Research on the Application of the Density-Based OPTICS Algorithm in Whole-Brain Functional Parcellation

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Abstract— **In the analysis of functional magnetic resonance imaging (fMRI) images, brain partitioning is a core step in the generation, analysis, and study of functional connectivity of human brain networks. Previous related research mainly relied on meta-analysis, random standards, or brain atlases generated based on original anatomical data to define the nodes of human brain networks. However, these methods have limitations in terms of functional specificity and may not accurately reflect the actual neural functional partitions. In contrast, brain functional partitioning can effectively avoid the above problems. Therefore, This paper, in light of the characteristics of resting-state fMRI data, proposes a Density First Clustering (DF-OPTICS) algorithm based on the OPTICS algorithm. By using local density to replace core distance and reachability distance metrics, this algorithm avoids clustering errors and ensures that the result sequence is output in order while considering the spatial continuity of the partition. Additionally, to prevent the original OPTICS algorithm from consuming a large amount of computing time in neighborhood search, DF-OPTICS utilizes the existing voxel spatial coordinate information for local voxel search, significantly reducing the computational load of neighborhood search. Simulation experiment results show that the algorithm proposed in this paper significantly outperforms other comparison algorithms in multiple comprehensive evaluation indicators and achieves satisfactory partitioning effects.**

Index Terms—Functional Magnetic Resonance Imaging；Brain Functional Parcellation；Clustering Algorithm；OPTICS

I. INTRODUCTION

The operational mechanisms of the human brain have long been a central theme in interdisciplinary research. Its intrinsic cognitive functions, encompassing perception, decision-making, emotional regulation, memory storage, and retrieval, not only form the foundation of individual behavior but also profoundly shape social interactions and cultural evolution[1]. Understanding how the brain integrates and processes information through the electrochemicaltransmission of signals between neurons is key to uncovering the nature of consciousness, the origins of intelligence, and the principles of neural plasticity[2].To analyze this dynamic process, researchers have developed a multi-level technological framework, ranging from microscopic approaches such as neurotransmitter receptor analysis and extracellular recordings to macroscopic techniques like electroencephalography (EEG) monitoring and blood oxygen metabolism imaging[3]. Among these, non-invasive techniques have emerged as essential tools for exploring brain functional networks and pathological mechanisms due to their safety, repeatability, and precision.Furthermore, research paradigms in neuroscience are profoundly influencing advancements in computational fields. Inspired by neuronal signal transmission and synaptic plasticity, artificial neural networks and deep learning models replicate the hierarchical information processing characteristics of the brain, demonstrating brain-like intelligence in tasks such as pattern recognition and natural language processing[4-6].

Whole-brain parcellation is a fundamental component of neuroscience research, playing a crucial role in understanding brain function and structure. For instance, the Human Connectome Project aims to construct a comprehensive atlas of human brain function and structure, further highlighting the critical importance of whole-brain parcellation in neuroscience[7]. Beyond these large-scale research initiatives, numerous other research teams are actively advancing work related to brain parcellation. Over the years, these efforts have accumulated a wealth of valuable findings, significantly contributing to the ongoing progress of brain science[8-10].Currently, widely used templates such as the Automated Anatomical Labeling (AAL) atlas and Brodmann Area (BA) maps segment the brain based on cytoarchitectonic features[11]. However, these structural templates do not fully account for functional connectivity between brain regions, inter-individual variability, or the distinct functional characteristics of each region. As a result, brain regions derived solely from these templates may have limitations in functional interpretation, potentially affecting the accuracy of disease diagnosis and treatment analysis.To address these challenges, functional brain parcellation methods based on functional magnetic resonance imaging (fMRI) data have emerged[12,13]. By delineating functional brain regions, researchers can gain deeper insights into the organizational principles of brain function. Moreover, functional parcellation serves as a foundation for constructing brain functional networks using abstracted nodes or defining regions of interest (ROIs) in functional connectivity analysis[14]. Therefore, functional brain parcellation is a core step in neuroscience research, essential for both fundamental studies and clinical applications[15-17].

Manuscript received March 08, 2025

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Whole-brain functional parcellation can be achieved through four primary approaches: clustering-based methods, boundary mapping methods, independent component analysis (ICA)-based methods, and graph theory-based methods[18].In recent years, advancements in brain imaging technologies—particularly multi-modal magnetic resonance imaging (MRI), including structural, functional, and diffusion MRI—have provided increasingly rich datasets, enabling researchers to explore more precise and comprehensive methods for delineating the organizational patterns of the cerebral cortex[19]. Despite these methodological developments, the fundamental principle of functional parcellation remains rooted in the concept of connectivity—the function of each brain region is defined by its input and output patterns relative to other regions. These connectivity patterns play a crucial role in determining the functional organization of the brain.While emerging brain parcellation methods differ in both technical implementation and theoretical foundations, their overarching goal remains consistent: to identify brain regions that are functionally coherent yet anatomically heterogeneous based on specific neurobiological measurements, ultimately enhancing our understanding of brain function and organization[20-22].

Clustering-based methods achieve brain functional parcellation by grouping voxels based on their feature distances, which typically reflect their similarity in connectivity patterns. During the clustering process, elements with similar connectivity characteristics are assigned to the same cluster, while those with significant differences are categorized into separate clusters.Numerous clustering algorithms have been applied to brain parcellation research. For example, Craddock et al. employed a spatially constrained spectral clustering method to partition the brain into 200 regions[23]. This approach segmented whole-brain fMRI data into spatially coherent regions with homogeneous functional connectivity, generating a region of interest (ROI) atlas. Building upon this work, Fan Lingzhong et al. introduced the Brainnetome Atlas, developing a spectral clustering-based framework for brain parcellation using structural connectivity data[24]. Their method produced 210 cortical and 36 subcortical regions across the entire brain, providing a comprehensive and cross-validated parcellation atlas.To address the need for multi-modal data integration, Joshi et al. proposed the USCBrain atlas, which combines the BCI-DNI anatomical atlas with resting-state fMRI data[25]. By employing hierarchical clustering, they refined the brain into 130 functional subregions, demonstrating the potential of cross-modal integration for achieving a finer-grained parcellation.

In summary, although significant methodological advancements have been made in brain functional parcellation, many unexplored areas remain. Future research should focus on further integrating multi-scale data, developing adaptive computational models, and establishing standardized evaluation frameworks to drive the transition of functional parcellation from methodological innovation to applications in precision medicine[26,27]. Ultimately, these advancements will provide stronger technological support for understanding the mechanisms of brain disorders and enabling personalized interventions.

II. MATERIAL AND METHODS

A. The 1000 Functional Connectomes Project

In this chapter, we utilize data from the Beijing_Zang dataset, which is part of the publicly available 1000 Functional Connectomes Project. This dataset, provided by Professor Yu-Feng Zang's team at Beijing Normal University, includes resting-state functional magnetic resonance imaging (rs-fMRI) data from 198 healthy adults aged 18-26 years with a balanced gender ratio.During scanning, all participants remained awake with their eyes closed and did not engage in any specific cognitive tasks to capture spontaneous brain activity signals. The data were acquired using a 3T Siemens Trio scanner, following a resting-state paradigm with the following parameters: repetition time (TR) = 2 seconds, voxel resolution = 3×3×3 mm³, and a scan duration of approximately 8 minutes (240 time points). Additionally, high-resolution T1-weighted structural images were collected for anatomical localization of brain regions.The dataset complies with ethical guidelines, with all participants providing informed consent and approval obtained from the institutional ethics committee. Due to its high quality and well-controlled conditions, this dataset has been widely used in studies on the default mode network (DMN), individual differences in functional connectivity, and methodological validation.Specifically, in this study, we use structural and resting-state fMRI data from 20 participants for further analysis.

B. *Density-First OPTICS Algorithm*

1. Algorithm Description and Initialization

The algorithm initialization settings as a dataset $D = \{u_1, u_2, \dots, u_n\}$ consisting of n voxels is assumed to exist in a three-dimensional brain space (x, y, z). Each voxel has m attributes, denoted as $u_i = \{u_{i1}, u_{i2}, \dots, u_{im}\}$, and its spatial coordinates are represented as $\{x_i, y_i, z_i\}$.In the dataset D, the feature distance between voxels u_i and $u_j$is defined using the Euclidean distance as:

$$d_{feature}(u_i, u_j) = \sqrt{\sum_{k=1}^{m} (u_{ik} - u_{jk})^2}$$

The spatial distance between voxels u_i and u_j is also defined using the Euclidean distance as:

$$d_{space}(u_i, u_j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

2. Definition of Neighborhood and Voxel Partitioning

For any voxel u_i, its neighborhood is defined as a spherical region centered at u_i with a radius r, denoted as $N(u_i, r)$. This can be expressed as:

$$N(u_i, r) = \{u_j \in D \mid d_{space}(u_i, u_j) \le r\}$$

To identify high-density regions within the data and thereby facilitate effective clustering analysis, voxels need to be categorized into core voxels (CoreVoxel) and boundary voxels (BounVoxel). For a given voxel u_i, a density threshold ρ_{Min} is defined. If the density of a voxel ρ_i satisfies $\rho_i \ge \rho_{Min}$, indicating that the voxel is located in a sufficiently dense region, it is classified as a core voxel. Conversely, if $\rho_i < \rho_{Min}$, meaning that the voxel's surrounding region is less densely populated, it is classified as a boundary voxel. This classification is formally defined as follows:

$$u_i = \begin{cases} CoreVoxel & \rho_i \geq \rho_{Min} \\ BounVoxel & \rho_i < \rho_{Min} \end{cases}$$

3. Generating the Result Sequence

(1) Initialize a max-heap PointTree and a result sequence ResultList. PointTree maintains the density of each voxel within its neighborhood, ensuring that the root node always corresponds to the voxel with the highest density. ResultList stores the visited voxels, forming the final ordered sequence.
(2) For each voxel, create an object containing feature distance $d_{feature}$, spatial distance d_{space}, voxel density ρ_i, and two flags: IsInList (indicating whether u_i is in ResultList) and IsInTree (indicating whether u_i is in PointTree).
(3) Iterate through each voxel. If the voxel is not a core voxel, skip it. Otherwise, update the density of its neighbors add u_i to PointTree while maintaining the heap property, and insert u_i into ResultList to mark it as visited.
(4) Construct PointTree by extracting the root node with the highest density voxel u_{Max}, expressed as:

$$u_{Max} = \arg Max_{k \in PointTree} \rho(k)$$

If u_{Max} is not a core voxel, directly add it to ResultList and mark it as visited, indicating that it is a boundary voxel. If u_{Max} is a core voxel but not yet in ResultList, visit its neighboring voxels and compute their densities. For voxels not already in PointTree, insert them, then update and adjust PointTree. Once the root node u_{Max} is fully processed, add it to ResultList and remove it from PointTree.

If PointTree is not empty, it indicates that the current cluster is still being traversed. In this case, jump to Step 4 and continue execution. Otherwise, if PointTree is empty, it means that the traversal of the current cluster has ended, and a new unvisited core voxel must be selected as the new starting point. Then, jump to Step 3 and continue execution.

When the algorithm terminates, the result sequence ResultList is output. Meanwhile, there may be some voxels that have not been visited. These voxels are considered outliers or noise points, denoted as NoiseVoxel.

4. Constructing the Density Map

After obtaining the result sequence ResultList , a density map can be constructed according to the ordering of voxels in the sequence and their corresponding density values. considering computational complexity and the spatial constraints required for functional parcellation, this chapter uses density values instead of reachability distance to evaluate the clustering structure of the data.

5. Cluster Extraction

Based on the density map, this section introduces a threshold parameter (thres) for cluster division. Inspired by the core principles of DBSCAN, this method is adapted specifically for the density map. Different thres values lead to varying clustering results, allowing adjustments to achieve different partitioning granularities.After setting the thres parameter, the algorithm iterates through each voxel in the density map using thres as the density threshold. If a voxel's density ρ_i is greater than or equal to thres, it is assigned to the same cluster as its preceding voxel. If the density is below thres, the algorithm further checks whether the voxel is a core voxel. If it is, the voxel is designated as the starting point of a new cluster; otherwise, it is marked as a noise voxel. Through this process, the algorithm dynamically merges continuous regions that meet the density threshold, ultimately forming the final clustering results.

III. RESULTS

a) *Spatial Continuity Results*

To evaluate spatial continuity, this section applies each clustering algorithm to 20 subjects and computes the Space Discontiguity (SD) index for each subject. The final spatial continuity measure for each algorithm is obtained by averaging the SD values across all subjects, providing a standardized evaluation of spatial consistency under a given number of partitions. A lower SD value indicates higher spatial continuity, meaning that the clustering results produce more spatially coherent functional regions.

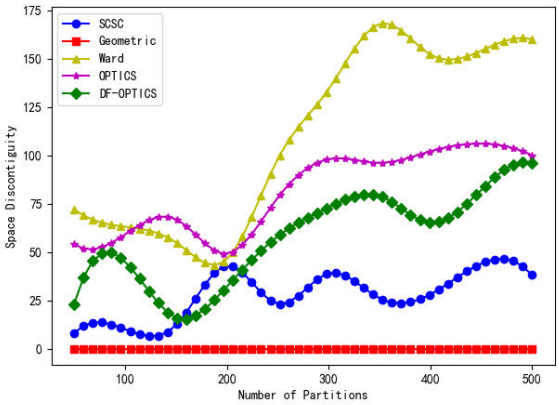

Fig.1.Spatial Continuity Results

As shown in Figure 1, the Geometric algorithm, used as a baseline method, clusters voxels solely based on spatial location. As a result, regardless of the partitioning strategy, each cluster consists of adjacent voxels, leading to an SD (Space Discontiguity) index of zero in all cases.The SCSC algorithm demonstrates the best spatial continuity, primarily due to its strong spatial constraints, which result in larger and more contiguous regions. However, this often comes at the cost of weaker functional connectivity within individual clusters.In contrast, the Ward algorithm relies primarily on functional feature similarity, leading to the formation of a greater number of disjoint regions and, consequently, a higher SD index.The DF-OPTICS algorithm proposed in this chapter exhibits slightly lower spatial continuity compared to SCSC. However, it significantly outperforms the original OPTICS and Ward algorithms, achieving 35.2% and 26.1% improvements in spatial continuity, respectively.

b) *Functional Consistency Results*

To evaluate functional consistency, a process similar to the assessment of spatial continuity is applied. The Silhouette Coefficient (SC) is computed for each of the 20 subjects, and the final evaluation metric for each algorithm is obtained by averaging the SC values across all subjects.Each algorithm produces an SC score corresponding to a specific number of partitions, where a higher SC value indicates better functional consistency within the clusters. A higher score suggests that voxels within the same partition share more similar functional properties, making the clustering results more functionally meaningful.

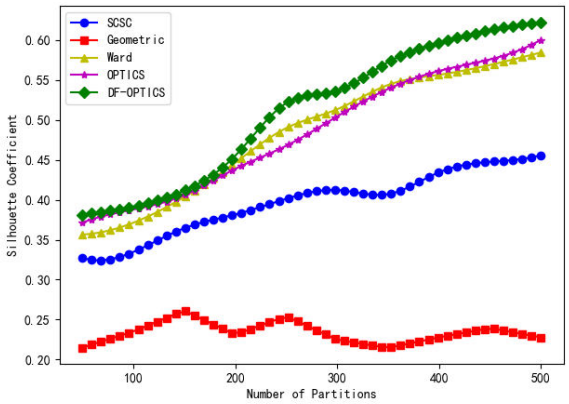

Fig.2.Functional Consistency Results

As shown in Figure 2, except for the Geometric algorithm, which serves as a baseline method, overall functional consistency improves as the number of partitions increases. However, unlike the results for spatial continuity, the SCSC algorithm exhibits poor functional consistency. This is primarily due to its strong spatial constraints, which reduce the functional homogeneity within clusters.The DF-OPTICS algorithm, proposed in this chapter, achieves the best functional consistency among all methods. Compared to the Ward algorithm, it improves functional consistency by 4.5%, and compared to the original OPTICS algorithm, it achieves a 4.1% improvement.

c) *Reproducibility Results*

To evaluate the reproducibility of the clustering algorithms, this study employs the bootstrap sampling method. Specifically, resampling with replacement is performed on the 20 subjects, selecting 20 samples per iteration, and this process is repeated 10 times.For each resampling iteration, the clustering results are pairwise compared, and the Dice coefficient is computed to measure the similarity between partitions. The final reproducibility score for a given number of partitions is obtained by averaging the Dice coefficients across all pairwise comparisons. This averaged Dice coefficient serves as the reproducibility metric, reflecting the stability and consistency of the clustering method under different subject selections.

As shown in Figure 3, the reproducibility of all algorithms declines as the number of partitions increases, indicating that inter-individual variability becomes more pronounced with finer-grained parcellation.Notably, the Ward algorithm exhibits even lower reproducibility than the baseline Geometric algorithm. This is primarily because Geometric is based on the k-means algorithm, which relies solely on spatial distance for clustering, whereas Ward's hierarchical clustering is more susceptible to individual differences.In contrast, SCSC and DF-OPTICS outperform other methods in terms of reproducibility, as both incorporate spatial information, which helps mitigate the impact of inter-subject variability. Among them, DF-OPTICS achieves the best reproducibility, improving by 9.8% compared to SCSC and by 32.6% compared to the original OPTICS algorithm.

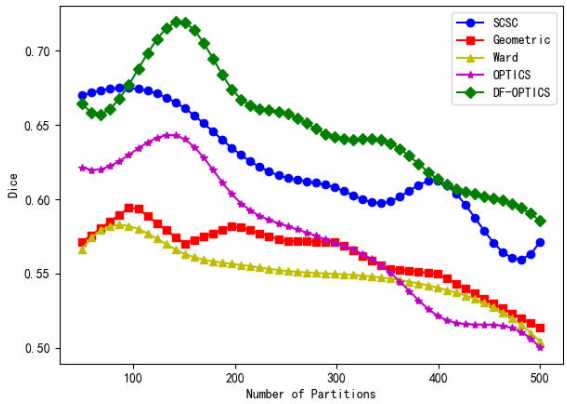

Fig.3.Reproducibility Results

d) *Runtime Results*

To quantify the computational efficiency of different clustering algorithms, we record their runtime performance under varying numbers of partitions. Specifically, we apply five clustering algorithms to the same set of fMRI data and measure their execution time for each partitioning setting. The recorded runtimes provide a direct comparison of the computational cost associated with each method, allowing for an evaluation of their scalability and efficiency.

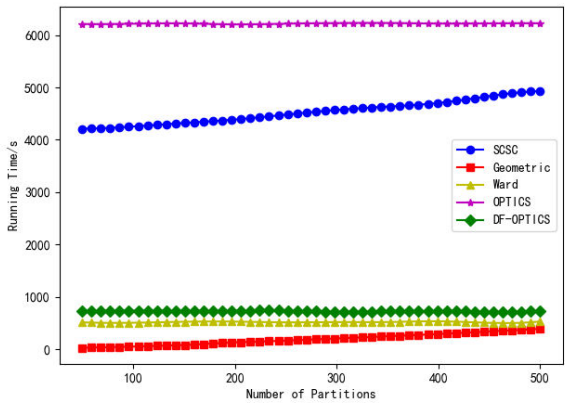

Fig.4.Runtime Results

As shown in Figure 4, the runtime trends indicate that, except for SCSC and the baseline Geometric algorithm, the execution time of the other clustering methods does not significantly increase with the number of partitions. This is primarily because SCSC relies on spectral decomposition, where computational complexity grows as the number of partitions increases. Similarly, Geometric clustering is based on k-means, whose computational cost is positively correlated with the number of partitions.In contrast, the execution time of the remaining algorithms is not directly dependent on the number of partitions, resulting in relatively stable runtime curves.From a numerical perspective, the DF-OPTICS algorithm, proposed in this study, demonstrates superior computational efficiency. Its runtime is reduced by 88.7% compared to the original OPTICS and by 83.3% compared to SCSC, making it a highly efficient clustering approach for brain functional parcellation.

e) *Brain Functional Parcellation Results*

As shown in Figure 5, different clustering algorithms exhibit significant variations in the overall spatial distribution of

brain parcellation results, where k represents the number of clusters.

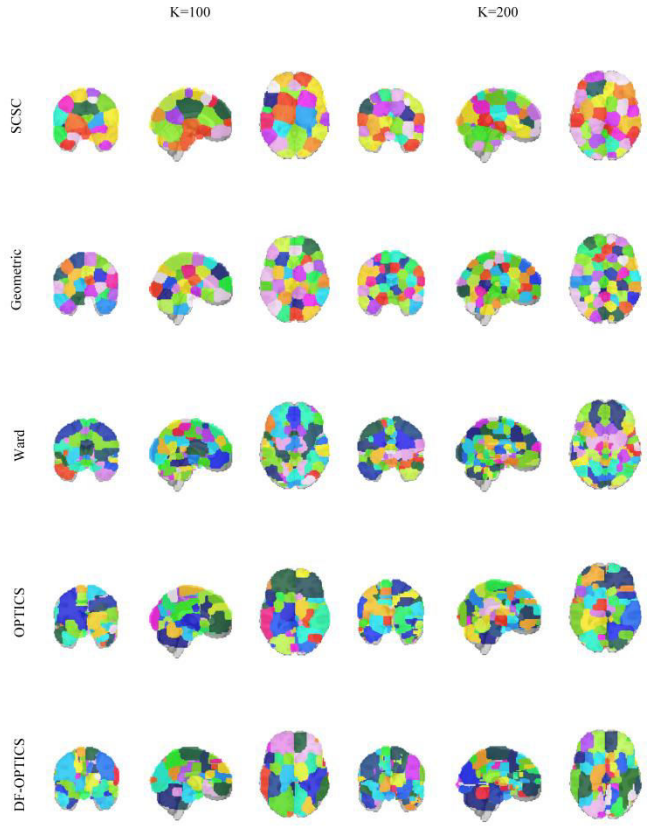

Fig.5.Brain Functional Parcellation Results

Specifically, the SCSC algorithm, due to its strong spatial constraints, produces more structured and regular partitions. In contrast, the Geometric algorithm, which clusters voxels solely based on spatial coordinates without considering functional features, maintains a highly uniform parcellation structure regardless of whether k = 100 or k = 200.The Ward and OPTICS algorithms, which primarily rely on feature distance for clustering, result in more spatially scattered brain regions. Notably, the Ward algorithm generates highly symmetric left and right brain regions. This is because Ward's hierarchical clustering follows a variance minimization principle, which favors grouping spatially adjacent and functionally similar regions into the same cluster. Such symmetry in brain parcellation reflects functional similarity between corresponding brain regions .For the DF-OPTICS algorithm, as k increases, some regions remain stable, while others undergo further refinement. This occurs because, with a higher density threshold, some voxel clusters that previously belonged to the same partition are split, whereas voxel groups that consistently exceed the threshold remain unaffected. A similar phenomenon is observed in the OPTICS algorithm, where density-based clustering dynamically adjusts the level of granularity in brain parcellation.

IV. DISCUSSION

This paper focuses on the Density-First OPTICS algorithm (DF-OPTICS) and its successful application in resting-state fMRI data clustering. First, the challenges associated with applying the original OPTICS algorithm to brain functional parcellation were analyzed, including issues related to computational complexity and distance metrics. Based on these considerations, a density-first optimization of the OPTICS algorithm was proposed.The DF-OPTICS algorithm replaces core distance and reachability distance with density-based measures, ensuring that the result sequence is output in an ordered manner while also maintaining spatial continuity within partitions. To address the high computational cost of neighborhood searches in the original OPTICS algorithm, existing voxel spatial coordinates were utilized to optimize the spatial neighborhood search process, significantly reducing computation time.To verify the effectiveness of the proposed method, simulation experiments were conducted. The algorithm parameters were first fine-tuned, followed by a comparative evaluation against other brain functional parcellation algorithms, including the original OPTICS algorithm, the commonly used Ward algorithm, the SCSC algorithm with spatial constraints, and the Geometric algorithm as a baseline.Experimental results demonstrate that, in terms of spatial continuity, functional consistency, reproducibility, and runtime efficiency, the proposed DF-OPTICS algorithm outperforms the other four methods, highlighting its feasibility and effectiveness for brain functional parcellation.

V. CONCLUSION

To address the distance metric bias and computational efficiency issues of the traditional OPTICS algorithm in brain parcellation, this paper proposes a Density-First OPTICS algorithm (DF-OPTICS). By replacing the core distance and reachability distance with local density measures, DF-OPTICS not only ensures the ordered output of the result sequence but also maintains the spatial continuity of the parcellation.To reduce the excessive computational cost of neighborhood searches in the original OPTICS algorithm, DF-OPTICS utilizes existing voxel spatial coordinates to perform localized voxel searches, significantly reducing the computational complexity of the neighborhood search process.Finally, the proposed algorithm was applied to brain parcellation experiments using resting-state fMRI data. The results demonstrate that DF-OPTICS achieves superior performance in terms of spatial continuity, functional consistency, reproducibility, and computational efficiency, making it a highly effective method for brain functional parcellation.With the continuous advancement of brain network analysis techniques and their expanding applications, brain functional parcellation remains a key research focus in the academic community. Although this study has made progress, several limitations remain, which will be explored and improved in future research:

1. The human brain is one of the most complex systems, and brain functional parcellation research is still evolving. Different parcellation methods employ varied evaluation criteria, and currently, there is no standardized evaluation metric in the field of brain functional parcellation. The clustering algorithm proposed in this study uses a limited set of evaluation metrics, which may not fully capture the accuracy and robustness of parcellation results. Future studies should explore more comprehensive and precise evaluation standards to improve the reliability and interpretability of brain parcellation outcomes.
2. This study primarily relies on BOLD signal features from functional magnetic resonance imaging (fMRI). However, the biological basis of brain functional parcellation should incorporate information from structural, metabolic, and electroph

ysiological data. Future research can explore multimodal fusi on algorithms to construct cross-scale brain parcellation mod els, which could uncover more intricate coupling mechanism s underlying brain function.

3. Functional regions extracted from fMRI data adjust dyna mically in response to changes in brain states, and the data it self also varies over time. Future research should focus on dy namic functional parcellation to further investigate time-depe ndent boundary shifts in functional regions and their underlyi ng mechanisms.

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