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CLUSTER VALIDITY WITH MINIMUM SPANNING TREE BASED CLUSTERING

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ABSTRACT

Clustering is a process of discovering groups of objects such that the objects of the same group are similar, and objects belonging to different groups are dissimilar. A number of clustering algorithms exist that can solve the problem of clustering, but most of them are very sensitive to their input parameters. Therefore it is very important to evaluate the result of them. The minimum spanning tree clustering algorithm is capable of detecting clusters with irregular boundaries. In this paper we propose a minimum spanning tree based clustering algorithm with cluster evaluation. The algorithm produces k clusters with center and guaranteed intra-cluster similarity. The radius and diameter of the k clusters are computed to find the tightness of the k clusters. The variance of the k clusters is also computed to find the compactness of the clusters. In this paper we computed tightness and compactness of clusters, which reflects good measure of the efficacy of clustering.

Key Words: *Euclidean minimum spanning tree, Subtree, Eccentricity, Center, Tightness. Hierarchical clustering, Radius, Diameter, Compactness*.

1. INTRODUCTION

One of the best known problems in the field of data mining is clustering. The problem of clustering is to partition a data set into groups (clusters) in such a way that the data elements within a cluster are more similar to each other than data elements in different clusters [11]. Clustering is the subject of active research in several fields such as statistics, pattern recognition, machine learning, and data mining. A wide variety of clustering algorithms have been proposed for different applications [2].

Clustering is mostly unsupervised process, thus evaluating the result of the clustering algorithms is very important. In the clustering process there are no predefined classes therefore it is difficult to find an appropriate metric for measuring whether the cluster configuration found during the process, is acceptable or not. Several clustering approaches have been developed [6].

The procedure of evaluating the results of a clustering algorithm is known under the term cluster validity. In general terms, there are three approaches to investigate cluster validity [23]. The first is based on *external criteria*. This implies that we evaluate the results of a clustering algorithm based on a pre-specified structure, which is imposed on a data set and reflects our intuition about the clustering structure of the data set. The second structure is based on *internal criteria*. In this case the clustering results are evaluated in terms of quantities that involve the vectors of the data set themselves (e.g. proximity matrix). The third approach of clustering validity is based on *relative criteria*. Here the basic idea is the evaluation of a clustering structure by comparing it to other clustering schemes, resulting by the same algorithm but with different input parameter values.

Given a connected, undirected graph $G=(V,E)$, where V is the set of 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 contain 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 [21], [16], [17]. 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 [15], [5], [9]. 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 ($\mathbf{E^n}$), 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 [25]. Unlike traditional clustering algorithms, the **MST** clustering algorithm does not assume a spherical shapes structure of the underlying data. The **EMST** clustering algorithm [20], [25] 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 [3]. 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 [3], [24].

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 $O(|V|^2 ln|V|)$ [22].

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

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

The *center* of *G* is the set

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

$\mathbf{C}$ (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

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

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].

In this paper we propose **EMST** based clustering algorithm to address the issues of undesired clustering structure and unnecessary large number of clusters. Our 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 and cluster evaluation. In Section 3 we propose **EMSTRDV** algorithm which produces *k* clusters with center, radius, diameter and variance. The radius, diameter and variance of sub tree (cluster) are used to find tightness and compactness of 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 [4] found an $O(n^2 \log^2 n)$ algorithm for the min-max diameter-2 clustering problem. Asano, Bhattacharya, Keil and Yao [3] 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 [14]. 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 [3]. 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 choice for all cases.

Zahn [25] 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. $w > \hat{W}N_1 + c \times \sigma N_1$ *or* $w > \hat{W}N_2 + c \times \sigma N_2$

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

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

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 [19] 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) [24] use 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.

Clustering algorithm proposed by S.C.Johnson [13] 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 [8] 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 [7] proposed another hierarchical algorithm from graph coloring.

Given n d-dimensional data objects or points in a cluster, we can define the centroid x_0, radius R, diameter D and variance of the cluster as

$$X_0 = \frac{\sum_{i=1}^{n} X_i}{n}$$

$$R = \left(\frac{\sum_{i=1}^{n} (X_i - X_0)^2}{n} \right)^{1/2}$$

$$D = \left(\frac{\sum_{i=1}^{n} \sum_{j=1}^{n} (X_i - X_j)^2}{n(n-1)} \right)^{1/2}$$

where *R* is the average distance from member objects to the centroid, and *D* is the average pairwise distance within a cluster. Both *R* and *D* reflect the tightness of the cluster around centroid[26].

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, i.e., 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, radius, diameter and variance of each cluster.

3.1Cluster Tightness and Compactness

In order to measure the efficacy of clustering, a measure based upon the radius and diameter of each subtree (cluster) is devised. The radius and diameter values of each cluster are expected low value for good cluster. If the values are large that the points (objects) are spread widely and may overlap. The cluster tightness measure is a within – cluster estimate of clustering effectiveness , however it is possible to devise inter- cluster measure also, to better measure the separation between the various clusters.

The Cluster compactness measure is based on the variance of the data points distributed in the subtrees (clusters). The variance of cluster *T* is computed as

$$\boldsymbol{\nu}(T) = \left(\frac{1}{n} \sum_{i=1}^{n} d^2(x_i, x_0) \right)^{1/2}$$

Where $d(x_i, x_j)$ is distance metric between two points(objects) x_i and x_j, where n is the number of objects in the subtree T_i and x_0 is the mean of the subtree *T*. A smaller the variance value indicates, a higher homogeneity of the objects in the data set, in terms of the distance measure *d ( )*. Since *d ( )* is the Euclidean distance, $v(T_i)$ becomes the statistical variance of data set $\sigma(T_i)$. The cluster compactness for the out put clusters generated by the algorithm is the defined as

$$Cmp = \frac{1}{k} \sum_{i=1}^{k} \frac{\boldsymbol{\nu}(T_i)}{\boldsymbol{\nu}(S)}$$

Where *k* is the number of clusters generated on the given data set *S*, $v(T_i)$ is the variance of the clusters T_i and $V(S)$ is the variance of data set *S*. [12]

The cluster compactness measure evaluates how well the subtrees (clusters) of the input is redistributed in the clustering process, compared with the whole input set, in terms of data homogeneity reflected by Euclidean distance metric used by the clustering process. Smaller the cluster compactness value indicates a higher average compactness in the out put clusters.

3.2 EMSTRDV Clustering Algorithm

Given a point set *S* in $\mathbf{E}^n$ 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 $\hat{W}$ 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 [18] which generates k clusters. We modified the algorithm in order to generate k clusters with centers. The algorithm is also find radius, diameter and variance of subtrees, which is useful in finding tightness and compactness of clusters. Hence we named the new algorithm as Euclidean Minimum Spanning Tree for Radius Diameter and Variance (**EMSTRDV**). 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 $C = \{c_1, c_2 \ldots\ldots c_k\}$

Algorithm: EMSTRDV(k)

Input : S the point set
Output : k number of clusters

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

1. Construct an **EMST** from S
2. Compute the average weight of $\hat{W}$ of all the edges
3. Compute standard deviation σ of the edges
4. Compute variance of the set S
5. $S_T = ø$; $n_c = 1$; C = ø ;
6. **Repeat**
7. **For** each $e \in$ **EMST**
8. If ($W_e > \hat{W} + \sigma$) or (current longest edge *e)*
9. Remove e from **EMST**
10. $S_T = S_T \cup \{T'\}$ // T'' is new disjoint subtree
11. $n_c = n_c + 1$
12. Compute the center C_i of T_i using eccentricity of points
13. Compute the diameter of T_i using eccentricity of points
14. Compute the variance of T_i
15. $C = U_{Ti} \in S_T \{C_i\}$
16 Until $n_c = k$
17. **Return** k clusters

Euclidean Minimum Spanning Tree is constructed at line 1. Average of edge weights and standard deviation are computed at lines 2-3. The variance of input data set S is computed at line 4. Using the average weight and standard deviation, the inconsistent edge is identified and removed from Euclidean Minimum Spanning Tree (**EMST**) at lines (8-9). Subtree (cluster) is created at line 10. Radius, diameter and variance of subtree are computed at lines 12-14. Lines 9-15 in the algorithm are repeated until k number of subtrees (clusters) are produced. The radius and diameter are good measure to find the tightness of clusters. The radius and diameter values of each cluster are expected low value for good cluster. If the values are large that the points (objects) are spread widely. However if the value of k increases the radius and diameter decreases.

The variance for each subtree (cluster) is computed to find the compactness of clusters. A smaller the variance value indicates, a higher homogeneity of the objects in the data set. The cluster compactness measure evaluates how well the subtrees (clusters) of the input is redistributed in the clustering process, compared with the whole input set, in terms of data homogeneity reflected by Euclidean distance metric used by the clustering process. Smaller the cluster compactness value indicates a higher average compactness in the out put clusters.

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, radius, diameter and variance 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 radius; diameter and also theirs center points 5 and 3. Figure 3 shows a graph which shows the relationship between radius and diameter with subtrees (clusters). Lower the radius and diameter value means higher the tightness. The compactness of the sub trees (clusters) is shown in the figure 4. Lower the values of variance means higher the homogeneity of the objects in subtree (cluster).

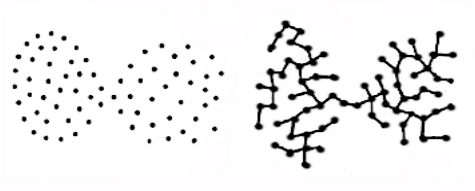

Figure 1. Clusters connected through a point

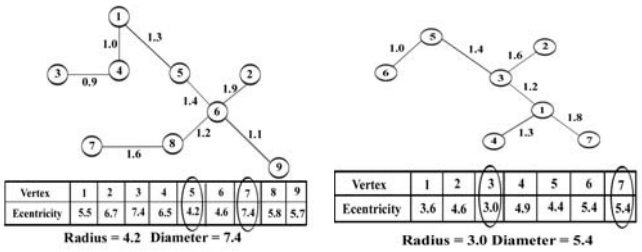

Figure 2. Two Clusters with radius and diameter (5 and 3 as center point)

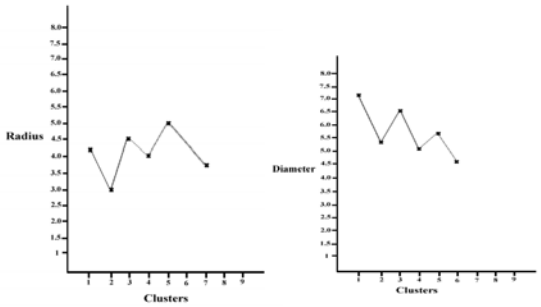

Figure 3: Tightness of clusters using radius and diameter

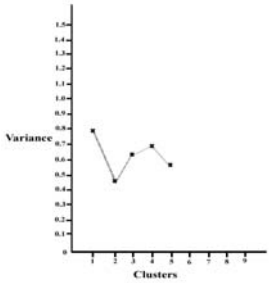

Figure 4. Compactness of clusters

4. CONCLUSION

Cluster validity is one of the most important issues in cluster analysis. It aims at the evaluation of clustering results and the selection of the scheme that best fit for the underlying data. The majority of algorithms are based on certain criteria in order to define the clusters in which a data set can be partitioned. Since clustering process is unsupervised process and there is no a-priori indication for the actual number of clusters presented in a data set, there is a need for clustering results validation. Our **EMSTRDV** 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. The algorithm also finds radius, diameter and variance of clusters using eccentricity of points in a cluster. The radius and diameter value gives the information about tightness of clusters. The variance value of the cluster is useful in finding the compactness of cluster. This information will be very useful in many applications. 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. There is a need for developing quality measures those asses the quality of the partitioning. The validity assessment approaches proposed in the **EMSTRDV** algorithm will works better in various domains.

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