Comparison of Validity Indexes for Fuzzy Clusters of fMRI Data

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Abstract. In computational neuroimaging, the analysis of functional Magnetic Resonance Images (fMRIs) using fuzzy clustering methods is a promising data driven approach to explore brain functional connectivity. In this complex domain, accurate evaluation procedures based on suitable indexes, able to identify optimal clustering results, are of great values strongly affecting the validity and interpretation of the overall fMRI data analysis. A large number of clustering validation indexes have been proposed in literature. This work proposes a comparison analysis of eight representative fuzzy and crisp clustering validation indexes. Salient aspects of the proposed strategy are the use of the widely adopted fuzzy c-means algorithm as underlying fuzzy clustering algorithm and the use of resting state fMRI data from the NITRC repository.

Keywords: Clustering · Clustering validation index · fMRI

1 Introduction

Data Clustering is one of the widely used methods to explore data in several domains. It utilizes only the statistical information inherent in the data without human supervision [5]. Fuzzy clustering computes degrees of membership of a single data to multiple clusters. In computational neuroimaging, the analysis of functional Magnetic Resonance Images (fMRIs) using fuzzy clustering methods is a promising data driven approach to explore brain functional connectivity. fMRI data have a complex content that regards both spatial and temporal information: the spatial ones are related to the mapping of brain regions that have common topological properties, whereas the temporal ones are referred to the detection of brain signal changes in correspondence to specific experimental times (see Fig. 1). In this context, clustering techniques find homogeneous spatio-temporal patterns without relying on any model of functional response are considered in principle more accurate than model-based methods when dealing with fMRI data analysis under complicated experimental conditions [9,17]. Clustering algorithms perform a partition of the complex fMRI content in homogeneous groups. Finding an optimized partition is a sophisticated task: not all the fMRI patterns are

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separable in distinguished crisp parcels since some of them could share common properties, as in the case of extended brain networks that vary the coactivation of different brain modules during an experimental task. Thus, the natural dynamic of the neuronal structures must be managed properly by clustering algorithms that should be able to handle both simple regularities of well-known patterns related to low-level active tasks and complex irregularities of partially-known patterns related to high-level active tasks or self-referred passive paradigms. Clustering has an important role in fMRI passive studies allowing to investigate the neurophysiological resting state that has debated biomarkers [9] and also evidence-based differences related both to gender and age [3]. In this context accurate evaluation procedures based on suitable indexes able to identify optimal (and suboptimal) clustering results are of great values strongly affecting the validity and interpretation of the overall fMRI data analysis which is still a controversial task in neuroimaging. Among the varied methods used for fMRI data clustering, fuzzy c-means [2] is certainly the most popular method [9,11,16,18]. An important issue in cluster analysis is the cluster validation aimed to measure how well the clustering results reflect the structure of the data set. For this purpose a large number of clustering validation indexes (CVIs) have been proposed in literature [4,7,13–16,19] to detect the optimal cluster number for a given dataset on the base of a balancing between the two opposite criteria of compactness within each cluster and separation between them. Several studies have been developed to investigate and compare the effectiveness of fuzzy and crisp CVIs in appropriately determining the number of clusters and measuring the goodness of clusters themselves produced by diverse algorithms [1,8]. Despite several achievements obtained, guidelines resulting from these general studies have not yet been adopted with large consensus and validation indexes are often selected basing on individual experience and/or arbitrary criteria. Critical aspects arise also in fMRI data analysis where clustering techniques are usually validated using external criteria based on prior knowledge about the data, whenever possible, or using internal different indexes depending on individual studies. The problem can be addressed by proposing comprehensive comparison studies oriented to specific clustering algorithm and specific application domains in such a way that resulting guidelines are applicable in future studies. Proceedings from these considerations, in this work we focus the attention on validation of fuzzy clustering of fMRI data and develop a comparison analysis of a set of representative fuzzy and crisp CVIs. Salient aspects of the proposed strategy are the use of the widely adopted fuzzy c-means (FCM) algorithm as underlying clustering algorithm and the use of resting state fMRI data from the NITRC repository [10]. The remaining part of the paper is organized as follows: Sect. 2 describes the clustering problem and the soft algorithm chosen to approach its solution, Sect. 3 lists the indexes used to validate the clustering results, Sect. 4 describes the general experimental procedure, the datasets used and the results obtained. Section 5 reports both the discussion of the results and the conclusions.

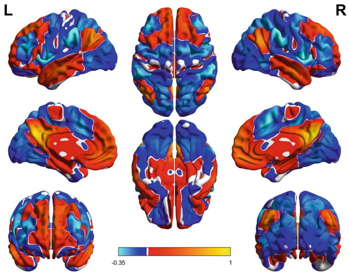

Fig. 1. This image displays resting-state functional connectivity as linear correlation for the seed region in a sample of 1,000 subjects. The seed chosen is the Precuneus (X/Y/Z MNI152 coordinates: 2 -60 30), that is the main core of the Default Mode Network (DMN), a candidate biomarker for the fMRI resting state studies. In the images, the Precuneus is in the zone with the highest functionality (yellow color).

2 Clustering Problem and Fuzzy C-Means Algorithm

The purpose of clustering is to partition a given set of data into groups (clusters) following a predefined criterion. These groups contain data that have both high similarity within clusters and high dissimilarity between the other clusters [5].

Let $X = \{x_1, x_2, \ldots, x_n\}$ a given dataset (with n elements), and let $C = \{c_1, c_2, \ldots, c_K\}$ the set of cluster, where K is the desired number of clusters. Regardless of the criterion chosen for the partition, the purpose of clustering is to develop a partition matrix of size $K \times n$ denoted as $U = [\mu_{ij}]$, with $i = 1, 2, \ldots, K$ and $j = 1, 2, \ldots, n$, where μ_{ij} is the grade of membership of point x_j to cluster c_i.

In crisp clustering, each point in the specified dataset belongs to a single cluster class. Then $\mu_{ij} = 1$ if $x_j \in c_i$, otherwise $\mu_{ij} = 0$. Instead, in fuzzy clustering, a point can be associated with more than one cluster, potentially also to all clusters, with a certain degree of membership, and the partition matrix in this case is represented as $U = [\mu_{ij}]$, where $\mu_{ij} \in [0, 1]$ indicates the degree of membership of the j-th element to the i-th cluster.

The FCM algorithm proposed by Bezdek [2] is used for the data analysis in a non-supervised way in several fields. The purpose of the FCM algorithm is to create vectors called centroids that minimize the value of the function J_m that is given by the sum of the intra-cluster quadratic error. J_m it is defined as:

$$J_m = \sum_{j=1}^{n} \sum_{i=1}^{K} \mu_{ij}^{m} ||x_j - z_i||^2 \tag{1}$$

where

- $m > 1$ is the exponent of the element of the fuzzy partition matrix to adjust the degree of fuzzy overlap.
- z_i is the centre of the i-th cluster.
- μ_{ij} is the degree of membership of x_j to the i-th cluster.

- $||\ldots||$ is the Euclidean norm between a point and the corresponding cluster center.

The FCM algorithm performs the following steps:

1. Randomly initialize the U matrix.
2. Calculate the cluster centroids with the following formula: $z_i = \frac{\sum_{j=1}^{n}(\mu_{ij})^m(x_j)}{\sum_{j=1}^{n}(\mu_{ij})^m}$
3. Update μ_{ij} according to the following formula: $\mu_{ij} = \frac{1}{\sum_{k=1}^{K}(\frac{||x_j - z_i||^2}{||x_j - z_k||^2})^{\frac{2}{(m-1)}}}$
4. Calculate the objective function J_m
5. Repeat steps 2–4 until J_m improves less than the prefixed threshold or until the specified maximum number of iterations is reached.

3 Cluster Validation Indexes

The use of a clustering algorithm must be complemented with the use of a validation index to detect the optimal cluster number for a given input dataset. A clustering validity index has two indicators: the compactness and the separation [12]. The compactness indicates the concentration of points that share the same cluster. The separation, evaluates the degree of isolation among clusters. A dataset is well partitioned if there is both high compactness and high separation. But often the two indicators conflict, e.g., if the compactness is high, the separation is low and *viceversa*. Therefore, a *rationale* between the two indicators is needed to design a clustering validation index.

The aim of the present work is to identify suitable CVIs for fMRI Clustering studies among a set of representative and widely used crisp and fuzzy indexes. A total of eight indexes is considered and their formal definition given below.

- The Pakhira Bandyopadhyay Maulik Index (PBMI) [13]. It evaluates the product between compactness and separation and its optimal value is towards the maximum. It is formalized as

$$PBMI(K) = \left(\frac{1}{K} \times \frac{E_1}{E_K} \times D_K\right)^2 \tag{2}$$

where K is the number of clusters used, i.e., $K = \{k^{'}, k^{''}, \ldots, k^K\}$, the $E_K = \sum_{k=1}^{K} E_k$ holds such that the compactness is defined as crisp functional

$$J(U, Z) = E_k = \sum_{n=1}^{N} u_{nk}||x_n - z_k|| \tag{3}$$

where $U(N) = [u_{nk}]_{N \times K}$ is the binary partition matrix of the clustered data and the crisp separation is formalized as

$$D_k = \max_{k', k''}^{K}\left\{||z_{k'} - z_{k''}||\right\} \tag{4}$$

with $z_{k'} \neq z_{k''}$ (that are different centroids). Note that x_n is the n-th point in the dataset and z_k is the center of the k-th cluster. $E_1 = \sum_{n=1}^{N}||x_n - z_1||$ z_1 is the centroid calculated on all points of the dataset

- The FPBMI is the fuzzy version of the index proposed by Pakhira et al. [13]. It evaluates the product between compactness and separation and its optimal value is towards the maximum. It is formalized similar as in the Eq. (2), except for the compactness of all clusters that it is defined as fuzzy functional, i.e.,

$$J_m(U, Z) = E_k = \sum_{k=1}^{K} \sum_{n=1}^{N} u_{nk}^m ||x_n - z_k|| \tag{5}$$

and E_1 that defined the fuzzy compactness of the cluster 1, i.e., $E_1 = \sum_{n=1}^{N} u_{n1}^m ||x_n - z_1||$. Both contain the membership value u_{nk}, where $U(N) = [u_{nk}]_{N \times K}$ is the fuzzy partition matrix of the clustered data.
- The Fukuyama Sugeno Index (FSI) [7]. It computes the difference between fuzzy compactness and fuzzy separation and its optimal value is towards the minimum., i.e.,

$$FSI(K) = \sum_{k=1}^{K} \sum_{n=1}^{N} u_{nk}^m ||x_n - z_k||^2 - \sum_{k=1}^{K} \sum_{n=1}^{N} u_{nk}^m ||z_k - \overline{z}||^2 \tag{6}$$

in which the $\overline{z}$ is the mean of all Z centroids and the u_{nk} is the membership value of the n-th point in the k-th cluster, and m is the fuzzy exponent.
- The Rezaee Lelieveldt Reider Index (RLRI) [14], also known as Compose Within and Between scattering Index (CWBI). It is the sum of compactness and separation and its optimal value is towards the minimum. In checks the average compactness and separation of fuzzy clustering by using the sum of two functions, i.e.,

$$RLR(K) = \alpha Scat(K) + Dis(K), \tag{7}$$

where α is a weighting factor equals to $Dis(K_{max})$ (the $Dis(K)$ with the maximum cluster number), and $Scat(K)$ that is the clustering compactness measure defined as

$$Scat(K) = \frac{\frac{1}{K} \sum_{k=1}^{K} ||\sigma^2(z_k)||}{||\sigma^2(X)||} \tag{8}$$

with $||x|| = (x^T \cdot x)^{1/2}$. Note that $\sigma^2(X)$ denotes the variance of all the dataset X and $\sigma^2(z_k)$ is the fuzzy variance of cluster k. The $Dis(K)$ is the clustering separation measure defined as

$$Dis(K) = \frac{D_{max}}{D_{min}} \sum_{k=1}^{K} \left[\sum_{k=1}^{K} ||z_{k'} - z_{k''}|| \right]^{-1} \tag{9}$$

with $z_{k'} \neq z_{k''}$ (different k centroids) and with Dis_{max} and Dis_{min} are the clustering separation with the maximum and minimum cluster number respectively.
- The Wang Sun Jiang Index (WSJI) [15]. It is the sum of compactness and separation and its optimal value is towards the minimum. It derived from the RLRI, adopting a linear combination of average fuzzy compactness and separation to evaluate clustering outcomes, i.e.,

$$WSJI(K) = Scat(K) + \frac{Sep(K)}{Sep(K_{max})} \tag{10}$$

where the separation $Sep(K)$ is differently defined as in Eq. 9, i.e.,

$$Dis(K) = \frac{D^2_{max}}{D^2_{min}} \sum_{k=1}^{K} \Big[\sum_{k=1}^{K} ||z_{k'} - z_{k''}||^2 \Big]^{-1}. \tag{11}$$

Instead, the $Scat(K)$ is the defined as in Eq. (8).

- The Xie Beni Index (XBI) [19]. It is the *ratio* between compactness and separation and its optimal value is toward the minimum. It measures the average within cluster fuzzy compactness *versus* the minimal value of the between-clusters separation, i.e.,

$$XBI(K) = \frac{\sum_{k=1}^{K} \sum_{n=1}^{N} u^2_{nk} ||x_n - z_k||^2}{N \cdot min_{k_\prime \neq k_{\prime\prime}} \{||z_{k_\prime} - z_{k_{\prime\prime}}||^2\}} \tag{12}$$

  with $K = \{k_\prime, k_{\prime\prime}, \ldots, k_K\}$ is the number of clusters used, N the number of data points, u_{nk} the membership values associated to the points n and a cluster k, the z_k is the centroid of a generic cluster k.
- The Davies Bouldin Index (DBI) [4]. It is the *ratio* between crisp compactness and separation and its optimal value is towards the minimum., i.e.,

$$DBI(K) = \frac{1}{K} \sum_{k=1}^{K} \max \Big\{ \frac{S_{k'} + S_{k''}}{||z_{k'} - z_{k''}||} \Big\} \tag{13}$$

  with $k_\prime \neq k_{\prime\prime}$ (different k centroids) and $S_{k'}$ the crisp clustering compactness of the $k' = k$-th cluster defined as

$$S_{k'} = \Big(\frac{1}{N_{k'}} \sum_{x_n \in k_i} ||x_n - z_{k'}||^2 \Big)^{1/2} \tag{14}$$

  where $N_{k'}$ is the cardinality of the cluster $k^{'}$.
- The SDBI is the soft (fuzzy) version of DBI [16]. It is the *ratio* between the fuzzy compactness and the separation and its optimal value is towards the minimum. It is defined as

$$SDBI(K) = \frac{1}{K} \sum_{k=1}^{K} \max \Big\{ \frac{S_{k'}\overline{U_{k'}} + S_{k''}\overline{U_{k''}}}{||z_{k'} - z_{k''}||} \Big\} \tag{15}$$

  where the fuzzy compactness $S_{k'}$ is the defined as follow

$$S_{k'} = \Big(\frac{1}{N} \sum_{x_n \in N} ||x_n - z_{k'}||^2 \Big)^{1/2} \tag{16}$$

  in which N is the cardinality of the used datasets, whereas the $\overline{U_{k'}}$ is the average of the membership values for the cluster $k^{'}$ (note that $k^{'}$ and $k^{''}$ are different clusters).

4 Experiments and Results

Performances of the eight indexes introduced in Sect. 3 are evaluated using clustering results obtained by processing fMRI datasets with different configuration of FCM algorithm and comparing the optimal number of clusters indicated by the indexes with those indicated by the available ground truth.

4.1 FMRI Dataset

From the NITRC repository [10] and 1000 Functional Connectome Project, we selected the Beijing dataset with 187 healthy subjects (73M/114F; ages 18–25; all righthanded). The subjects did a resting state experimental paradigm with eyes closed. The fMRI parameters were the following: TR = 2, slices = 33 acquired with interleaved ascending procedure, time-points = 225, magnet = 3 [T]. The selection of this dataset is motivated by the specific age range and because it was just used by Biswal et al. [3] to discover resting state functional properties and their gender determinants. The brain resting state measured with fMRI has a bunch of possible biomarkers that allow researchers to build a likely ground truth (or experimental-based ground truth). The common knowledge about those biomarkers are presented in [3,9,11]. Since we want to get an empirical ground truth to validate the indexes, we defined it taking in account the acquired common knowledge about resting state fMRI biomarkers, obtaining a two classes ground truth and a four classes ground truth. The first has two labels associated to the presence/absence of regions related to the so-called Default Mode Network (DMN) [6] and the second has four labels associated to regions part of DMN and other three candidate resting networks, i.e., the Visual Network (VN), the Sensory/Motor Network (SMN) and the Other Resting Networks (ORN) (the last one encompasses all the regions that are not classified as DMN, VN or SMN).

4.2 Experiments

Two experiments have been developed by using fMRI data. In the first experiment two classes of truth are considered: what is DMN network and what is not. In the second experiment, 4 classes are considered: DMN network, VN network, SMN network and other resting networks. The FCM algorithm was configured with number of clusters $K = 2, 3, .., \sqrt{n}$ and weighting exponent $m = 1.1, 1.2, \ldots, 2.5$. To improve robustness in the evaluation, each FCM implementation was executed 200 times for each configuration and clustering result having the lowest Jm value was considered for the CVIs evaluation. In both the experiments the 8 CVIs were applied to evaluate clustering results obtained by the allowed FCM implementations distinguished by the different values of K and m parameters. To enable the quantitative comparison analysis, CVIs values were normalized taking into consideration the fact that some indexes designate the optimal number of clusters by using the maximum value, while the others the minimum value. In particular, the z-score normalization has been implemented in a positive way for the indexes that minimize their optimal value, and in a negative way for the indexes that maximize their optimal value. After normalization, the indexes indicated the number of optimal clusters with the lowest value, making them to be well comparable. Table 1 illustrates the CVIs values resulting from the evaluation of clustering fMRI dataset by FCM with $m = 2$ and i ranging from 2 to 10.

Table 1. Values of CVIs resulting from the evaluation of clustering fMRI dataset by FCM with $m = 2$ and i ranging from 2 to 10.

Index	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 6$	$i = 7$	$i = 8$	$i = 9$	$i = 10$
FPBMI	1.66	1.59	−1.66	−0.12	1.95	−0.44	0.62	1.62	−0.12
PBMI	1.02	0.89	−1.19	−0.47	0.69	−0.67	0.93	1.12	−0.44
FSI	0.75	0.81	−0.08	−0.53	0.07	−0.64	0.93	−0.42	−0.54
WSJI	−0.27	0.02	0.02	−0.44	0.05	−0.35	1.09	−0.95	−0.61
XBI	−0.73	−0.90	0.11	−0.46	−0.81	−0.40	−0.61	−0.63	−0.41
RLRI	−0.82	−0.98	0.65	−0.31	−0.96	−0.11	−0.57	−1.05	−0.63
DBI	−0.92	−0.97	0.93	−0.07	−1.03	0.28	−0.94	−0.29	0.46
SDBI	−0.67	−0.46	1.21	2.43	0.02	2.35	−1.44	0.61	2.30

To summarize the set of results generated and develop systematically a comparative evaluation of CVIs, we introduced a measure E defined as:

$$E = |ni - nr| \tag{17}$$

where ni is the optimal number of clusters designated by the index, nr the number of cluster by reference. Table 2 illustrates performance of E values of the 8 CVIs, computed as average of E values obtained varying parameter m in the two experiments mentioned above.

Table 2. Mean and variance of E values for the 8 index evaluating clustering of fMRI data with 2 (Experiment 1) and 4 (Experiment 2) reference classes, the CVIs are in ascending order based on the E mean.

Index	Experiment 1		Index	Experiment 2	
	E mean	Var		E mean	Var
FSI	0.58	0.13	WSJI	0.78	0.08
RLRI	0.65	0.18	RLRI	1.35	0.17
WSJI	1.28	0.10	FSI	1.47	0.08
SDBI	1.54	1.50	SDBI	1.55	0.49
DBI	4.76	5.02	DBI	3.31	2.35
XBI	5.50	0.40	XBI	3.69	0.39
PBMI	6.22	0.42	PBMI	4.22	0.42
FPBMI	6.36	0.25	FPBMI	4.36	0.25

5 Discussion and Conclusions

In this work the performance of 8 well-known CVIs was quantitatively evaluated by using the FCM algorithm to process fMRI data. The use of the selected dataset allows to investigate the behavior of CVIs under two different levels of organizing data in two and four reference classes. The results obtained are preliminary but useful to suggests guidelines for a reliable use of cluster evaluation indexes and to contribute to a proper use of data driven, clustering techniques in the complex and more and more investigated brain function evaluation domain. Looking into the details of the results listed in Table 2, we noticed that RLRI, WSJI and FSI gained the top three positions in both the experiments even if with a different internal order. This fact leads to the conclusion that each one of them is able to both mediate between different characteristics of cluster structures and efficiently create a balance between compactness and separation. It was found also that widely used indexes such XBI, DBI and PBMI showed values considerable lower the three indexes mentioned above. The major differences between the two sets of CVIs lie in the formalization of separation component that plays an important role when dealing with clusters allocated closely as probably in case of fMRI data, and in the management of the two measures (compactness and separation) in the case of RLRI and WSJI is the sum of the two components, FSI subtraction while XBI, DBI, SDBI apply the ratio and FPBMI, PBMI the product. The novel SDBI index showed better values than crisp standard version and gained a position just below the top three positions. The XBI, PBM, FPBM, and DBI indices seem to be more suitable for contexts in which data distribution with little overlap is hypothesized, or in which cluster compactness is preferred.

Main conclusions obtained by our experimental work are consistent with results obtained in previous works [12] while considering the different experimental strategies and different domains. However caution must be exercised when applying results to other fMRI contexts taking into account the variability and complexity of these data and the different processing strategies. Future work contemplates a refinement of the metric adopted in the comparison to include other evaluation criteria and the use of a broader set of fMRI data with different levels of complexity and inter-cluster overlap, to obtain results more robust and extensible to other similar contexts.

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