achieve some measures of optimality, such as minimum intra-cluster distance or maximum inter-cluster distance [2]. The **EMST** algorithm has been widely used in practice.

Clustering by minimal spanning tree can be viewed as a hierarchical clustering algorithm which follows a divisive approach. Using this method firstly **MST** is constructed for a given input. There are different methods to produce group of clusters. If the number of clusters k is given in advance, the simplest way to obtain k clusters is to sort the edges of minimum spanning tree in descending order of their weights and remove edges with first k-1 heaviest weights [2, 19].

Geometric notion of centrality are closely linked to facility location problem. The distance matrix D can computed rather efficiently using Dijkstra's algorithm with time complexity $O(| V|^2 \ln | V |)$ [18].

The *eccentricity* of a vertex x in G and radius ρ(G), respectively are defined as

$$e(x) = \max_{y\in V} d(x , y) \quad \text{and} \quad \rho(G) = \min_{x\in V} e(x)$$

The *center* of G is the set

$$\boldsymbol{C}(G) = \{x \in V \mid e(x) = \rho(G)\}$$

C (G) is the center to the "*emergency facility location problem*" which is always contain single block of G. The length of the longest path in the graph is called *diameter* of the graph G. we can define diameter D (G) as

$$\mathbf{D}(G) = \max_{x\in V} e(x)$$

The *diameter* set of G is

$$\boldsymbol{Dia}(G) = \{x\in V \mid e(x) = \mathbf{D}(G)\}$$

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All existing clustering Algorithm require a number of parameters as their inputs and these parameters can significantly affect the cluster quality. In this paper we want to avoid experimental methods and advocate the idea of need-specific as opposed to care-specific because users always know the needs of their applications. We believe it is a good idea to allow users to define their desired similarity within a cluster and allow them to have some flexibility to adjust the similarity if the adjustment is needed. Our Algorithm produces clusters of *n*-dimensional points with a given cluster number and a naturally approximate intra-cluster distance.

Hierarchical clustering is a sequence of partitions in which each partition is nested into the next in sequence. An Agglomerative algorithm for hierarchical clustering starts with disjoint clustering, which places each of the *n* objects in an individual cluster [1]. The hierarchical clustering algorithm being employed dictates how the proximity matrix or proximity graph should be interpreted to merge two or more of these trivial clusters, thus nesting the trivial clusters into second partition. The process is repeated to form a sequence of nested clustering in which the number of clusters decreases as a sequence progress until single cluster containing all *n* objects, called the *conjoint clustering*, remains[1].

An important objective of hierarchical cluster analysis is to provide picture of data that can easily be interpreted. A picture of a hierarchical clustering is much easier for a human being to comprehend than is a list of abstract symbols. A *dendrogram* is a special type of tree structure that provides a convenient way to represent hierarchical clustering. A dendrogram consists of layers of nodes, each representing a cluster.

In this paper we propose two **EMST** based clustering algorithm to address the issues of undesired clustering structure and unnecessary large number of clusters. Our first algorithm assumes the number of clusters is given. The algorithm constructs an **EMST** of a point set and removes the inconsistent edges that satisfy the inconsistence measure. The process is repeated to create a hierarchy of clusters until *k* clusters are obtained. In section 2 we review some of the existing works on graph based clustering algorithm. In Section 3 we propose **CEMST** algorithm which produces *k* clusters with center. We also propose another algorithm called **EMSTU** for finding cluster of clusters using the *k* clusters which are from previous **CEMST** algorithm. Hence we named this new cluster as *Meta similarity clusters.* Finally in conclusion we summarize the strength of our methods and possible improvements.

2. Related Work

Clustering by minimal spanning tree can be viewed as a hierarchical clustering algorithm which follows the divisive approach. Clustering Algorithm based on minimum and maximum spanning tree were extensively studied. Avis [3] found an $O(n^2 \log^2 n)$ algorithm for the min-max diameter-2 clustering problem. Asano, Bhattacharya, Keil and Yao [2] later gave optimal O $(n \log n)$ algorithm using maximum spanning trees for minimizing the maximum diameter of a bipartition. The problem becomes NP-complete when the number of partitions is beyond two [10]. Asano, Bhattacharya, Keil and Yao also considered the clustering problem in which the goal to maximize the minimum inter-cluster distance. They gave a *k*-partition of point set removing the *k*-1 longest edges from the minimum spanning tree constructed from that point set [2]. The identification of inconsistent edges causes problem in the **MST** clustering algorithm. There exist numerous ways to divide clusters successively, but there is not suitable a suitable choice for all cases.

Zahn [20] proposes to construct **MST** of point set and delete inconsistent edges – the edges, whose weights are significantly larger than the average weight of the nearby edges in the tree. Zahn's inconsistent measure is defined as follows. Let *e* denote an edge in the **MST** of the point set, v_1 and v_2 be the end nodes of *e, w* be the weight of *e*. A *depth neighborhood* ***N*** of an end node *v* of an edge *e* defined as a set of all edges that belong to all the path of length *d* originating from *v*, excluding the path that include the edge *e*. Let N_1 and N_2 be the depth *d* neighborhood of the node v_1 and v_2. Let $\hat{W}_{N1}$ be the average weight of edges in N_1 and σN_1 be its standard deviation. Similarly, let $\hat{W}_{N2}$ be the average weight of edges in N_2 and σN_2 be its standard deviation. The inconsistency measure requires one of the three conditions hold:

1. $w > \hat{W}N_1 + c \text{ x } \sigma N_1$ or $w > \hat{W}N_2 + \text{c x } \sigma N_2$

2. $w > \max(\hat{W}N_1 + c \text{ x } \sigma N_1 , \hat{W}N_2 + c \text{ x } \sigma N_2)$

3. $$\frac{w}{\max(c \text{ x } \sigma N_1 , c \text{ x } \sigma N_2)} > f$$

where *c* and *f* are preset constants. All the edges of a tree that satisfy the inconsistency measure are considered inconsistent and are removed from the tree. This result in set of disjoint subtrees each represents a separate cluster. Paivinen [15] proposed a Scale Free Minimum Spanning Tree **(SFMST)** clustering algorithm which constructs scale free networks and outputs clusters containing highly connected vertices and those connected to them.

The **MST** clustering algorithm has been widely used in practice. Xu (Ying), Olman and Xu (Dong) [19] fuse MST as multidimensional gene expression data. They point out that **MST**- based clustering algorithm does not assume that data points are grouped around centers or separated by regular geometric curve. Thus the shape of the cluster boundary has little impact on the performance of the algorithm. They described three objective functions and the corresponding cluster algorithm for computing *k*-partition of spanning tree for predefined $k > 0$. The algorithm simply removes *k*-1 longest edges so that the weight of the subtrees is minimized. The second objective function is defined to minimize the total distance between the center and each data point in the cluster. The algorithm removes first *k*-1 edges from the tree, which creates a *k*-partitions.

The clustering algorithm proposed by S.C.Johnson [9] uses proximity matrix as input data. The algorithm is an agglomerative scheme that erases rows and columns in the proximity matrix as old clusters are merged into new ones. The algorithm is simplified by assuming no ties in the proximity matrix. Graph based algorithm was proposed by Hubert [6] using single link and complete link methods. He used threshold graph for formation of hierarchical clustering. An algorithm for single-link hierarchical clustering begins with the minimum spanning tree (MST) for G (∞), which is a proximity graph containing *n(n-1)/2* edge was proposed by Gower and Ross [8]. Later Hansen and DeLattre [5] proposed another hierarchical algorithm from graph coloring.

3. Our Clustering Algorithm

A tree is a simple structure for representing binary relationship, and any connected components of tree is called *subtree*. Through this **MST** representation, we can convert a multi-dimensional clustering problem to a tree partitioning problem, ie., finding particular set of tree edges and then cutting them. Representing a set of multi-dimensional data points as simple tree structure will clearly lose some of the inter data relationship. However many clustering algorithm proved that no essential information is lost for the purpose of clustering. This is achieved through rigorous proof that each cluster corresponds to one subtree, which does not overlap the representing subtree of any other cluster. Clustering problem is equivalent to a problem of identifying these subtrees through solving a tree partitioning problem. The inherent cluster structure of a point set in a metric space is closely related to how objects or concepts are embedded in the point set. In practice, the approximate number of embedded objects can sometimes be acquired with the help of domain experts. Other times this information is hidden and unavailable to the clustering algorithm. In this section we preset clustering algorithm which produce *k* clusters, with center of each cluster. We also present another algorithm to find the hierarchy of *k* clusters.

3.1 CEMST Clustering Algorithm

Given a point set *S* in $\mathbf{E}^\mathbf{n}$ and the desired number of clusters *k*, the hierarchical method starts by constructing an **MST** from the points in *S*. The weight of the edge in the tree is Euclidean distance between the two end points. Next the average weight Ŵ of the edges in the entire **EMST** and its standard deviation σ are computed; any edge with $W > \hat{W} + \sigma$ or *current longest edge* is removed from the tree. This leads to a set of disjoint subtrees $S_T = \{T_1, T_2 \ldots\}$ *(divisive approach)*. Each of these subtrees T_i is treated as cluster. Oleksandr Grygorash et al proposed algorithm [14] which generates *k* clusters. We modified the algorithm in order to generate *k* clusters with centers. Hence we named the new algorithm as Center Euclidean Minimum Spanning Tree (**CEMST**). Each center point of *k* clusters is a representative point for the each subtree S_T. A point c_i is assigned to a cluster i if $c_i \in T_i$. The group of center points is represented as $S = \{c_1, c_2 \ldots\ldots c_k\}$

```
Algorithm : CEMST(k)
 Input   : S the point set
 Output  : k number of clusters with S (set of
           center points)
 Let e be an edge in the EMST constructed from S
 Let W_e be the weight of e
 Let σ be the standard deviation of the edge
 weights
 Let S_T be the set of disjoint subtrees of the
 EMST
 Let n_c be the number of clusters
 Construct an EMST from S
 Compute the average weight of Ŵ of all the
   edges
 Compute standard deviation σ of the edges
 S_T = ø; n_c = 1
 Repeat
   For each e ∈ EMST
     If (W_e > Ŵ + σ) or (current longest edge e)
       Remove e from EMST
       S_T = S_T U { T' } // T'' is new disjoint
       subtree
       n_c = n_c+1
       Compute the center C_i of T_i using
       eccentricity of points
       S = U_Ti ∈ S_T {C_i}
 Until n_c = k
 Return k clusters with S
```

Figure 1 illustrate a typical example of cases in which simply remove the *k*-1 longest edges does not necessarily output the desired cluster structure. Our algorithm finds the center of the each cluster, which will be useful in many applications. Our algorithm will find 7 cluster structures (*k*=7). Figure 2 shows the possible distribution of the points in the two cluster structures with their center vertex as 5 and 3.

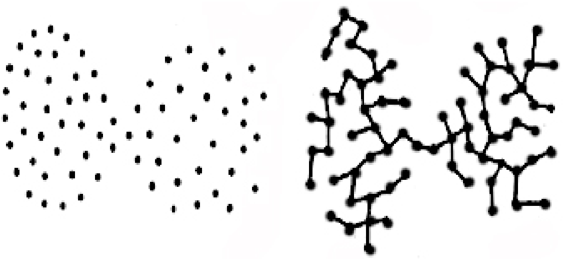
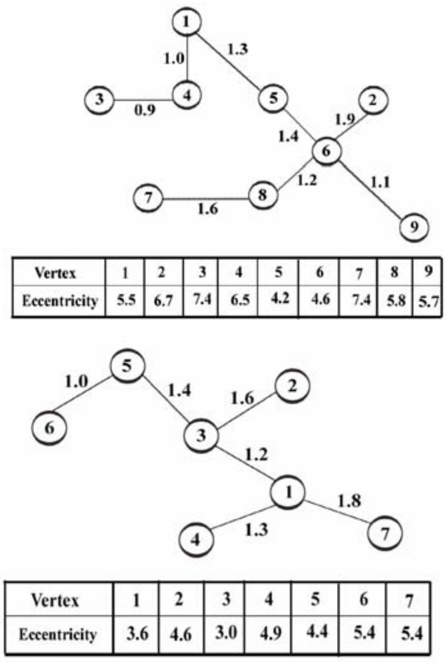


Figure 1: Clusters connected through a point



Vertex	1	2	3	4	5	6	7	8	9
Eccentricity	5.5	6.7	7.4	6.5	4.2	4.6	7.4	5.8	5.7

Vertex	1	2	3	4	5	6	7
Eccentricity	3.6	4.6	3.0	4.9	4.4	5.4	5.4

Figure 2. Two Clusters with Center vertices 5 and 3

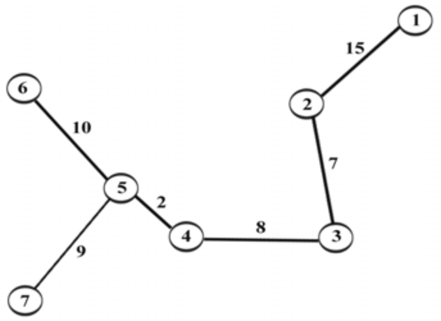


Figure 3. EMST From 7 cluster center points

3.2. EMSTU Clustering Algorithm

The result of the **CEMST** algorithm consists of k number clusters with their center. These center points c_1, c_2 ….c_k are connected and again minimum spanning tree is constructed is shown in the Figure 3. A Euclidean distance between pair of clusters can be represented by a corresponding weighted edge. Our Algorithm is also based on the minimum spanning tree but not limited to two-dimensional points. There were two kinds of clustering problem; one that minimizes the maximum intra-cluster distance and the other maximizes the minimum inter-cluster distances. Our Algorithms produces clusters with both intra-cluster and inter-cluster similarity. We propose Euclidean Minimum Spanning Updation algorithm (**EMSTU**) converts the minimum spanning tree into dendrogram, which can be used to interpret about inter-cluster distances. This new algorithm is neither single link clustering algorithm (SLCA) nor complete link clustering algorithm (CLCA) type of hierarchical clustering, but it is based on the distance between centers of clusters. This approach leads to new developments in hierarchical clustering. The level function, *L,* records the proximity at which each clustering is formed. The levels in the dendrogram tell us the least amount of similarity that points between clusters differ. This piece of information can be very useful in several medical and image processing applications.

Algorithm: EMSTU

```
Input:  the point set $S = \{c_1, c_2……c_k\}$
Output: dendrogram
 1. Construct an EMST $T$ from $S$
 2. Begin with disjoint clusters with level $L$ (0) =
    0 and sequence number $m$ = 0
 3. If ($T$ has some edge)
 4. $e$ = get-min-edge($T$) // for least dissimilar pair
    of clusters
 5. ($i, j$) = get-vertices ($e$)
 6. Increment the sequence number $m = m + 1$,
    merge the clusters ($i$) and ($j$), into single
    cluster to form next clustering $m$ and set the
    level of this cluster to L($m$) = $e$;
 7. Update $T$ by forming new vertex by
    combining the vertices $i, j$; go to step 3.
 8. Else Stop.
```

We use the graph of Figure 3 as example to illustrate the **EMSTU** algorithm. The **EMSTU** algorithm construct minimum spanning tree *T* from the points c_1, c_2, c_3….c_k and convert the *T* into dendrogram is shown in figure 5. It places the entire disjoint cluster at level 0 (line 2). It then checks to see if *T* still contains some edge (line 3). If so, it finds minimum edge *e* (line 4). It then finds the vertices i, j of an edge *e* (line 5). It then merges the vertices (clusters) and forms a new vertex (*agglomerative approach*). At the same time the sequence number is increased by one and the level of the new cluster is set to the edge weight (line 6). Finally, the Updation of minimum spanning tree is performed at line 7. The lines 3-7 in the algorithm are repeated until the minimum spanning tree *T* has no edge. The algorithm takes O *(*| *E* | ^{2}*)* time. The various stages of minimum spanning tree during hierarchical cluster formation are shown in the figure 4.

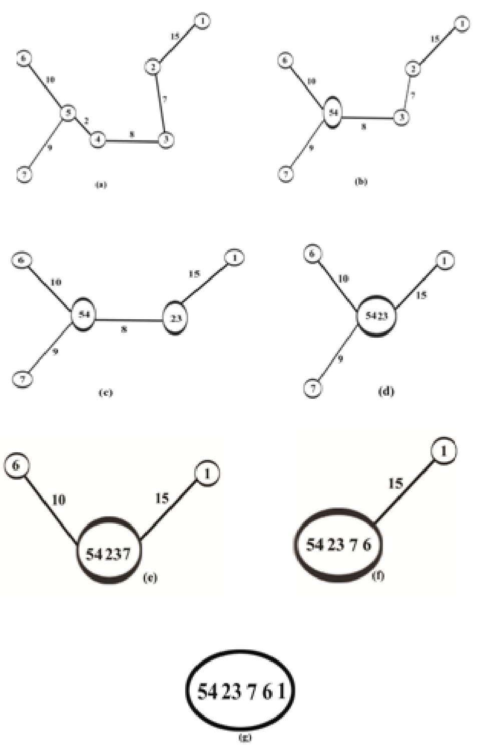


Figure 4. Various stages of Updating Minimum Spanning Tree T

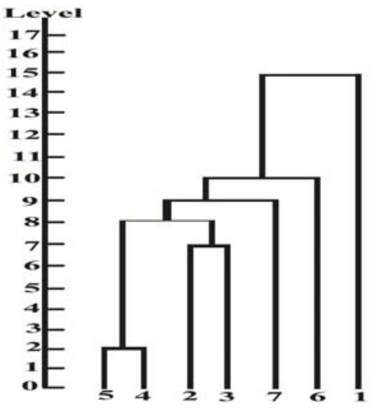


Figure 5. Dendrogram for Meta cluster

4. Conclusion

Our **CEMST** clustering algorithm assumes a given cluster number. The algorithm gradually finds *k* clusters with center for each cluster. These *k* clusters ensures guaranteed intra-cluster similarity. Our algorithm does not require the users to select and try various parameters combinations in order to get the desired output. All of these look nice from theoretical point of view. However from practical point of view, there is still some room for improvement for running time of the clustering algorithm. This could perhaps be accomplished by using some appropriate data structure. Our **EMSTU** clustering algorithm generates dendrogram which is used to find the relationship between the *k* number clusters produced from the **CEMST** algorithm. The inter- cluster distance between *k* clusters are shown in the Dendrogram. This will be very useful in many applications. In the future we will explore and test our proposed clustering algorithm in various domains. The **CEMST** algorithm uses divisive approach, where as the **EMSTU** algorithm uses agglomerative approach. In this paper we used both the approaches to find Meta similarity clusters. We will further study the rich properties of EMST-based clustering methods in solving different clustering problems.

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