An Efficient Minimum Spanning Tree based Clustering Algorithm

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Abstract— **Clustering analysis has been an emerging research issue in data mining due its variety of applications. In the recent years, it has become an essential tool for gene expression analysis. Many clustering algorithms have been proposed so far. However, each algorithm has its own merits and demerits and can not work for all real situations. In this paper, we present a clustering algorithm that is inspired by minimum spanning tree. To automate and evaluate our algorithm, we incorporate the concept of ratio between the intra-cluster distance (measuring compactness) and the inter-cluster distance (measuring isolation). Experimental results on some complex as well as real world data sets reveal that the proposed algorithm is efficient and competitive with the existing clustering algorithms.**

Keywords-Clustering; minimum spanning tree; gene expression data;* k-*means algorithm

I. INTRODUCTION

Clustering is a process which partitions a given dataset into homogeneous groups based on given features such that similar objects are kept in a group whereas dissimilar objects are in different groups. Clustering plays an important role in various fields including image processing, computational biology, mobile communication, medicine and economics. With the recent advances of microarray technology, there has been tremendous growth of the microarray data. Identifying co-regulated genes to organize them into meaningful groups has been an important research in bioinformatics. Therefore, clustering analysis has become an essential and valuable tool in microarray or gene expression data analysis [1]. In the recent years, although a number of clustering algorithms [2], [3], [4], [5], [6], [7] have been developed, most of them are confronted in meeting the robustness, quality and fastness at the same time. Minimum spanning tree (MST) is an useful data structure that has been used to design many clustering algorithms. Initially, Zahn [8] proposed an MST based clustering algorithm. Later MST has been extensively studied for clustering by several researchers in biological data analysis [9], image processing [10], [11], [12] pattern recognition [13], etc. One approach [8] of the MST based clustering algorithm is to first construct MST over the whole dataset. Then the inconsistent edges are repeatedly removed to form connected components until some terminating criterion is met. The resultant connected components represent the different clustering groups. The other approach is to maximize or minimize the degrees of the vertices [14], which is usually computationally expensive. Recently, Wang et al. [15] proposed a MST based clustering algorithm using divide and conquer paradigm. Gryorash et al. proposed another MST based clustering algorithm that can be found in [16]. As stated in [9] that MST based clustering algorithm does not depend on the detailed geometric structure of a cluster and therefore, it can overcome many of the problems that are faced by many classical clustering algorithms. The other graphical structures such as relative neighborhood graph (RNG) Gabriel graph (GG), Delaunay triangulation (DT) have also been used for cluster analysis. The relationship among these graphs can be seen as $MST \subseteq RNG \subseteq GG \subseteq DT$ [18]. However, they may not produce good clustering results for the dimension more than five [15].

Motivated with this, we propose, in this paper, a new MST based clustering algorithm. Our algorithm has no specific requirement of prior knowledge of some parameters and the dimensionality of the data sets. We run our algorithm on a number of synthetic dataset as well as real world dataset. For visual judgment of the performance of the proposed algorithm, we show the experimental results on some already known data sets as well as some real world data sets from UCI machine learning repository [17].

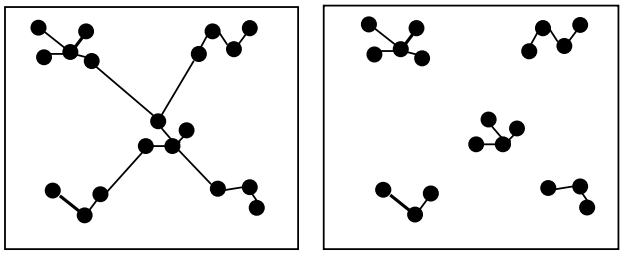
The rest of the paper is organized as follows. We introduce the necessary concept of MST and other terminologies in section II. The proposed algorithm is presented in section III. The experimental results are shown in section IV followed by the conclusion in section V.

II. TERMINOLOGIES

A. Minimum Spanning Tree (*MST*)

Given a set of N data points, a minimum spanning tree is a spanning tree that connects all the data points either by a direct edge or by a path and has minimum total weight. The total weight is the sum of the weights of all the edges of the spanning tree. In MST based clustering analysis, the weight

for each edge, is usually considered as the distance between the end points forming the edge. Removal of the longest edge results into two-group clustering. Removal of the next longest edge results into three-group clustering and so on [15]. Five-group clustering after removal of successive longest edges (four) is shown in Fig. 1.



(b) An MST connecting all the data points

(a) Clusters after removal of longest edges

Figure 1. MST representation and five-group clustering

B. Validity Index

Validity index is generally used to evaluate the clustering results quantitatively. In this paper we focus on the validity index, which is based on compactness and isolation. Compactness measures the internal cohesion among the data elements whereas isolation measures separation between the clusters [18]. We measure the compactness by Intra-cluster distance and separation by Inter-cluster distance, which are defined as follows.

Intra-cluster distance: This is the average distance of all the points within a cluster from the cluster centre given by

$$Intra = \frac{1}{N}\sum_{i=1}^{k}\sum_{x\in C_i}\left\|x - z_i\right\|^2 \qquad (1)$$

Inter-cluster distance: This is the minimum of the pair wise distance between any two cluster centers given by

$$Inter = Min\left\|z_i - z_j\right\|^2 \qquad (2)$$

In the evaluation of our clustering algorithm, we use the validity index proposed by Ray and Turi [19] as follows

$$Ratio\ (validity) = \frac{Intra}{Inter} \qquad (3)$$

Threshold value: This denotes the limit when two points get disconnected if the distance between them is greater than this limit.

III. PROPOSED ALGORITHM

The basic idea of our proposed algorithm is as follows.

We first construct MST using Kruskal algorithm and then set a threshold value and a step size. We then remove those edges from the MST, whose lengths are greater than the threshold value. We next calculate the ratio between the intra-cluster distance and inter-cluster distance using equation (3) and record the ratio as well as the threshold. We update the threshold value by incrementing the step size. Every time we obtain the new (updated) threshold value, we repeat the above procedure. We stop repeating, when we encounter a situation such that the threshold value is maximum and as such no MST edges can be removed. In such situation, all the data points belong to a single cluster. Finally we obtain the minimum value of the recorded ratio and form the clusters corresponding to the stored threshold value. The above algorithm has two extreme cases: 1) with the zero threshold value, each point remains within a single cluster; 2) with the maximum threshold value all the points lie within a single cluster. Therefore, the proposed algorithm searches for that optimum value of the threshold for which the Intra-Inter distance ratio is minimum. It needs not to mention that this optimum value of the threshold must lie between these two extreme values of the threshold. However, in order to reduce the number of iteration we never set the initial threshold value to zero.

Let us now describe the notations used in the pseudocode of our algorithm as follows.

Notations used:

N: Number of data points; D: Dimension of each data point
Data[N][D]: Data matrix
Step_size: Step size by which to increment the threshold after each iteration.
Signal: Variable used to check termination criterion.
ARatio[N]: Array which holds ratio (equation 3) after each iteration.
AThreshold[ ]: Array which holds threshold value after each iteration.
T[N][N]: Adjacency matrix returned by Kruskal algorithm.
Storage[2(N-1)][D+1]: Matrix used to store the end points of the edges that are removed from MST .
Counter1: Variable to keep track of the rows of the Storage matrix.
Index[N]: Array to hold the cluster number, a data point belongs to.
Store[N - 1]: Array used to store connected components.
Cluster_no[ ]: Stores the number of cluster center.
Counter2, Counter3, Cluster_no, iteration: Temporary variable.
$d(i, j)$: denotes Euclidean distance between data points i and j.
*: denotes all the columns (dimensions) for multivariate data.

Pseudocode of Algorithm MST_Clustering:

Initialize Threshold, Step_size, Signal:= 0; iteration := 1
Apply Kruskal algorithm to get adjacency matrix T
while (Signal = 0) do // checking whether all the data point are in a single cluster //
Counter:= 1; Cluster_no:= 0;

```
Index [i]:= 0.0, 1 ≤ i ≤ N
AThreshold[iteration] := Threshold
// storing end points with edge weight > Threshold and
   removing that edge from MST //
Storage[i][j]:= 0.0,  1 ≤ i ≤ 2(N - 1), 1 ≤ j ≤ D + 1
for i := 1 to (N - 1) do
   j := i + 1
   while (j <=  N) do
      if ((T[i][j] = 1) & (d(i, j) > threshold))
       {
        T[i][j]:= 0;   T[j][i]:= 0;
        Storage[Counter1][k] := Data[i][k], 1 ≤ k ≤ D
        Storage[Counter1][D + 1] := i
        Storage[Counter1 + 1][k] :=Data[j][k], 1 ≤ k ≤ D
        Storage[Counter1 + 1][D + 1] := j
        Counter1 := Counter1 + 2
        j := j + 1
       }
   endwhile
end for
Cluster_no := (Counter1 + 1)  /  2
Counter1 := 1
// Finding cluster number of each data point //
while (Storage[Counter1][D+1]  >  0) do
    Store[i]:= 0.0, 1 ≤ i ≤ N
    Counter3:= 1;  Counter2:= 1
     while (Index[Storage[Counter1][D+1]] > 0) do
         Counter1:= Counter1 + 1;
         if (Storage[Counter1][D + 1] = 0)
            {
             Counter1:= Counter1 – 1;
             break
            }
      endwhile
        if (Storage[Counter1][D+1]  > 0)
          {
            Index[Storage[Counter1][D+1]] := Counter1
            for i := 1 to N do
               if (T[Storage[Counter1][D+1][i] > 0)
                  {
                    Index[i] := Counter1;
                    Store[Counter3] := i ;
                    Counter3 := Counter3 + 1
                  }
             endfor
          }
          while (Store[Counter2] > 0) do
               for i := 1 to N do
                  if ((T[Store[Counter2]][i] > 0) AND
                    (Index[i] := 0))
                       {
                        Index[i]:=Counter1;
                        Store[Counter3] := i;
                         Counter3:= Counter3 + 1
                       }
                  endfor
                  Counter2:= Counter2 + 1
          end while
          Counter1:= Counter1 + 1
      endwhile
       ARatio[iteration]:= Intra / Inter ; // from (1) and (2) //
       iteration:= iteration + 1
       for i := 1 to N do
            if (Index[i] ≠ 1)
              {
                Signal := 0
              }
            else
              {
                break
              }
       endfor
       if (i = N+1)
         {
          Signal:= 1
         }
       Threshold:= Threshold + Step_size
endwhile
```

Time Complexity: It can be seen that the proposed algorithm consists of two phases. In the first phase, we construct the MST using Kruskal algorithm that requires O(N log N) time. In the second phase we find the connected components by removing those edges from MST whose edge weight (length) is greater than the chosen threshold. The outermost while loop of this iterates k times. Inside it, the nested while-for / for-while loops may run at most N^2 times. Therefore, the overall time complexity is $O(kN^2)$ .This is comparable with k-means.

IV. EXPERIMENTAL RESULTS

We have tested our algorithm on a number of synthetic datasets as well as the real world data sets (Iris, Wine and Spect heart) using MATLAB. The experiments were performed on a Intel Core 2 Duo Processor machine with T9400 chipset, 2.53 GHz CPU and 2 GB RAM running on the platform Microsoft Windows Vista. To investigate, we first run our algorithm on one simple and two complicated clustering problems and exclusively use two dimensional data points for the visual convenience of their performance. The first set consisting of 510 data points has well separated clusters, referred as easy clustering problem here. Like the other researchers [2], [15], [21], we also run the k-means algorithm [20] on the same sets of data to measure the relative performance. For the run of the k-means, we input the same number of clusters as have been produced by our algorithm. The experimental results of the proposed and the k-means algorithm are shown in Fig. 2 and Fig. 3 respectively. Both the algorithms successfully create five well separated clusters shown by different colors with the same color for all the data points inside a cluster. Note that all the points inside a cluster are connected for our proposed algorithm as it is basically an MST. The next two sets of 550 and 491 data points have

curve and kernel (ring inside a ring) shapes which are known to be difficult clustering. The results of the proposed and the *k*-means algorithm are shown in Figs. 4-7. This is important to note that the clusters generated by the *k*-means are interspersed (see Fig. 5 and Fig. 7), whereas our proposed algorithm has successfully created two clusters as shown in Fig. 4 and Fig. 6.

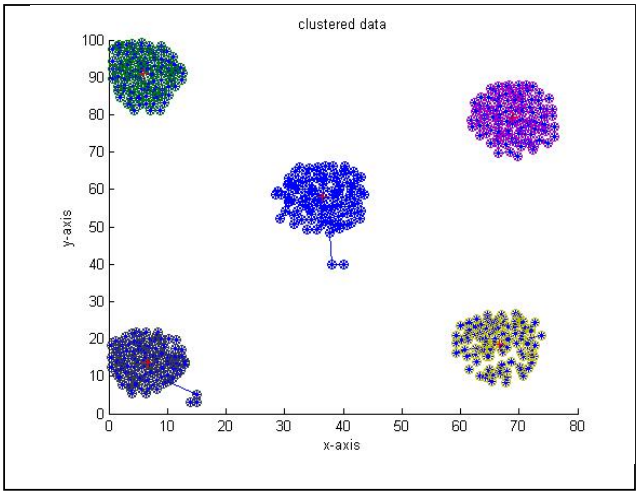


Figure 2. Result of the proposed algorithm on synthetic data of size 510

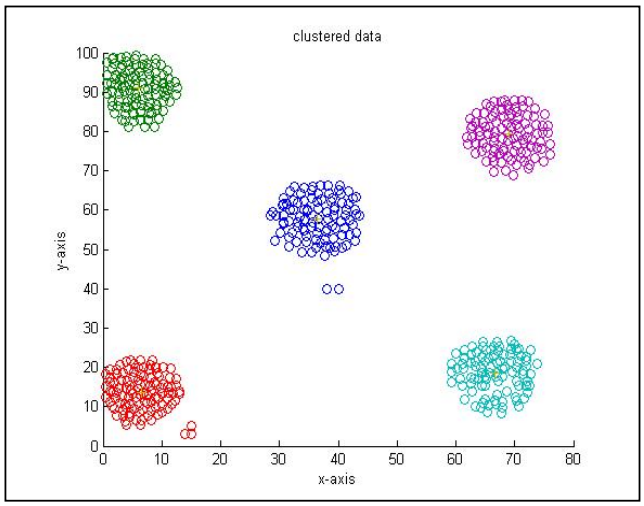


Figure 3. Result of *k*-means on synthetic data of size 510

We next run on multi-dimensional data sets, namely Iris, Wine and Spect heart [17] with 4, 14 and 22 attributes form UCI machine learning repository. The descriptions of these data sets can be found in [17]. The results of the runs of our algorithm are compared with the *k*-means algorithm with respect to the Intra-inter ratio (equation 3) as shown in Table 1. It clearly shows that our proposed algorithm has better intra-inter ratios than the *k*-means.

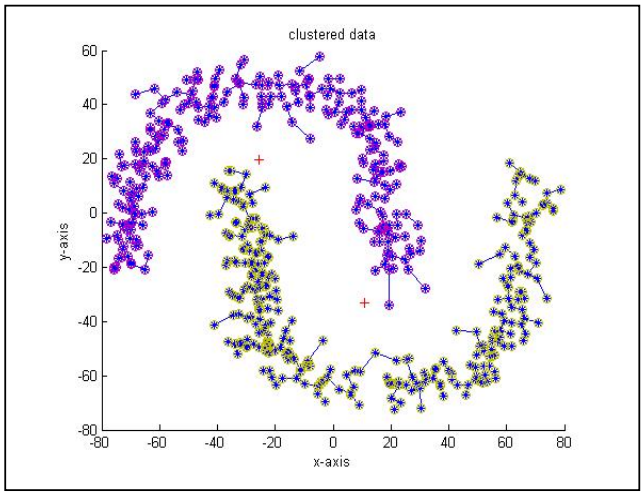


Figure 4. Result of the proposed algorithm on curve data of size 550

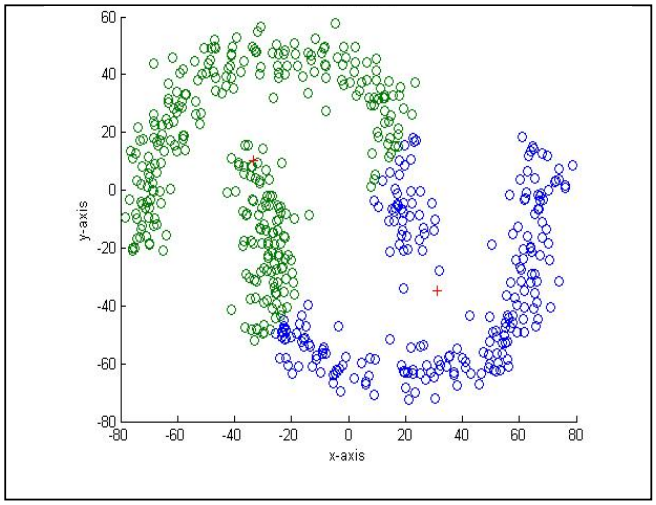


Figure 5. Result of *k*-means on curve data of size 550

V. CONCLUSION

In this paper, we have presented a clustering algorithm which is based on minimum spanning tree. Unlike the other algorithms such as *k*-means, the algorithm does not require any prior parametric value, e.g., number of clusters, initial cluster seeds etc. We have shown the experimental results of our algorithm on some synthetic as well as multivariate real data sets, namely Iris, Wine and Spect heart. Experimental results demonstrate that the proposed algorithm performs better than the *k*-means.

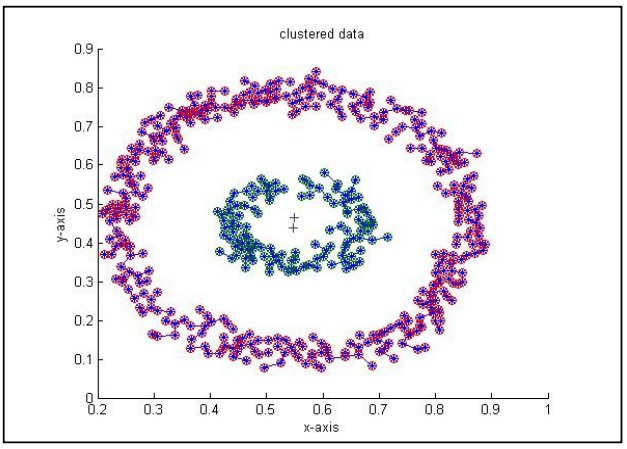


Figure 6. Result of the proposed algorithm on kernel data

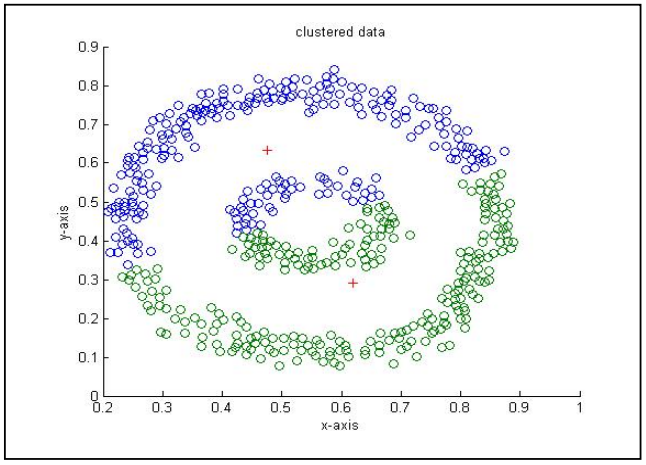


Figure 7. Result of *k*-means on kernel data of size 491

TABLE 1 COMPARISON WITH RESPECT TO INTRA-INTER DISTANCE RATIO

Name	Attributes	Data Size	Cluster Number	Ratio (*K*-means)	Ratio (Ours)
Iris	4	150	3	0.2888	0.1492
Wine	13	178	3	0.1895	0.0924
Spect-heart	22	267	2	2.3652	1.8806

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