

Evidence-Based Information Granulation for Three-Way FCM Clustering

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Abstract: *High-dimensional data often contain inherent ambiguity and complex local structures, which limit the performance of deep clustering methods. To address this, we propose a deep three-way FCM clustering method based on evidential information granulation. Our approach integrates contrastive learning into a deep FCM network to learn discriminative features. Using three-way decision theory, samples are divided into positive and boundary regions. A semi-ball neighborhood granulation method is then designed, and evidential theory is applied to fuse neighborhood trust degrees for precise sample reassignment. Experimental results on benchmark datasets show that our method outperforms state-of-the-art approaches in accuracy and normalized mutual information, demonstrating its effectiveness.*

Keywords: Clustering, Fuzzy C-Means Clustering, Three-Way Decision, Information Granulation, Evidential Theory, Contrastive Learning, Data Uncertainty.

1. Introduction

In complex data analysis and intelligent system applications, data objects often exhibit characteristics such as noise interference, inter-class overlap and blurred boundaries, which poses a significant challenge to traditional unsupervised learning methods in practical applications [1]. Existing research shows that when the data distribution deviates from the ideal assumption, classical clustering algorithms are difficult to guarantee in terms of stability and reliability [2]. Hard clustering methods usually assume that samples can be uniquely classified into a certain category and achieve the clustering goal by minimizing intra-class distance, but this assumption is often difficult to hold in high-dimensional or overlapping data scenarios [3]. In particular, algorithms represented by K-means are more sensitive to initial conditions and noisy samples, and are prone to producing unstable clustering results in complex distributed data [4]. In order to improve the model's ability to characterize uncertainty, fuzzy clustering methods introduce a membership mechanism so that samples can belong to multiple clusters at different degrees at the same time [5]. Among them, the Fuzzy C-Means (FCM) algorithm is widely used in unsupervised clustering research due to its clear optimization goal and good interpretability [6][7]. However, the classic FCM method mainly relies on the global distance information between the sample and the cluster center to update the membership degree. When there are many noisy samples or the cluster boundaries are unclear, the membership degree distribution is prone to instability [8]. To this end, researchers have proposed a variety of robust fuzzy clustering methods to reduce the influence of abnormal samples by introducing penalty mechanisms or weight adjustment [9][10].

In recent years, information granulation theory has provided a new research perspective for modeling the uncertainty of complex data. Its core idea is to express the multi-level structure of data by constructing information particles of different granularities [11].

Related studies have shown that information granulation can effectively improve the model's ability to characterize local

structures in high-dimensional mixed distribution and overlapping data scenarios [12][13].

In clustering tasks, introducing the idea of information granulation into model design helps to combine local neighborhood features with overall distribution features, thereby enhancing the stability of clustering results. Information granulation-based clustering methods have shown good application potential in complex data analysis [14]. However, there are often inconsistencies between multi-source information, and it is still difficult to achieve effective fusion by relying solely on granulation structure [15]. Evidence theory provides a unified mathematical framework for the fusion of multi-source uncertain information through basic probability allocation and evidence synthesis rules, and can explicitly express the state of "unknown" and "incompletely uncertain" [16][17].

At the decision-making level, the three-branch decision theory divides the sample into a deterministic region and a boundary region by introducing a delayed decision mechanism, providing a more flexible processing strategy for uncertain samples [18]. This theory has obvious advantages in reducing the risk of misjudgment and improving the robustness of decision-making, and has been gradually applied to machine learning tasks [19][20].

Based on the aforementioned research progress, in recent years scholars have begun to introduce information granulation, evidence theory, and a three-branch decision framework into clustering tasks, forming an information granulation three-branch clustering method. This type of method can more reasonably handle boundary and uncertain samples while maintaining the original clustering objective function structure, thereby improving the stability and interpretability of the clustering results. Building upon the standard fuzzy C-means (FCM) clustering framework, three-branch decision theory is introduced to explicitly divide samples into deterministic and boundary domains at the decision level, thus distinguishing between high-confidence samples and uncertain samples, avoiding the interference caused by the "one-size-fits-all" approach of traditional fuzzy clustering. Furthermore, for boundary domain samples, a

hemispherical neighborhood construction strategy combining directional and distance constraints is proposed, selecting only deterministic samples that are spatially aligned with and close to the cluster center as local evidence sources to improve the reliability of the evidence. Furthermore, by utilizing the membership information of locally determined samples, the membership of boundary samples is redistributed through evidence fusion rules. Without changing the original FCM optimization objective, neighborhood consistency constraints are introduced, making the assignment of boundary samples more robust and improving the overall clustering performance and intra-cluster consistency.

2. Basic Theory

2.1 FCM Clustering

2.1.1 Basic Idea

In the fuzzy clustering framework, given a sample set, $X = \{x_1, x_2, \dots, x_N\}, x_i \in R^d$, the goal is to divide the samples into C clusters. Each sample x_i has a membership degree $u_{ij} \in [0,1]$ with each cluster c_j , representing the degree to which the sample belongs to that cluster. The membership degree matrix $U = [u_{ij}]_{N \times C}$ must satisfy the following constraints:

$$\sum_{j=1}^C u_{ij} = 1, \forall i = 1, 2, \dots, N, \quad (1)$$

$$0 < u_{ij} < 1, \forall i, j.$$

2.1.2 FCM objective function

The Fuzzy C-Means (FCM) algorithm achieves clustering by minimizing the weighted within-class squared error. Its objective function is defined as:

$$J_m(U, V) = \sum_{i=1}^N \sum_{j=1}^C u_{ij}^m \|x_i - v_j\|^2, \quad (2)$$

in:

$V = \{v_1, v_2, \dots, v_C\}$ For the set of cluster centers; $m > 1$ The fuzzy index is used to adjust the degree of fuzziness in membership; $\|\cdot\|$ it is usually Euclidean distance. m The value of this parameter has a significant impact on the clustering results. When the value is low, FCM degenerates into hard clustering; when $m \rightarrow 1$ the value is high, the membership tends to be uniformly distributed, and the clustering discriminative power weakens. In practical applications, a value of [value missing] is often used $m \in [1.5, 2.5]$.

2.1.3 Parameter update formula

Given the membership matrix U , by taking the partial derivative of the objective function and introducing constraints, we can obtain the update formula for the cluster centers:

$$v_j = \frac{\sum_{i=1}^N u_{ij}^m x_i}{\sum_{i=1}^N u_{ij}^m}, j = 1, 2, \dots, C. \quad (3)$$

Given cluster centers V , the membership update formula is:

$$u_{ij} = \frac{1}{\sum_{k=1}^C \left(\frac{\|x_i - v_j\|}{\|x_i - v_k\|} \right)^{\frac{2}{m-1}}}, i = 1, \dots, N, j = 1, \dots, C. \quad (4)$$

continuously reduces the objective function value by alternately updating the membership matrix U and cluster centers until the convergence condition is met V .

2.2 Evidence Theory

By narrowing the representational distance between semantically similar samples and widening the representational distance between dissimilar samples, discriminative feature representations are learned. Unlike supervised learning that relies on manual annotation, contrastive learning generates supervisory signals by constructing relative relationships between samples, demonstrating significant advantages in unlabeled or weakly labeled scenarios.

Given a sample x_i , construct a positive sample through data augmentation or semantic consistency constraints x_i^+ , and treat the remaining samples as negative samples x_k^+ . After encoder $f_\theta(\cdot)$ mapping, the embedded representation is obtained:

$$z_i = f_\theta(x_i), z_i^+ = f_\theta(x_i^+), z_k^- = f_\theta(x_k^-). \quad (5)$$

The goal of contrastive learning is to maximize (z_i, z_i^+) the similarity between two learning methods and minimize (z_i, z_k^-) the similarity between two learning methods.

InfoNCE contrastive loss is currently the most widely used contrastive loss function, and its definition is as follows:

$$\mathcal{L}_{NCE} = -\log \frac{\exp(\text{sim}(z_i, z_i^+)/\tau)}{\sum_{k=1}^{|\mathcal{B}|} \exp(\text{sim}(z_i, z_k)/\tau)}, \quad (6)$$

Where: $\text{sim}(z_i, z_j)$ represents the similarity function (usually cosine similarity or dot product); \mathcal{B} represents the comparison batch containing positive and negative samples; $\tau > 0$ represents the temperature parameter used to adjust the smoothness of the similarity distribution. This loss function encourages the model to form a compact intra-class and segregated inter-class structure in the embedding space. From an information theory perspective, the InfoNCE loss can be interpreted as maximizing the lower bound of mutual information. Ignoring the constant term, we have:

$$I(\mathbf{Z}; \mathbf{Z}^+) \gtrsim \log |\mathcal{B}| - \mathcal{L}_{NCE}, \quad (7)$$

Minimizing the contrastive loss is equivalent to maximizing the mutual information between the sample representation and its positive sample representation, thereby improving the discriminative power of the feature representation.

3. Algorithm

3.1 Algorithm Flowchart

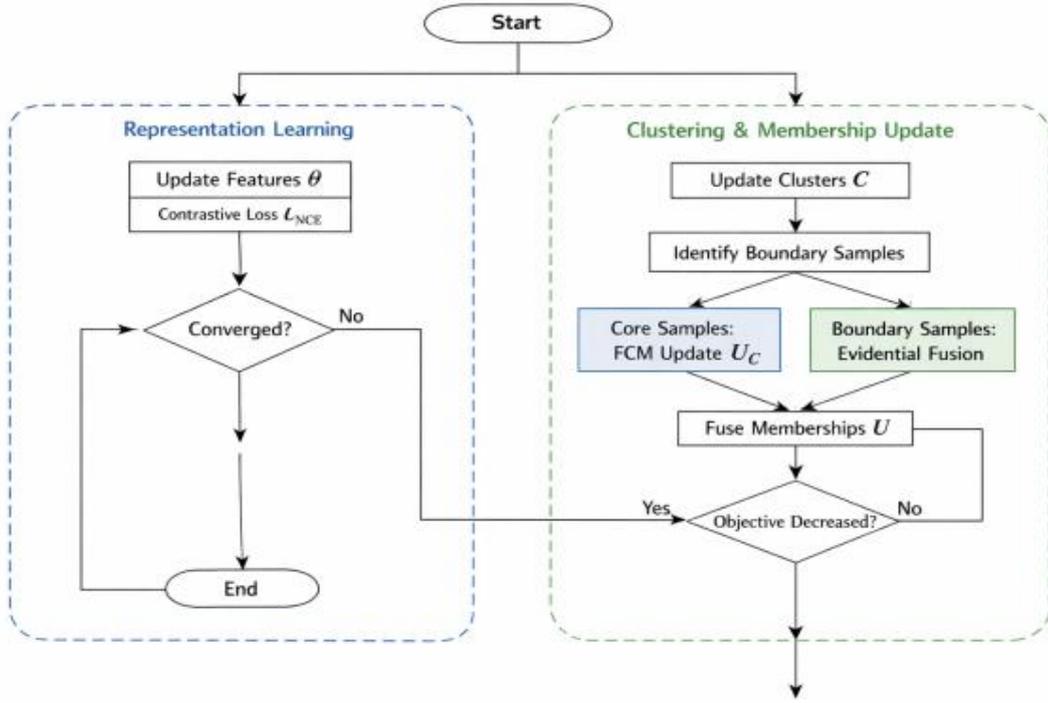


Figure 1: Algorithm Flowchart

3.2 Basic FCM Optimization Process

Given dataset

$\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^d$ And the number of clusters k , the classic fuzzy C-means (FCM) is optimized by minimizing the following objective function:

$$J(\mathbf{U}, \mathbf{C}) = \sum_{i=1}^n \sum_{j=1}^k u_{ij}^m \|\mathbf{x}_i - \mathbf{c}_j\|^2, m > 1, \quad (8)$$

Where $\mathbf{U} = [u_{ij}]$ represents the membership matrix, satisfying $\sum_j u_{ij} = 1$; $\mathbf{C} = \{\mathbf{c}_j\}$ is the set of cluster centers.

By iteratively updating membership degree and cluster center, the following analytical update formula is obtained:

$$\mathbf{c}_j = \frac{\sum_i u_{ij}^m \mathbf{x}_i}{\sum_i u_{ij}^m}, \mathbf{u}_{ij} = \left(\sum_{t=1}^k \left(\frac{\|\mathbf{x}_i - \mathbf{c}_j\|}{\|\mathbf{x}_i - \mathbf{c}_t\|} \right)^{\frac{2}{m-1}} \right)^{-1}. \quad (9)$$

After the algorithm converges, the initial solution is obtained $(\mathbf{U}^{(0)}, \mathbf{C})$.

3.3 Sample Partitioning Based on Three-Way Decision Making

To explicitly distinguish between certain and uncertain samples, this paper adopts a three-branch decision strategy based on membership confidence.

For any sample \mathbf{x}_i , its maximum membership degree is defined as $\mathbf{u}_i^{\max} = \max_j \mathbf{u}_{ij}$. Given a threshold $\epsilon \in (0, 1)$, the sample splitting rule is defined as follows:

$$\text{mask}(\mathbf{x}_i) = \begin{cases} \mathbf{1}, & \mathbf{u}_i^{\max} \geq \epsilon (\text{确定域}), \\ \mathbf{0}, & \mathbf{u}_i^{\max} < \epsilon (\text{边界域}). \end{cases} \quad (10)$$

Among them, the samples in the defined domain have a high clustering confidence, while the samples in the boundary domain have an uncertain membership relationship due to their relatively uniform membership distribution, and require further processing.

3.4 Neighborhood Construction

For boundary domain samples, this paper \mathbf{z}_i constructs a local neighborhood for each cluster center to extract reliable local evidence \mathbf{c}_j .

Let the radius

$$R_{ij} = \|\mathbf{z}_i - \mathbf{c}_j\|. \quad (11)$$

If a given sample \mathbf{x}_a simultaneously satisfies:

$$(\mathbf{x}_a - \mathbf{z}_i) \cdot (\mathbf{c}_j - \mathbf{z}_i) \geq 0, \|\mathbf{x}_a - \mathbf{z}_i\| \leq R_{ij}, \quad (12)$$

It is then included in the neighborhood $N(\mathbf{z}_i, \mathbf{c}_j)$.

This geometric constraint ensures that the selected evidence is oriented in alignment with the cluster center and spatially close enough to the boundary samples.

3.5 Evidence Fusion and Membership Reassignment for Boundary Samples

For each boundary sample \mathbf{z}_i , extract the evidence set from its hemispherical neighborhood.

$$\mathcal{E}_{ij} = \{\mathbf{u}_{aj} \mid \mathbf{x}_a \in N(\mathbf{z}_i, \mathbf{c}_j)\}. \quad (13)$$

When the number of pieces of evidence is not less than the minimum threshold, the product rule is used for evidence fusion, and the membership degree is updated as follows:

$$\mathbf{u}'_{ij} = \frac{\prod_{u \in \mathcal{E}_{ij}} u}{\sum_{t=1}^k \prod_{u \in \mathcal{E}_{it}} u}. \quad (14)$$

If the evidence is insufficient, the original FCM membership values are retained as backoff values. The updated membership matrix is then obtained U^* .

3.5 Loss Function

$$L = \lambda_1 L_{FCM} + \lambda_2 L_{CON}$$

Where L_{FCM} is the overall objective function of FCM clustering, and L_{CON} is the overall comparison function.

3.6 Computational Complexity Analysis

Let the number of FCM iterations be $*I* T$, and its time complexity be $*O(Tnkd)*$.

The worst-case complexity of the evidence fusion stage is $*O(|X_{uncertain}| \cdot |X_{certain}| \cdot k \cdot d)*$.

Since the three-branch partition and hemispherical constraints significantly reduce the number of samples effectively involved in the computation, this method exhibits good computational efficiency in practical applications.

4. Experimental Setup

4.1 Dataset

Table 1: Dataset Table

Dataset	Sample size	Feature Dimension	Number of categories
USPS	2,000	256	10
ORL	400	1,024	40
JAFFE	213	1,024	10

This paper conducts experimental validation on three public datasets: USPS, ORL, and JAFFE.

4.2 Evaluation Indicators

This paper uses three commonly used metrics—accuracy (ACC), normalized mutual information (NMI), and purity — to evaluate clustering performance.

4.2.1 Accuracy (ACC)

Clustering accuracy measures the consistency between clustering results and true labels, and is defined as follows:

$$ACC = \frac{1}{n} \max_{\pi} \sum_{i=1}^n \mathbf{1}(y_i = \pi(c_i)), \quad (15)$$

Wherein $\pi(\cdot)$ represents the optimal mapping from cluster labels to real labels, $\mathbf{1}(\cdot)$ and is an indicator function.

4.2.2 Standardized Mutual Information (NMI)

NMI is used to measure the relevance between cluster labels and true labels, and it is defined as follows:

$$NMI = \frac{I(\mathbf{y}, \mathbf{c})}{\sqrt{H(\mathbf{y})H(\mathbf{c})}} \quad (16)$$

Here, $I(\mathbf{y}, \mathbf{c})$ mutual information is represented, $H(\cdot)$ and entropy is represented.

4.2.3 Purity

Purity measures the consistency within a cluster, and is defined as follows:

$$Purity = \frac{1}{n} \sum_{l=1}^L \max_k |c_l \cap y_k|. \quad (17)$$

4.3 Comparison Algorithm

(1) K-means K-means [9] is a classic hard clustering method that minimizes the intra-cluster squared error and maximizes the inter-cluster difference by alternately updating the cluster center and sample assignment results. This method is computationally efficient and simple to implement, but due to the hard partitioning strategy, it is difficult to effectively characterize the fuzzy belonging relationship between samples and is more sensitive to noise and boundary samples.

(2) FKM (Fuzzy K-means) FKM [15] introduces fuzzy membership degree on the basis of K-means, and assigns each sample a probabilistic membership degree to each cluster. This method maximizes the similarity within the cluster by iteratively optimizing the membership degree matrix and cluster center, thereby alleviating the problem of insufficient ability of hard clustering to handle boundary samples to a certain extent.

(3) DEKM (Deep Embedded K-means) DEKM [20] constructs a K-means in-class divergence signal... The eigenvectors are then used to introduce an orthogonal transformation matrix for the embedding. The space is reconstructed to map the original embedding space to a space that can... This method more explicitly reveals a new space of clustering structure. The ability to express cluster structure information in the input features helps to improve clustering performance.

Table 2: Clustering Results

Model	index	USPS	ORL	JAFFE
KM	ACC	63.97	58.75	85.34
	NMI	61.98	76.89	88.56
	Purity	71.35	63.17	87.01
FKM	ACC	60.83	55.68	72.28
	NMI	56.62	76.24	81.35
	Purity	65.94	59.76	75.01
DEKM	ACC	74.31	42.95	75.02
	NMI	74.52	67.48	80.95
	Purity	80.46	47.33	77.69
Ours	ACC	75.34	64.30	91.78
Ours	NMI	71.54	81.02	92.25
Ours	Purity	80.21	67.55	92.00

4.4 Hyperparameter Analysis

The proposed method has five adjustable hyperparameters: λ_1 , λ_2 , γ , σ , and ϵ . λ_1 represents the number of complete dataset traversals during formal training, λ_2 and γ are trade-off parameters in the final loss function of the proposed framework, γ is a trade-off parameter controlling u_{ij} in the clustering loss, σ is a trade-off parameter controlling the robustness of various types of outliers in the clustering loss, and ϵ is the threshold for the three-branch decision to separate confirmed and uncertain samples. For most datasets, the search is performed on the grid of [0.1, 0.2, 0.3, 0.5, 0.7, 0.9]

for λ_1 , [0.001, 0.01, 0.1, 1, 10, 100] for λ_2 , and [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9] for ϵ . Similar to general deep

learning models, all hyperparameters significantly influence the clustering results.

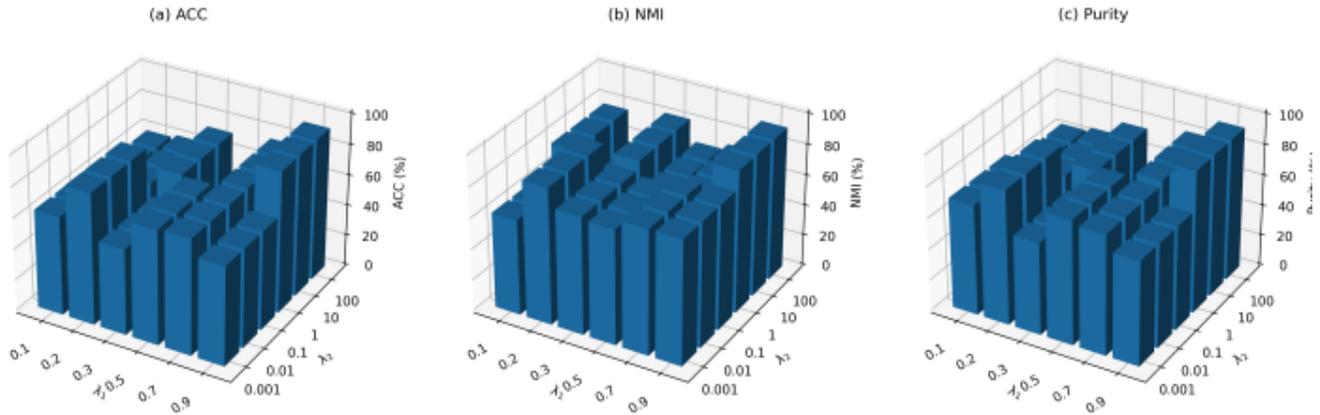


Figure 2: Experimental results

On the USPS dataset, our proposed method achieves state-of-the-art results in both ACC and Purity metrics, with an ACC of 75.34%, significantly outperforming KM, FKM, and DEKM methods. This demonstrates that in handwritten digit data where intra-class variation is significant, the introduced three-way decision and local evidence fusion mechanism effectively handles the uncertainty introduced by boundary samples, thereby improving overall clustering accuracy. Although slightly lower than DEKM in the NMI metric, the overall performance remains stable, reflecting the method's continued advantage in sample-level consistency.

On the ORL face dataset, our proposed method outperforms in all three metrics: ACC, NMI, and Purity, with a particularly significant improvement in ACC. This reflects that in high-dimensional face feature spaces, traditional distance-based or embedding-transformation-based methods often struggle to effectively address the uncertainties caused by inter-class overlap and pose variations. Our proposed method explicitly partitions uncertain samples into boundary regions through a three-branch partition and redistributes them based on local evidence, thereby enhancing the clustering and discrimination capabilities for complex face structures.

On the JAFFE facial expression dataset, our proposed method achieves the best results across all evaluation metrics, with a particularly significant advantage in the NMI metric, indicating a higher consistency between the obtained clustering results and the actual facial expression categories. These results demonstrate that, on facial expression data with a small sample size and subtle differences between categories, the three-branch decision mechanism can avoid premature judgments on uncertain samples, while the evidence fusion strategy further enhances the structural consistency within clusters.

5. Conclusion

This paper proposes a three-branch fuzzy C-means (FCM) clustering method based on evidence information granulation. First, a contrastive deep FCM clustering network framework is designed to map data from the original space to a deeper feature space more suitable for clustering analysis. Then, drawing on the three-branch decision-making approach, the

initial clustering results are divided into positive and boundary regions to handle the uncertainty inherent in the data. Based on this, a hemispherical neighborhood granulation method is introduced to construct information granules for uncertain samples in the boundary region, and evidence theory is used to fuse the trust levels of each information granule, thereby enhancing the model's ability to perceive local structures and more accurately capturing the inherent distribution characteristics of the data. Experiments on multiple public datasets show that this method outperforms existing contrastive methods. The main limitation of this work is the use of a fully connected network in the autoencoder part; future plans aim to further improve feature extraction capabilities by introducing more complex network structures.

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