Novel Clustering based on Discrete Morse Technique

Jian Ping Zhang¹, Xi Yu Liu¹ and Yong Li²

¹School of Management Science and Engineering, Shandong Normal University, No.88 Culture East Road, Ji'nan, China ²Institute of Information Engineering, BinZhou University, No.391 Huanghe Road, BinZhou, China

Keywords: Density Clustering, Simplicial Complexes, Discrete Morse Function, Discrete Gradient Vector Field.

Abstract: A new clustering algorithm based on discrete Morse theory is proposed for cluster analysis in this paper. Firstly, an energy surface is defined on data set by Gaussian kernel functions. Secondly, a simplicial complex can be obtained by hull Triangulation on the energy surface. Finally, the optimization model based on discrete Morse theory is adopted to find cluster centers and clusters on a simplicial complex. It is a novel approach. The experimental results on some synthetic and UCI data sets have demonstrated that the new algorithm can discover clusters with arbitrary shapes and densities at different levels, moreover it can successfully divide data points overlapping into many meaningful clusters. The results show the feasibility and effectiveness of the new clustering algorithm.

1 INTRODUCTION

Clustering analysis (Han and Kamber, 2006) is used to handle classification problem by mathematical methods, and is an important part of non-supervised pattern classification in pattern recognition. In recent 30 years, it has been developed drastically. The aim of Clustering (Chan et al., 2003) (Kaufman and Rousseeuw, 2009) (Hubert et al., 1999) (Chen et al., 1996)is that the intracluster similarity is maximized and the intercluster similarity is minimized. Clustering in the sample space is an optimization problem of objective function. There have been many kinds of clustering algorithms based on computational intelligence(CI) techniques, such as fuzzy control, neural networks, evolutionary computation, swarm intelligence, artificial life and DNA computation (Graves and Pedrycz, 2007) (Pal et al., 1993) (Babu and Murty, 1994) (Bader et al., 2004). The CI-based clustering analysis models have a good ability to adapt to characteristics of objects and it can make up for the disadvantages of classical clustering algorithms. However, the data mining system should process more complex data sets with arbitrary shapes, arbitrary distribution and densities at different levels with the application fields of data technology continuously. mining expanding Therefore, new techniques are still a good choice to get more insight into cluster analysis.

Morse theory appears in topology of smooth

manifolds (Milnor, 1963). Discrete Morse theory is a combinatorial analogue of Morse theory developed by Forman (Forman, 1995) (Forman, 1998). Making the points more dense does not allow one to use smooth methods to analyze the qualitative behavior of f. This problem was addressed by Edelsbrunner in (Edelsbrunner et al., 2003). Researchers find that discrete Morse theory is a discrete analogue of a technology called steepest descent method, which has extreme importance in optimization. In (Zhang and Liu, 2014), we propose a method to construct discrete Morse function that mirrors the large-scale behavior of f and has the minimum possible number of critical cells by optimization analysis on given f in 3-D or higher dimension space and present an optimization model based on discrete Morse theory that can obtain an optimal value or approximate optimal one

In this paper, we have proposed a new clustering algorithm based on discrete Morse optimization model. The algorithm is mainly to adopt to the thought of hierarchical clustering based on kernel density estimation. In our approach, local minima (the density attractors) are chosen to generate the center-defined data partition, and finally the center-defined clusters are iteratively merged into one cluster by cancelling critical cells. The experimental results on two synthetic data sets and UCI data sets have demonstrated that the new algorithm can discover clusters with arbitrary shapes, arbitrary distribution and densities at

different levels. The comparisons with DBSCAN method further show that the proposed algorithm can successfully divide data points overlapping in the feature space into many meaningful clusters.

2 OPTIMIZATION MODEL BASED ON DISCRETE MORSE THEORY

In this section we present a general discrete structure which will be useful for clustering and propose an optimization model based on discrete Morse theory.

Now we will present some notation. A finite data set is denoted by $X = \{x_1, x_2, ..., x_n\} \subset \mathbb{R}^n$, $x_i = [x_{i_1}, x_{i_2}, ..., x_{i_d}]$, $i = 1, 2, ..., n \cdot h : X \to \mathbb{R}$ is a map function defined on a data set X. A function $S = \{(x_i, h(x_i)) | i = 1, 2, ..., n\} \subset \mathbb{R}^{n+1}$ is called a discrete surface. A q-simplex σ (denoted by $\sigma^{(q)}$) is the convex hull of q+1 affinely independent points $A = (a_0, a_1, ..., a_q)$. The cone from a vertex $x(x_i \notin \sigma^{(q)})$ to a q-simplex $\sigma^{(q)}$ is the convex hull of x and $\sigma^{(q)}$ which yields a (q+1)-simplex $\sigma^{(q+1)}$. A simplicial complex K is a set of simplices that satisfies the following conditions: 1. $v \in K$ if $\sigma \in K$ and $v < \sigma$ 2. $\sigma_1 \cap \sigma_2 = \phi$ or $\sigma_1 \cap \sigma_2 = \tau, \tau \in \sigma_1, \tau \in \sigma_2$ if $\sigma_1, \sigma_2 \in K$.

2.1 The Discrete Structure: A Simplicial Complex

In order to get discrete surfaces, we define a hull triangulation. Let the convex hull of $X = \{x_1, x_2, ..., x_n\} \subset \mathbb{R}^n$ be hull(X). If $x_i \in X$ is an interior point of hull(X), then there exists a neighbor in *S* of $(x_i, h(x_i))$ homeomorphic to \mathbb{R}^n . Otherwise if $x_i \in X$ is an boundary point of hull(X), then there exists a neighbor in *S* of $(x_i, h(x_i))$ homeomorphic to \mathbb{R}^n . Otherwise if $x_i \in X$ is an boundary point of hull(X), then there exists a neighbor in *S* of $(x_i, h(x_i))$ homeomorphic to the halfspace of \mathbb{R}^n . Clearly the hull triangulation is a n-dimensional manifold with boundary.

We take Delaunay Triangulation as a tool of hull triangulation. Firstly we generate a Delaunay triangulation of $X = \{x_1, x_2, ..., x_n\} \subset \mathbb{R}^n$. A q+1 simplex is generated by q-simplex connecting one point $x_i \in X$. For each simplex, the unique ball circumscribed about the simplex contains no data points other than the vertices. Secondly generate simplicial complex K by replacing the vertices with its corresponding vertices on the surface. a simplicial complex K is composed by the following way (Figure 1).



Figure 1: The generating process of a simplicial complex.

Figure1(b) denotes that D-Triangulation on DataSet1 in 2D and Figure1(d) means surface based on the probability density function(σ =1) on based on DataSet1 in 2D.

Table 1 shows the running time of generating a simplicial complex K based on the probability density function (the window width $\sigma = 1$) on a data set $X = \{x_1, x_2, ..., x_n\} \subset \mathbb{R}^n$

Table 1: The running time of generating a simplicial complex.

dat	CPU (s)	
DataSet1	(300 2-D points)	0.002
DataSet2	(500 2-D points)	0.003
Haberman's Survival	(306 3-D points)	0.018
Iris	(150 4-D points)	0.055

2.2 Discrete Morse Theory

Definition 1[12] (discrete Morse function). A function $f: K \to R$ is a discrete Morse function, if for every $\sigma^{(p)} \in K$, the following two conditions hold:

$$\#\{\tau^{(p+1)} > \sigma^{(p)} : f(\tau) \le f(\sigma)\} \le 1$$

and $\#\{\upsilon^{(p-1)} < \sigma^{(p)} : f(\upsilon) \ge f(\sigma)\} \le 1$ (1)

Definition 2[12] (critical simplex). Let $f: K \to R$ be

a discrete Morse function. A simplex $\sigma^{(p)}$ is critical if the following two conditions hold:

$$\#\{\tau^{(p+1)} > \sigma^{(p)} : f(\tau) \le f(\sigma)\} = 0$$

and $\#\{\upsilon^{(p-1)} < \sigma^{(p)} : f(\upsilon) \ge f(\sigma)\} = 0$ (2)

A simplex that is not critical is called regular. **Definition 3 (discrete gradient vector field).** A discrete gradient vector field *V* is a collection of pairs $< \alpha^{(p)}, \beta^{(p+1)} >$ of simplices of *K*. for α, β , the following two conditions hold: $\alpha < \beta$ and

 $f(\beta) \leq f(\alpha)$.

Property 1. A discrete Morse function f is generated on the discrete gradient vector field v, then the function f is descending along v - path.

Definition 4 (level cut). Level cut on the simplicial complex *K* is a collection of simplices, where a simplex α is included if values of all its vertices $x \in \alpha$ are below the threshold *t*. i.e, $K(t) = \{\alpha \in K \mid h(x) \le t, \forall x \in \alpha\}$.

Definition 5 (Simple homotopy). (Lewiner and Lopes,2003)A simple homotopy(i.e, a continuous deformation) is a succession of collapses and extensions. If two complexes are related by a simple homotopy, we say they have the same simple homotopy type.

In this paper, discrete gradient vector field is generated based on discrete Morse theory by using simple homotopy expansions to grow from one subcomplex to the next.

2.3 Optimization Algorithm: DVF-Algorithm

The goal of our algorithm is to construct a discrete Morse function on the simplicial complex which can obtain the extreme value of given function. The algorithm is based on simple homotopy expansions which grow from K(t-1) to K(t) iteratively. Now we will present two definitions.

Definition 6 (lower star). (Lewiner and Lopes,2003) The lower star S(x) of a vertex *x* contains of all simplices that contain *x* as a face, including *x* itself, and hold $g(x) = \max g(\alpha)$.i.e.

 $S(x) = \{ \alpha \in K \mid x \in \alpha, g(x) = \max g(y) \}.$

Definition 7 (lower link). The lower link L(x) of a vertex x consists of all faces of simplices in the lower star that are disjoint from x. i,e. $L(x) = \{v \in K | v \subseteq \alpha \in S(x), v \cap x = \phi\}$

According Definition6 and Definition7, we present a definition of the closed lower star of a vertex x: $\overline{S(x)} = S(x) \cup L(x)$.

DVF-Algorithm contains two steps: ConstructDVF(K,g) and CancelCriticalCell(K,g,j,p). *ConstructDVF*(K,g) generates critical cells C and constructs discrete gradient vector field V; *CancelCriticalCell*(K,g,j,p) modifies C and V so that it can produce the minimum possible number of critical cells. Algorithm1. *ConstructDVF*(K,g)

Step1 input a complex K, a mapping function $h: K_0 \to R$;

Step2 $x \in K_0$, if $L(x) = \phi$, add x to C; otherwise let $h': K_0 \to R$ be the restriction of h;

Step3 find the $y \in L(x)$ so that h'(y) is the smallest; denote $\omega = xy$ and define $V[x] = \omega$; add all other 1-cells from S(x) to *QueueZero*, add all cells $\alpha \in S(x)$ to *QueueOne* such that $\alpha > \omega$ and num_unpaired_faces(α) = 1;

Step4 assign the front cell from *QueueOne* to α , if *num_unpaired_faces*(α) $\neq 0$, then $V[pair(\alpha)] = \alpha$, delete $pair(\alpha)$ from QueueZero; add the cells $\beta \in S(x)$ to QueueOne such that $\beta > \alpha$ or $\beta > pair(\alpha)$ and num_unpaired_faces(α) = 1, until *QueueOne* = ϕ ; if *QueueZero* $\neq \phi$, then assign the front cell γ from *QueueOne* to *C* ; add $\alpha \in S(x)$ that $\alpha > \gamma$ to QueueOne such and $num_unpaired_faces(\alpha) = 1$; repeat Step4 , until *QueueOne* = ϕ and *QueueZero* = ϕ

Step5 Return to Step2, until $K_0 = \phi$

The algorithm1 works on the links of vertices. There is an alternative definition of h in the lower link of x with the property that the vertex with the minimum value of h more closely approximates the direction of steepest decrease of h. In the alternative definition, we set

$$h'(y) = (h(y) - h(x)) / l([x, y])$$
 (3)

where l([x, y]) is the length of the edge [x, y]. The function *num_unpaired_faces*(α) which returns the number of faces of α are in S(x) have not yet either C or been inserted in V . If $num_unpaired_faces(\alpha) = 0$ in QueueZero , it is denoted that there is no $pair(\alpha)$ for the cell α ; $num_unpaired_faces(\alpha) = 1$ otherwise if in *QueueOne*, then there is exactly one $pair(\alpha)$ for the cell α , which is a candidate for homotopic expansion. In Step2, If $L(x) = \phi$, x is critical and is a local minimum . Otherwise, x is paired with its lowest incident edge $\omega = xy$, denoted $V[x] = \omega$. this

is a simple homotopy expansion. In *Step4*, there is a pair $V[pair(\alpha)] = \alpha$, if two conditions hold: $\alpha \in L(x)$ and *num_unpaired_faces*(α) = 1. The expansion proceeds until *QueueOne* = ϕ and *QueueZero* $\neq \phi$, then a critical cell is created and the expansions then proceed from the new cell. The algorithm terminates because there are a finite number of 0-cells selected. Each cell in *S*(*x*) will be paired and included in *V* or inserted into *C* by the algorithm1.

In order to construct optimal discrete Morse function which has the minimum possible number of critical present cells, we Algorithm2 CancelCriticalCell(K, g, j, p). In the discrete gradient vector field V, it is necessary to wait to cancel until we found the pair $\sigma \in C_{i-1}$, $\tau \in C_i$ connected by exactly one gradient path so that $\max h(\tau) - \max h(\sigma)$ is minimized. In optimization model based on discrete Morse theory, the value of the parameter p that controls cancellation is as large as possible. In our new clustering framework, we obtain a different number of critical 0-cells by adjusting the parameter p, and the critical 0-cells can be taken as clustering centers.

Algorithm2. *CancelCriticalCell*(*K*, *g*, *j*, *p*)

Step1 $\tau \in C_i$;

Step2 find all gradient paths $\tau = \tau_{i1} \rightarrow \tau_{i2} \rightarrow ... \rightarrow \tau_{il_i} \in C_{j-1}$ with $\max h(\tau) - \max h(\tau_{il_i}) < p$; if the pair $\tau_{il_i} \in C_{j-1}$, $\tau \in C_j$ connected by exactly one gradient path, let $m_i = \max\{h(\tau_{il_i})\}$;

Step3 if at least one m_i is defined, pick $m_j = \max\{m_i\}$. if each cell β in the gradient path holds $h(\beta) < \delta$, execute Step4; otherwise return to Step1;

Step4 find the unique gradient path

 $\begin{aligned} \tau &= \tau_1 \rightarrow \sigma_1 \rightarrow \tau_2 \rightarrow \sigma_2 \rightarrow \dots \rightarrow \sigma_j = \sigma \in C_{j-1} \quad \text{,thus} \quad V(\sigma_i) = \tau_{i+1} \quad \text{,} \\ \sigma_i \text{ is a face of } \tau_i \text{ and } \sigma_i \neq \sigma_{i+1}; \end{aligned}$

Step5 delete σ and τ from *C*; reverse direction from τ to σ , $V(\sigma_i) = \tau_i$;

Step6 repeat Step1 , until no $\tau \in C_j$ to be selected.

Then we propose a method to construct discrete Morse function. The method for constructing discrete Morse function on a simplicial complex Kis motivated by the techniques of an extension of hto a discrete Morse function f with the same modified Hasse diagram in (King et al., 2005). Let *x* be a vertex and let S(x) be its lower star. We record the order that cells from S(x) inserted into *V* or *C* by **Definition1** that if $V(x) = \delta$, then δ will precede *x*. This algorithm ordering is $\delta, x_i, \alpha_{i_1}, \alpha_{i_2}, ..., \alpha_{i_{k-2}}$ for $i_j \in 1, ..., k-2$ ($S(x_i)$ has k > 2 cells). Now we can define a discrete Morse function on $S(x_i)$ as follows: given $\varepsilon > 0$

$$\begin{cases} f(\delta) = h(x_i) - \varepsilon; \\ f(x_i) = h(x_i); \\ f(\alpha_{i_i}) = h(x_i) + j\varepsilon; \end{cases}$$
(4)

The definition for f extends to all vertices $x \in X$, and all cells $\alpha \in K$. then f is a discrete Morse function on the simplicial complex K.

According to Algorithm1, All other faces of β must have been inserted into *V* or *C* at an earlier point, so α is the single face of β with greater *f* - value. If $\gamma \in C$, it shows that all faces of γ inserted earlier and all of its cofaces are added later, so the conditions for a critical cell of a discrete Morse function are also satisfied by *f*.

3 NEW CLUSTER FRAMEWORK BASED ON DISCRETE MORSE OPTIMIZATION MODEL

In our density-based clustering framework, we choose discrete Morse theory as a clustering tool, which can efficiently partition each data point into the corresponding cluster. It's a novel method. The new cluster framework based on discrete Morse optimization model (CADMOM) is a graph-based theoretic (King et al., 2005) clustering method. Each tree represents a cluster, many trees can form a forest. The root node of each tree represents one vertex in bottom regions whereas most leaf nodes are regarded as vertices situated in the valley regions.

Definition 8 (Kernel Density Estimation). (Fukunag, 1990) The discrete Morse optimization model is based on the steepest descent characteristic on discrete gradient vector field, which follows negative gradient flow. Let *n* data points in the d-dimensional space, $X = \{x_1, x_2, ..., x_n\}$, where the data vector is $x_i = [x_{i1}, x_{i2}, ..., x_{id}]$, i = 1, 2, ..., n. The probability density of the data is given by the following kernel density estimation:

$$h(x) = -\frac{1}{(N)} \sum_{i=1}^{N} K(\frac{x - x_i}{\sigma})$$
(5)

then we choose the Gaussian function as the kernel, which can be described as follows:

$$K(\frac{x-x_i}{\sigma}) = \exp(-\frac{\|x-x_i\|^2}{2\sigma^2})$$
(6)

We can obtain the local minima of the overall density function h(x) in their local regions, which are root nodes of trees and can determine mathematically clusters.

3.1 The Formation of Initial Clusters

Each cell in S(x) will be paired and included in V or inserted into C by Algorithm1, so we can obtain the Hasse diagram of vector field. On 0-1 level, one vertex v_0 following steepest descent path (V – Path) reaches the next vertex v_1 that can be called the predecessor of v_0 . v_2 continues to look for its predecessor v_3 . If a node does not have a predecessor, we call it the root node of a tree. Correspondingly, the nodes cannot be the predecessor of other nodes, we call them leaf nodes. In this way, a series of branches is called a directed path, which is discrete gradient path. Clustering on discrete gradient vector field forms a directed tree. When all the data points are visited, a forest will be generated and each tree in this forest represents a cluster. Several V - paths: $\alpha_0^{(p)}, \beta_0^{(p+1)}, \alpha_1^{(p)}, \beta_1^{(p+1)}, ..., \beta_r^{(p+1)}, \alpha_{r+1}^{(p)}$ can be obtained by Algorithm1. Data points can be quickly divided into the corresponding clusters by searching predecessors of nodes.

In the new clustering framework, we can take $\alpha \in C_0$ as a cluster center, whose cluster contains 0-cells in V-Path taking a critical cell $\alpha \in C_0$ as the end points. thus the initial clusters can be formed.

3.2 The Mergence of Clusters

Consider 0-1 level. A critical 1-simplex $\tau \in C_1$ is the start of exactly two gradient paths, if τ is connected to $v \in C_0$ by a single gradient path, it must be connected to some other vertex $w \in C_0$ by a single gradient path. If any 0-cell $y \in V - paths$ that are from $\tau \in C_1$ to $v \in C_0$ and from $\tau \in C_1$ to $w \in C_0$ holds $f(y) \ge \delta$, then we can choose min{max $h(\tau) - \max h(v), \max h(\tau) - \max h(w)$ } to merge clusters. These steps can be repeated until the

desired number of clusters is obtained by Algorithm2.

3.3 The New Clustering Framework based on Discrete Morse Optimization Model

Through the above analyses, the total algorithm can be divided into two parts: constructing the simplicial complex on an energy surface and clustering on the simplicial complex. Now, we can describe the whole algorithm steps for our discrete Morse optimization model-based clustering framework as follows:

Step1 Input the data set $X = \{x_1, x_2, ..., x_n\}$;

Step2 Compute the probability density $h(x_i)(i=1;2;...;n)$ for each data according to (5) with Gaussian kernel in (6);

*Step*3 construct the simplicial complex on a discrete surface according to 2.1;

*Step*4 compute each initial clusters according Algorithm1;

Step5 merge clusters that meet conditions based on hierarchical clustering (Wang et al., 2009) by Algrithm2;

In this paper, the computation is based on a discrete surface generated by the density function, so we should restore clustering results to clusters about the data set $X = \{x_1, x_2, ..., x_n\} \subset \mathbb{R}^n$. the distribution of data points is determined by level sets. Now we present the new clustering framework, See Figure 2.



Figure 2: Procedure of the new clustering framework.

4 EXPERIMENTAL RESULTS AND ANALYSIS

In this section, we present the experimental results and analysis of our discrete Morse optimization model-based clustering framework on some synthetic and UCI data sets. The implementation of these algorithms is in Visual C++ 2010. Matlab7.0 and Geomview are adopted to display graphics.

4.1 Parameter Setting

As shown in the algorithm in Section 3.3, the new algorithm requires three input parameters, i.e., the window width σ , the cancelling critical simplex parameter p, the threshold of the density δ . the window width σ can be set to a value in the scope of 0.1-2. the cancelling critical simplex parameter p can be set to a value in the scope of 0.01-0.5. the threshold of the density δ is fixed $\delta = 0$ for all experiments.

4.2 Experimental Results of Synthetic Data Sets

The first data set, Dataset1, contains 300 points and has two clusters that are of irregular shapes. The new clustering algorithm is used for clustering in Figure 3(c) for ten times. Expected result can be achieved every time, see Figure 3(b). One cluster contains data points represented by '+', the other contains data points represented by '+'. The total processing time of our clustering framework is 1.3s.



Figure 3: Clustering 2D- Dataset1 using the new clustering algorithm.

The second data set, Dataset2, contains 600 points and has three clusters that are of different shape, size, density. The clusters partially overlap. The new clustering algorithm is used for Clustering in Figure 4(a) for ten times. Expected result can be achieved every time, see Figure 4(b). One cluster contains data points represented by '+', one contains data points represented by '+'. The total processing time of our clustering framework is 1.8s.



Figure 4: Clustering 2D- Dataset2 using the new clustering algorithm.

4.3 **Experimental Results of UCI**

Haberman's Survival data set and *Iris* data set are used to test our clustering algorithms in this section that are taken from UCI Machine Learning repository. *Gemview* is adopted to display graphics. In the window, there are some black dots (which are the vertices) and some colored balls, some with lines coming from them (these are the critical simplices, The balls are around the barycenter of the simplex and the lines go to the barycenters of its codimension one faces. a purple ball represents a critical vertex.)

The third data set, Haberman's Survival, contains 306 points represented by three features and consists of two classes that partially overlap in the feature space. The proposed clustering framework is used to address the Haberman's Survival data set in 4D space. The proposed clustering framework is used for Clustering in Figure5(a). After implementation of Algorithm1 ConstructDVF(K,g), the number of critical simplices is (4,11,8,0): 4 0critical simplices, 11 1-critical simplices, 8 2-critical simplices, 0 3-critical simplices. a purple ball represents a critical vertex, a green ball represents a 1-critical simplex, An orange ball represents a 2critical simplex, see Figure 5(b). Figure 5(c) and Figure 5(d) show the discrete gradient vector fields of 0-1 level and 1-2 level. Figure 5(e) gives the result cancelling 1-2 level discrete gradient paths by performing Algorithm2 CancelCriticalCell(K, g, j, p), the number of critical simplices is (4,3,0,0). 8 2critical simplices and 8 1-critical simplices are cancelled. 0-critical cells can be cancelled in ascending order by cancelling 0-1 level discrete gradient paths, the remaining ones are taken as the cluster centers separately. A cluster that the cluster center is $\alpha \in C_0$ contains 0-cells in discrete gradient paths taking $\alpha \in C_0$ as the end point.



Figure 5: Clustering 3D-Haberman's Survival using the new clustering algorithm.

From Figure 5, We can see that: (a) Delaunay triangulation on the surface.(b) clustering result executing Algorithm1.(c) 0-1 level discrete gradient paths(denoted by gray lines). (d) 1-2 level discrete gradient paths(denoted by gray lines).(e) Result cancelling 1-2 level discrete gradient paths.

The new clustering algorithm is used for clustering in Figure 5(a) for ten times. The value of σ is in the scope of 0.5~2. The correct clustering rate is 98 percent due to the overlapping between the classes. The overall processing time is 4.3s.

The fourth data set, *Iris*, contains 150 points and consists of three classes(Setosa, ersicolor, and Virginica), with 50 points per classes, represented by four features. Setosa class is linearly separable from the remaining two classes, while the other two classes partially overlap in the feature space. The proposed clustering framework is used to address the *Iris* data set in 5D space and used for Clustering for ten times. σ is in the scope of 0.1~1. The correct clustering rate based on *Iris* data set is 96 percent due to the overlapping between the Versicolor and Virginica classes and the overall processing time was 5.1s.

4.4 Comparisons with DBSCAN Methods

The four data sets shown in 4.2 and 4.3 have been considered to illustrate the advantages of our new framework over other density-based clustering methods. The DBSCAN method (Ester et al., 1996) was used to cluster the four data sets separately. We have set the values of MinPts = [1, 10] and that of Eps = [0.1,1]. The DBSCAN method could produce a correct clustering of DataSet1, otherwise the DBSCAN method failed to find meaningful clusters in DataSet2, Haberman's Survival and Iris due to the overlapping in the clusters. However, the proposed density clustering framework based on the discrete Morse theory method succeeded in detecting the correct clusters, as shown in Figure 4(b), Figure 5(e). Now we present comparisons with DBSCAN methods. See Table 2 and Figure 6.

Table 2: Comparisons with DBSCAN methods.

	datasets	Execution times	DBSCAN	CADMOM
			(correct rate	(correct rate
			%)	%)
	DataSet1	10	class1:100;	class1:100;
			calss2:100	class2:100
	DataSet2	10	class1:31.3;	calss1:99.1;
			calss2:26.4	calss2:96.3
			calss3:60	calss3:100
	DataSet3	10	class1:10.2;	class1:99.1;
			calss2:17.3	calss2:97.5
			class1:13.5;	class1:97.2;
	Iris	10	calss2:10.7	calss2:95.3
			calss3:67.3	calss3:100



Figure 6: Comparisons with DBSCAN methods.

Viewing the experimental results, the new clustering algorithm based on discrete Morse theory can produce satisfactory clusters and generate more

accurate clusters even in the case of the failure of classical clustering algorithms.

5 CONCLUSIONS

Inspired by an optimization model based on discrete Morse theory, we propose the new clustering framework that is mainly to adopt to the thought of hierarchical clustering based on kernel density estimation. The experimental results on some synthetic and UCI data sets have demonstrated that the new algorithm can discover clusters with arbitrary shapes and densities at different levels, moreover it can successfully divide data points overlapping to the feature space into many correct clusters. The results show the feasibility and effectiveness of the new clustering algorithm.

ACKNOWLEDGEMENTS

This work is carried out under the "Taishan Scholar" project of Shandong China. It is also supported in part by the Natural Science Foundation of China (61472231, 61640201) and the Scientific and Technology Project of Shandong Education Bureau.

REFERENCES

- Han, J., Kamber, M., 2006. Data Mining Concepts and Techniques, Morgan Kaufmann Publishers, San Francisco, 2nd edition.
- Chan, E., Ching, W., Ng, M., and Huang J. 2004. An optimization algorithm for clustering using weighted dissimilarity measures. Pattern Recognition.
- Kaufman, L., Rousseeuw, P.J., 2009. Finding Groups in Data: an Introduction to Cluster Analysis. John Wiley & Sons, New Jersey, 3nd edition.
- Hubert, L.J., Arabie, P., and Soete G., 1999 Clustering and Classification. World Scientific, London, 2nd edition.
- Chen, M.S., Han, J., and Yu, P.S., 1996. Data mining: An overview from database perspective. IEEE Transactions on Knowledge and Data Engineering.
- Graves, D., Pedrycz, w., 2007. Performance of Kernel-Based Fuzzy Clustering. Electronics Letters.
- Pal, N. R., Bezdek, J.C. and Tsao, E.C.-K., 1993. Generalized clustering networks and Kohonen's selforganization. IEEE Trans. Neural Network.
- Babu, G.P., Murty, M. N., 1994. Clustering with evolution strategies. Pattern Recognition.
- Bader, J.S., A. Chaudhuri, et al. 2004. Gaining confidence in high-throughput protein interaction networks. Nat Biotechnol.

- Milnor, J.W., 1963. Morse theory. Princeton University Press, Princeton, NJ,
- Forman, R., 1995. A discrete Morse theory for cell complexes. Geometry, Topology and Physics for Raoul Bott. International Press, Boston.
- Forman, R., 1998. Morse Theory for Cell Complexes, Advances in Mathematics.
- Edelsbrunner, H., Harer, J., and Zomorodian, A., 2003. Hierarchical Morse-Smale Complexes for Piecewise Linear 2-Manifolds. Discrete Comput. Geom.
- Zhang, J.P., Liu, X.Y., 2014. An Optimization Model Based on Discrete Morse theory. Systems Engineering - Theory & Practice. In press.
- Lewiner, T., Lopes, H., 2003. Gavares. Toward Optimality in Discrete Morse Theory. J. Experimental Math.
- Edelsbrunner, H., Harer, J., Natarajan, V., and Pascucci, V., 2003. Morse-Smale Complexes for Piecewise Linear 3-Manifolds. In Proc. 19th Ann. Sympos. Comput. Geom. ACM Press, New York.
- King, H., Knudson, K., and Mramor, N., 2005. Generating Discrete Morse Functions from Point Data, Experimental Mathematics.
- Fukunaga, K., 1990. Introduction to Statistical Pattern Recognition, second ed. Academic Press, Boston.
- Wang, X.C., Wang, X.L., and Wilkes, D.M., 2009. A Divide-and-Conquer Approach for Minimum Spanning Tree-Based Clustering. IEEE Transactions on Knowledge and Data Engineering.
- Ester, M., Kriege I, H., Sander, J., and Xu, X., 1996. A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise. Proc. Int'l Conf. Knowledge Discovery and Data Mining.