THE UNIVERSITY OF ALABAMA AT BIRMINGHAM.

An Approach to Compare Clustering Results of Two Temporal fMRI Dataset

Presented By: Group 16

Ahmedur Rahman Shovon (ashovon) Ashraful Islam (aislam) Pratim Saha (psaha) Shahariar Rabby (arabby)

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Introduction

- Topological data analysis is an important topic in the field of data mining.
- This is especially useful to handle high-dimensional and noisy data.
- In this paper, we show an approach to compare different clustering results on an fMRI dataset of two temporal frequencies for a subject.
- fMRI (Functional Magnetic Resonance Imaging) is a non-invasive and non-detrimental process to quantify the neuronal activity of the brain during normal and diseased conditions
- We explore the similarity between two fMRI scans of the same people taken at two-time points.

Motivation

- Time-varying data analysis has increasingly become an integral part of fields such as Data Mining.
- Major objectives of understanding this type of data is to extrapolate meaningful information and correlation among the data points to forecast future outcome.
- fMRI is a time series data.
- We formulate the hypothesis that fMRI data for the same subjects at two time points should have similar natures.

Dataset Description

- Dataset was collected from Auburn University MRI research center.
- Two fMRI scan of 316 subjects were used in our experiment.
 - Dynamic_FC_2500:
 - Number of slices: 86
 - Dimension of each slice: 114*114
 - Dynamic_FC_1400:
 - Number of slices: 336
 - Dimension of each slice: 114*114
- Dataset was provided in the matrix format.

Methodology



Workflow Diagram





Normalization of Dataset

- We normalized the input matrix data within a range of 0 to 1.
- The following formula was used to normalize the data:

$$[x]' = \sqrt{1 - \mathcal{C}([x]^T)}$$

- [x]' = normlized matrix
- *C* = *correlation coefficient*
- $[x]^T = transposed input matrix [x]$

Persistent Homology

- Computed 0-dimensional persistent homology (PH) for time frames of each subjects
- Generated 0-dimensional barcodes from calculated
 PH value with maximum value of 1
- Generated 316 * 2 JSON files, 1 for each subject for 1-Wasserstein distance matrix of the timeframe barcodes
- Matrix size 86 * 86 and 336 * 336



Multidimensional Scaling

- Applied classical metric Multidimensional scaling (MDS) with precomputed distance (1-Wasserstein)
- It represents a low-dimensional view of the data in which the distances respect well the distances in the original high-dimensional space
- Generated 316 * 2 JSON files, 1 for each subject for MDS matrix
- Matrix size 86 * 2 and 336 * 2



Algorithms Used

We've used 8 clustering algorithms:

- KMEANS
- KMEANS++
- Affinity Propagation
- Birch
- Mean Shift
- Spectral Clustering
- DBSCAN
- OPTICS

Clustering Parameters

• Silhouette Score:

It is a metric used to calculate the goodness of a clustering techniques.

- For iterative(Kmeans, Kmean++) and graph-based (Spectral) clustering we generated Silhouette Score for the number of clusters ranging from 2 to 15.
- The number with the highest score was picked as the number of cluster.
- For DBSCAN, OPTICS we set the $\in = 1.5$ and min_point = 5 and generate clusters for each fMRI scan.
- For Mean Shift we set the *bandwidth* = 2, BIRCH $n_{cluster} = None, threshold = 1.5$ and For Affinity Propagation we set the *iteration* = 200, with *damping* = 0.5.

Affinity Propagation

- Affinity Propagation creates clusters by sending messages between pairs of samples until convergence.
- A dataset is then described using a small number of exemplars, which are identified as those most representative of other samples.
- The messages sent between pairs represent the suitability for one sample to be the exemplar of the other, which is updated in response to the values from other pairs.
- This updating happens iteratively until convergence, at which point the final exemplars are chosen, and hence the final clustering is given.

Mean Shift

- Mean Shift clustering aims to discover blobs in a smooth density of samples.
- It is a centroid-based algorithm
- It works by updating candidates for centroids to be the mean of the points within a given region.
- Each point try to find its group by moving towards the weighted mean of its local area in each step.
- The destination of each point will be the centroid of the data cluster that the point belongs to.
- All the data points with the same destination point can be labeled with the same cluster.

Spectral Clustering

- Graph based clustering algorithm
- Spectral Clustering performs a low-dimension embedding of the affinity matrix between samples,
- Find the Laplacian matrix of the input matrix by subtracting the adjacency matrix from input matrix.
- First non-zero eigenvalue is called spectral gap which gives us the notion about the density of the graph.
- First large gap of the eigenvalues determines the number of clusters
- Eigenvectors correspond to the eigenvalues determine the actual cluster label.

BIRCH (Balanced Iterative Reducing & Clustering using Hierarchies)

- The Birch builds a tree called the Clustering Feature Tree (CFT) for the given data.
- The data is essentially lossy compressed to a set of Clustering Feature nodes (CF Nodes).
- The CF Nodes have several subclusters called Clustering Feature subclusters (CF Subclusters)
- These CF Subclusters located in the non-terminal CF Nodes can have CF Nodes as children.



Evaluation

- We compare the number of clusters for fMRI of a subject.
- We find the percentage of population with same number of clusters in both fMRI data.
- For mismatched clusters, we find the difference in cluster number between 2 scans and calculated the mean mismatch distance.
- Percentage match and mean mismatch distance was used to evaluate the clustering algorithms.
- K-means++ provides the best performance with 56.33% matches and MMD of 1.28.

Figure OPTICS clustering for Subject 1



Fig. Clusters generated by OPTICS



Figure KMeans clustering for Subject 1



Fig. Clusters generated by KMeans clustering algorithm



Figure DBSCAN clustering for Subject 1



Fig. Clusters generated by DBSCAN clustering algorithm



Figure Spectral clustering for Subject 1



Fig. Clusters generated by Spectral Clustering



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Figure Clustering summary

Clustering Method: KMeans Best cluster selection using Silhouette Score in 2-15 range Total subjects: 316 Total matches: 172 Total match percentage: 54.43 Mean mismatch distance: 1.50

```
Clustering Method: dbscan
Parameters: eps=1.5, min_samples=5
Total subjects: 316
Total matches: 137
Total match percentage: 43.35
Mean mismatch distance: 0.81
```

Clustering Method: spectral Best cluster selection using Silhouette Score in 2-15 range Total subjects: 316 Total matches: 161 Total match percentage: 50.95 Mean mismatch distance: 1.58

Fig. Clustering result summary using KMeans, DBSCAN, and Spectral



Evaluation

	Method	Algorithm Type	Subjects	Matches	Match (%)	Mean Mismatch Distance
1	K-means	Iterative	316	172	54.43	1.50
2	K-mean++	Iterative	316	178	56.33	1.28
3	Affinity propagation	Hierarchical Clustering	316	1	0.32	6.95
4	Spectral Clustering	Graph based	316	161	50.95	1.58
5	DBSCAN	Density Based	316	137	43.35	0.81
6	OPTICS	Density Based	316	137	43.35	0.81
7	BIRCH	Hierarchical Clustering	316	5	1.58	14.56
8	Mean Shift	Centroid based	316	37	11.08	1.86



Conclusion and Future Work

- Time-varying fMRI data is becoming increasingly important in data analysis.
- Analyze the structural changes of time-varying fMRI data at different time points using unsupervised machine learning techniques.
- Applied different clustering algorithms to all fMRI scans to find their clustered nature.
- Found the difference between the number of clusters over two-time points to log the quality of data changes over time.
- Performance of the clustering result was evaluated by percentage similarity of matches and MMD.
- KMeans++ achieves a maximum of 56.33% matches and 1.28 MMD which outperformed other clustering algorithms we have adopted in this work.
- In future we are planning to apply deep learning-based algorithm.
 - Auto-encoder to analyze quality of clusters.

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