A New Fuzzy Clustering Validity Index Based on Kullback-Leibler Divergence

Abstract. Determining the optimal number of clusters, a critical step in clustering analysis, is typically guided by domain expertise or assessed through clustering validity indexes. This study evaluates the effectiveness of such indexes for centroid-based partitional clustering algorithm. We propose a new clustering validity index, termed KLDCVI, which mitigates instability by incorporating Kullback-Leibler Divergence. This adjustment allows KLDCVI to tolerate closely allocated centroids to a reasonable degree, enhancing robustness in evaluation. We assess the performance of KLDCVI against existing validity indexes by applying the fuzzy c-means algorithm to real-world images. Experimental results demonstrate that KLDCVI achieves superior accuracy and reliability compared to conventional indexes.

Keywords: Clustering validity index, Fuzzy c-means method, KuLLback-Leibler Divergence.

1 Introduction

Clustering is an unsupervised learning technique and fundamental in image segmentation. It is used to partition in groups by analyzing similarities among their attributes. It organizes homogeneous pixels into cohesive clusters while separating heterogeneous pixels into distinct groups. The core objective of clustering is to efficiently generate well-defined and meaningful clusters, making it vital for image processing. Since its introduction as intelligent techniques based on fuzzy theory, Fuzzy C-Means (FCM) methods are widely studied and used as a powerful tool in a wide range of applications(1)(2)(3) and successfully applied in medical image segmentation(4)(5) (6)(7)(8). It was first proposed by Dunn(9) and improved by Bezdek (10). The main idea of FCM is to use fuzzy membership to cluster iteratively image into subsets, the fuzzy membership allows each pixel to belong to clusters with different degrees. To enhance FCM performance, many authors have focused their researches for developing new ideas or techniques to overcome some limitations such as noise and initialization sensitiveness, high-time complexity and use of Euclidian distance as the similarity criterion (11)(12) (13).

To overcome these limitations, Ahmed in (4) adds a spatial constraint by using the labels in the neighborhood of a pixel to compute its label, but it was very time-consuming, treated later in (14) given birth to two variants of algorithms by simplifying this proposed objective function. Kang (15) modified the objective function in the conventional FCM and introducing an adaptive weighted averaging filter to indicate the spatial influence of the neighboring pixels on the central pixel. Kernels methods are successfully incorporated in FCM to deal with corrupted data by noise or outliers (16). To calculate distance between the examples and the cluster centers, Chen and Zhang (17) apply the idea of kernel methods and demonstrates that such distances are more robust to noises. In (16), Zanaty et al. present an alternative Kernelized FCM (KFCM) for automatic magnetic resonance image (MRI) segmentation and incorporate spatial information into the membership function (Spatial KFCM). Authors in (18) propose Multiple KFCM (MKFCM) algorithm that provides a new flexible vehicle to fuse different pixel information in image-segmentation problems. This algorithm was enhanced later by incorporating spatial information (Spatial MKFCM)(19) (20). Hybrid clustering methods are also used to enhance FCM effectiveness like Evolutionary algorithms, deformable model, neural networks and more techniques (21) (22) (23) (24)(25) (26) (27) (28)(8)

Recently many researchers introduce Kullback–Leibler divergence (KL-Divergence)(29) in FCM in different ways. Zou et al. in (30) surrogate the Euclidian distance by the KL- Divergence in the objective function, while in (31), authors modify the objective function by incorporating weighted membership KL-Divergence and local data information. Authors in (32) use the KL-Divergence to handle the memberships. First, they classified the image with distinct fuzzy clustering methods and then the resulting soft clustering are aggregated by an objective function based on fuzzy KL-Divergence. Authors confirm that the proposed method gives good results compared with other methods.

To achieve the clustering process, most of these approaches require the appropriate number of clusters to start with. But for new or unknown data this information is crucial and the segmentation accuracy depends highly on it and when it is incorrect serious problems may arise. To get the right number of clusters, many studies deal with this problem which is known as cluster validity index. Since images lack prior reference information, determining the optimal number of clusters remains a significant challenge. In this work we develop a novel fuzzy index based on KL-Divergence that allows getting the right number of clusters for a given image.

2 FCM algorithm

The FCM algorithm belongs to the family of clustering algorithms based on fuzzy function optimization. The standard version is firstly introduced by Dunn and generalized by Bezdek (10). It has undergone many interventions leading to a lot of algorithms. All these algorithms are considered as soft clustering in the way that each element of the data to be clustered may belong to more than one cluster with deferent degrees of membership. The objective function is optimized in an iterative way and at the end of the process; each element is assigned to the cluster in which it has the highest membership.

Let $I = (x_1, x_2, \dots, x_N)$ an image of *N* pixels to be clustered into C $(2 < K \ll N)$ clusters, where x_i represents data features. The standard FCM objective function is formulated as (10):

$$J(U) = \sum_{i=1}^{C} \sum_{j=1}^{N} u_{i,j}^{m} d^2(x_j, c_i) \tag{1.1}$$

U is the memberships degrees matrix, c_i is the *ith* center and C is the total number of clusters centers. m ∈ [1, ∞[is to control fuzziness, $d^2(x_j, c_i)$ is the grayscale Euclidean distance and $u_{i,j}$ is the membership degree of the pixel *j* in the *ith* cluster c_i.

An alternate optimization is applied on the membership function U and clusters centers using the following formulas:

$$u_{ij} = \frac{(d^2(x_j,c_i))^{\frac{1}{1-m}}}{\sum_{l=1}^{C}(d^2(x_j,c_l))^{\frac{1}{1-m}}} \quad (1.2)$$

and

$$c_i = \frac{\sum_{j=1}^{N}(u_{ij})^m .x_j}{\sum_{j=1}^{N}(u_{ij})^m} \quad (1.3)$$

From a random initialization of clusters centers and using formulas (1.2) and (1.3), FCM algorithm recomputed clusters centers until no improvement of these centers. Once the clusters centers fixed, the algorithm assign each pixel *j* of the image to a cluster having maximum fuzzy membership degree.

3 Cluster validity index for fuzzy clustering algorithms

In the field of cluster analysis, cluster validity is a very important and large topic; it began to appear in the 1980s (33)(34). The main purpose of any cluster validity index (CVI) is to find the optimal number of clusters that corresponds to the natural partition of the given data, image in our case. CVI focuses on incorporating measures of compactness and separation (35) (36) (37) (38). In image segmentation field, compactness measures the concentration of pixels belonging to the same cluster around the cluster center while separation represents isolation of clusters from each other. In this section, we will list some popular CVI.

(i) The partition coefficient Index (PCI) and partition entropy Index(PEI) are proposed by Bezdeck (39) in association with FCM Algorithm

$$PCI = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{C} u_{ij}^2 \quad (1.4)$$

$$PEI = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{C} u_{ij}\, log\left(u_{ij}\right) \quad (1.5)$$

PCI is a max optimum index and *PEI* is min optimum index.

(ii) To reduce the monotonic tendency with *C (number of cluster)* of the both index *PCI* and *PEI*, Dave (40) proposed Modification of *PCI* (*MPC*). This index is defined as

$$MPC = \frac{C * PCI - 1}{C - 1} \tag{1.6}$$

(iii) Xie and Beni (41) defied a new CVI called in this paper *XBI*. It take account the fuzzy membership degrees and the structure of the data to be clustered in order to have compact and well-separated clusters. *XBI* is defined as

$$XBI = \frac{J_m(U, C, X)}{N(min_{i,j}\|c_i - c_j\|)} \tag{1.7}$$

where J_m is the fuzzy objective function of the FCM algorithm. *XBI* is a min optimum index.

(iv) In the same way of XBI, Fukayama and Sugno (42) defined another CVI called *FSI* as (*FSI* is a min optimum index):

$$FSI = J_m(U, C, X) - \sum_{i=1}^{N} \sum_{j=1}^{C} u_{ij}^{m} \|c_j - \bar{x}\|^2 \tag{1.8}$$

where $\bar{x} = \frac{\sum_{i=1}^{N} x_i}{N}$, the mean of the whole data to be clustered.

(v) The Separation-Compactness Index (*SCI*) is a fuzzy clustering validity metric that balances intra-cluster compactness and inter-cluster separation. SCI is min optimum index. It's typically defined as:

$$SCI = \frac{J_m(U, C, X)}{\sum_{i=1}^{C} \sum_{j=i+1}^{C} \|c_i - c_j\|^2} \tag{1.9}$$

(vi) The Davies-Bouldin Index (*DBI*) measures the compactness and separation of clusters. It is defined as:

$$DBI = \frac{1}{K} \sum_{i=1}^{K} \max_{i \neq j} \left(\frac{S_i + S_j}{D_{i,j}} \right) \tag{1.10}$$

Where S_i is the mean distance between the center of the cluster *I* and all the points belonging to this cluster and $D_{i,j}$ denotes the distance between the centroids of the clusters *I* and *J*. *DBI* is min optimum index.

(vii) The MBMF (Mean Bounded Membership Function) is a fuzzy max optimum clustering validity index that evaluates the crispness or definiteness of the clustering results. It is defined as

$$MBMF = \frac{1}{C} \sum_{j=1}^{N} \max_{i} (U_{ij}) \tag{1.11}$$

(viii) *IMI* is also a min optimum index for evaluating fuzzy clustering results. It inspired from WLI. It deal with impact of the uniform effect on the separation and compactness metrics

$$IMI = \frac{\sum_{i=1}^{C_i} \frac{\sum_{j=1}^{N} u_{k,j}^{m} d^2(x_j, c_i)}{\sum_{j=1}^{N} u_{ij}^{2}}}{\min_{l \neq k} \delta_{l,k} d^2(c_l, c_k) + \underset{l \neq k}{median}\, \delta_{l,i} d^2(c_l, c_k)} \tag{1.12}$$

where $\delta_{l,k} = \frac{\sum_{j=1}^{N} u_{l,j}}{\sum_{j=1}^{N} u_{k,j}}$.

The characteristics of the clustering validity index (CVIs) discussed above revolve around their ability to measure the quality of clustering by evaluating two main aspects: compactness and separation. Compactness refers to the degree to which data objects within the same cluster are similar and closely packed, typically measured using intra-cluster distances such as between pairs of objects or between each object and the cluster centroid. In contrast, separation assesses how well distinct clusters are isolated, often using inter-cluster distances between centroids or between objects from different clusters. CVIs mentioned above incorporate fuzzy membership degrees and structural properties of clusters. Some CVIs, like PC and PE, focus solely on compactness, whereas others, like DBI, XBI, FSI, and SCI, account for both compactness and data structure but may not address compactness–separation trade-offs at the cluster level. CVIs also differ in how they treat centroid distances: PBMF emphasizes maximum centroid distance (which can misrepresent image clustering), while XBI and CSI focus on the minimum. Simpler CVIs like PC and PE use membership degrees alone, whereas advanced ones also incorporate distance metrics averaged like FSI, minimal like XBI and CSI, or maximal (MBMF). Typically, CVIs are used as post-processing tools independent of the clustering method, helping determine the optimal number of clusters by identifying the value of number of clusters where the CVI reaches its maximum (PC, Dunn, SCI, WLI, IMI, …) or minimum (PE, DBI, XBI, FSI, CSI, …).
For convenience, this paper denotes a larger-the-better CVI as CVI^{+} and a smaller-the-better CVI as CVI^{-}.

4 The Proposed CVI

We propose a novel cluster validity index based on the Kullback-Leibler Divergence named KLDCVI (Kullback-Leibler Divergence-Cluster Validity Index). The main purpose of KLDCVI is to evaluate the fuzzy clustering results considering the Kullback-Leibler Divergence between clusters in the separation metric.

4.1 Kullback-Leibler Divergence

Kullback-Leibler Divergence (KLD) is a measure of how one probability distribution differs from a second, reference probability distribution. It quantifies the "distance" between two distributions in terms of information loss when using one to approximate the other (43). For two discrete probability distributions *P* and *Q* the Kullback–Leibler Divergence of *P* with respect to *Q* is defined by :

$$D_{KL}(P\|Q) = \sum_{i} P(i) log \frac{P(i)}{Q(i)} \quad (1.13)$$

4.2 Structure of KLDCVI

In a general context, clustering is a process of grouping or classifying a collection of objects into homogeneous "clusters." Ideally, members of the same cluster are characterized by strong similarity to each other and strong dissimilarity to members of other clusters. In fuzzy classification methods such as FCM (Fuzzy C-Means) and its variants, each individual (a pixel in the case of images) is assigned a membership degree indicating its association with each cluster. This can be interpreted as the probability of belonging to a given cluster. Therefore, we will leverage this measure to compute the divergence between clusters resulting from a classification. By maximizing this measure, we ensure separation between the clusters.

Like conventional CVIs, the KLDCVI index is defined as the ratio between fuzzy compactness and separation measures. The distinguishing characteristic of KLDCVI lies in its explicit incorporation of Kullback-Leibler Divergence into the separation metric.

4.2.1 Separation measure

The notion of KLD divergence is based on two probability variables, P and Q. In our application, the proposed measure defines P and Q as follows: For each pixel j belonging to cluster i, if we define $P_{i,j}$ as the membership probability of pixel j in cluster i, then $P_{i,j}$ is simply U_{ij} (from FCM algorithms), i.e., $P_{i,j} = U_{ij}$.

Similarly, we define $Q_{i,j}$ as the sum of membership probabilities of pixel j to all other clusters (excluding cluster i). Thus, $Q_{i,j}$ represents the complement of the pixel's membership probability in cluster i, meaning:

$Q_{i,j} = 1 - P_{i,j}$ (i.e., $Q_{i,j} = 1 - U_{ij}$) since the sum of a pixel's membership degrees across all clusters must equal 1. The figure below illustrates the principle of separation measure. The separation measure must ensure the isolation of the cluster C_i over the rest of clusters.

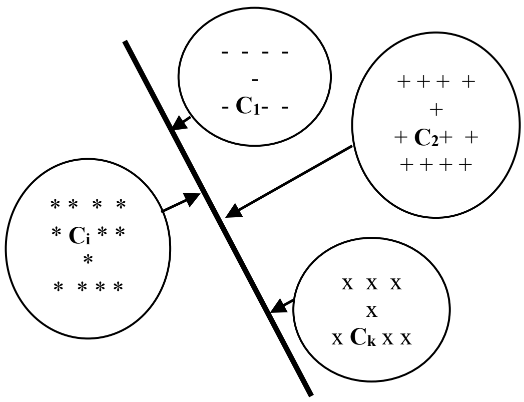

Fig.1. Principle of KLD-CIV separation measurement

The divergence of cluster i relative to the remaining clusters is calculated using the formula:

$$kld_i = \sum_{j=1}^{N} \delta_{ij} U_{ij} * Log\left(\frac{U_{ij}}{1 - U_{ij}}\right) \quad (1.14)$$

where $\delta_{ij} = \begin{cases} 1 & if\ U_{i,j} = Max(U_{ij}) \quad i = 1, \dots, C \\ 0 & otherwise \end{cases}$.

According to this presentation, the separation measure is defined as the average divergence of the *C* clusters in the partition. This new separation metric is

$$KLDIV = \frac{1}{C} \sum_{i=1}^{C} kld_i \quad (1.15)$$

4.2.2 Compactness measure

The fuzzy compactness metric serves as a fundamental criterion in numerous CVIs, such as XBI, FSI, WLI and IMI indexes. Conventionally, this metric is mathematically defined as the aggregate compactness measure across all clusters. It is defined as:

$$\sum_{i=1}^{C} \frac{\sum_{j=1}^{N} u_{ij}^m d^2(x_j, c_i)}{\sum_{j=1}^{N} u_{ij}^2} \quad (1.16)$$

Building upon the mathematical foundations established in Equations (15) and (16), the KLDCVI index is formally defined as:

$$KLDCVI = \frac{\sum_{i=1}^{C_i} \frac{\sum_{j=1}^{N} u_{kj}^m d^2(x_j, c_i)}{\sum_{j=1}^{N} u_{ij}^2}}{\frac{1}{C} \sum_{i=1}^{C} kld_i} \quad (1.17)$$

Like other CVIs, the KLDCVI assesses the compactness-separation trade-off in clustering. The numerator in Eq. (1.19) computes the average fuzzy distance of data points to all cluster centroids, smaller values indicate tighter, more compact clusters. This principle aligns with other CVIs, such as XBI, SCI, and MBMF.

The denominator measures cluster separation, where a larger value signifies more distinct, well-separated clusters. Thus, lower KLDCVI values correspond to better clustering performance, as they reflect higher compactness and greater separation.

5 Experiments

To demonstrate the effectiveness of our KLDCVI index, several experiments are conducted on different images. In these experiments, the images were clustered using FCM with varying numbers of clusters. The clustering outcomes were assessed using a cluster validity index (CVI) to determine the optimal number of clusters. The

proposed KLDCVI was compared against eight established indexes mentioned in section (3).
First, the proposed CVI was tested on synthetic image. This later contains 6 clusters (Fig.2). The proposed CVI was also tested on four remote sensing images from a prior study (35) (Fig. 3). Each image measures 128 × 128 pixels, comprising 16,384 3D data points with 24-bit RGB values (3D features) for clustering.
In (35), domain experts determined the number of clusters by identifying distinct objects—such as roads, sandbanks, sea areas, rooftops, and aircraft—that clustering should resolve. Based on this, Img2 and Img4 were assigned 3–4 clusters, while Img3 and Img5 were assigned 4–5 clusters. Furthermore, KLDCVI was tested on medical images (Fig.4). Img6 and Img7 were assigned 3-5 clusters where Img8 is assigned 3-4 clusters.
For computational efficiency, all images were converted to grayscale prior to clustering.

Img1

Fig.2. Synthetic image

Img2 Img3 Img4 Img5

Fig.3. Remote sensing images

Img6 Img7 Img8

Fig.4. Medical images

Table 1 bellow presents the result obtained for image Img6. For this image KLDCVI find the right number of cluster with DBI, PCI, MPC, XBI and MBMF. Table 2 provides results obtained on all images

Table 1. Clustering result metrics for Img6
Bold numbers presents optimum values

C	DBI^-	PCI^+	PEI^-	MPC^+	XBI^-	FSI^-	$MBMF^+$	IMI^-	$KLDCVI^-$
2	1.0000	0.0000	1.0000	0.0000	0.8652	**0.0000**	0.0000	**0.0000**	1.0000
3	**0.0000**	**1.0000**	**0.0000**	0.9683	0.0910	0.9933	**1.0000**	0.9947	0.0981
4	0.2774	0.8877	0.2485	**1.0000**	**0.0000**	1.0000	0.8593	1.0000	0.0006
5	0.2871	0.7546	0.5271	0.9866	0.2469	0.9415	0.7362	0.9702	**0.0000**
6	0.4198	0.5139	0.9635	0.9135	1.0000	0.8212	0.5229	0.9036	0.0273

Table 2. cluster numbers decided by CVIs

Image	#C	DBI	PCI	PEI	MPC	XBI	FSI	MBMF	IMI	KLDCVI
Img1	6	**-**	**6**	**6**	**6**	**6**	**6**	**6**	**6**	**6**
Img2	3-4	**3**	2	2	**3**	**3**	**3**	2	2	**3**
Img3	4-5	3	3	2	3	3	2	3	**4**	3
Img4	3-4	2	2	2	2	2	**3**	2	**4**	2
Img5	4-5	3	2	2	3	3	6	2	2	**4**
Img6	3-5	**3**	**3**	**3**	**4**	**4**	2	**3**	2	**5**
Img7	3-5	**3**	**3**	**3**	**3**	**3**	2	**3**	2	**3**
Img8	3-4	**3**	**3**	2	**3**	**3**	6	**3**	2	**3**

We Remarque that our KLDCVI index detects the right number of clusters for 6 images over 8. This confirms the robustness of our CVI.

6 Conclusion

FCM is widely used in lots of fields. But it needs to preset the number of clusters and is greatly influenced by the initial cluster centroids. This paper presents a method for determining the number of clusters by using of FCM algorithm. In this method, a Kullback-Leibler Divergence is used for developing a new cluster validity index termed KLDCVI. This CVI can estimates the right number of clusters for a given image. This new fuzzy clustering validity index was put forward based on fuzzy compactness and separation based on Kullback-Leibler Divergence so that the clustering result is closer to global optimum. The index is robust and interpretable when the number of clusters tends to that of objects in the dataset. The contributions are validated by experimental results.

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