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Improvement of Functional Brain Parcellation Using Machine Learning Techniques

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Abstract: Functional brain parcellation is fundamental to understanding large-scale neural organization and improving downstream neuroimaging analyses. Traditional atlas-based and classical clustering approaches, while widely used, often fail to capture complex, non-linear functional connectivity patterns and inter-individual variability present in high-dimensional resting-state fMRI data. This study proposes a machine learning-driven framework to enhance functional brain parcellation using large-scale datasets, including those from the Human Connectome Project. The methodology integrates advanced preprocessing, feature extraction from functional connectivity matrices, and multiple machine learning models, including unsupervised clustering, deep learning architectures, and graph-based neural networks. Model performance was evaluated using functional homogeneity metrics (Silhouette Score, Davies–Bouldin Index), spatial consistency measures (Dice Similarity Coefficient), and predictive utility in cognitive outcome modeling. Results demonstrate that the proposed framework outperformed traditional atlas-based, spectral clustering, and graph modularity approaches. The machine learning model achieved a higher mean silhouette score (0.61), a lower Davies–Bouldin Index (0.94), and improved Dice similarity (0.76), indicating enhanced intra-parcel coherence and inter-subject reproducibility. Furthermore, predictive modeling accuracy improved by 9–14%, with an 11% reduction in mean absolute error compared to atlas-based features. Statistical testing confirmed that these improvements were significant ($p < 0.05$). The findings suggest that machine learning techniques substantially improve the accuracy, stability, and practical utility of functional brain parcellation. By capturing non-linear connectivity structures and adapting to individual variability, the proposed framework advances computational brain mapping and supports more reliable neuroimaging analyses for research and potential clinical applications.

Keywords: Functional Brain Parcellation; Machine Learning; Resting-State fMRI; Functional Connectivity; Deep Learning.

I. INTRODUCTION

Understanding the structural and functional organization of the human brain remains one of the central challenges in contemporary neuroscience[1]. Functional brain parcellation the process of dividing the brain into spatially distinct and functionally homogeneous regions serves as a foundational step in mapping neural networks, interpreting brain activity, and identifying biomarkers of neurological and psychiatric disorders [2]. Traditional parcellation approaches, including atlas-based methods and connectivity-driven clustering techniques, have significantly advanced insights into large-scale brain organization [3]. However, these conventional strategies often rely on predefined anatomical boundaries or linear assumptions that may not fully capture the complex, high-dimensional patterns embedded within neuroimaging data.

With the emergence of advanced neuroimaging modalities such as functional magnetic resonance imaging (fMRI), large-scale datasets particularly those generated by initiatives like the Human Connectome Project have made it possible to study functional connectivity at unprecedented spatial and temporal resolutions [4]. Yet, the increasing dimensionality and variability of such data pose significant analytical challenges. Variations across individuals, noise contamination, and non-linear interactions between brain regions can limit the reliability and reproducibility of traditional parcellation methods. Consequently, there is a growing need for adaptive, data-driven techniques capable of capturing subtle and complex functional relationships.

Machine learning techniques offer a promising avenue for addressing these limitations. By leveraging supervised, unsupervised, and deep learning frameworks, machine learning algorithms can model non-linear dependencies, integrate multimodal features, and enhance robustness against noise [4]. Clustering algorithms, graph-based learning models, and convolutional neural networks have demonstrated considerable potential in identifying functionally coherent regions beyond rigid anatomical constraints. These approaches enable individualized parcellation schemes that reflect subject-specific connectivity patterns, thereby improving both sensitivity and specificity in downstream analyses such as disease classification, cognitive mapping, and predictive modeling[5]. Despite these advances, challenges remain regarding interpretability, generalizability, and computational efficiency. The integration of machine learning into functional brain parcellation requires careful validation, methodological transparency, and comparison with established atlases. Therefore, this study aims to explore and evaluate machine learning-based strategies for improving functional brain parcellation, emphasizing enhanced accuracy, reproducibility, and adaptability to diverse neuroimaging datasets. By advancing computational methodologies in brain mapping, this work contributes to the broader objective of achieving more precise and personalized representations of functional brain organization.

II. REVIEW OF RELATED LITERATURE

A. Conceptual Foundations of Functional Brain Parcellation

Functional brain parcellation refers to the subdivision of the cerebral cortex or whole brain into regions that exhibit coherent functional activity or connectivity patterns. Early efforts relied heavily on cytoarchitectonic and anatomical atlases derived from post-mortem studies, most notably the Korbinian Brodmann map, which divided the cortex into distinct areas based on cellular architecture. While these anatomical atlases provided a foundational framework, they do not fully reflect functional heterogeneity or dynamic connectivity patterns observed in vivo [6].

With the advent of functional magnetic resonance imaging (fMRI), connectivity-based parcellation emerged as a data-driven alternative. Functional connectivity, defined as the temporal correlation between spatially remote neurophysiological events, became central to identifying intrinsic brain networks. Resting-state fMRI studies revealed reproducible large-scale networks such as the default mode network (DMN), attention networks, and sensorimotor networks. These discoveries highlighted the importance of functional rather than purely anatomical segmentation [7].

B. Atlas-Based and Connectivity-Driven Approaches

Atlas-based parcellation methods typically apply predefined brain templates to neuroimaging data. Notable examples include the Montreal Neurological Institute (MNI) coordinate system and multi-resolution cortical parcellations developed from large cohorts. A widely cited functional atlas is the Thomas Yeo 7- and 17-network parcellation, derived from resting-state connectivity clustering across a large population [8]. While atlas-based methods promote reproducibility and standardization, they may oversimplify inter-individual variability. Connectivity-driven clustering methods, including k-means clustering, hierarchical clustering, and spectral clustering, attempt to partition the brain based on similarity in functional connectivity profiles. These unsupervised methods improved functional homogeneity within parcels but often depend on linear similarity metrics and require predefined cluster numbers, which can bias outcomes[9].

Graph-theoretical approaches further advanced the field by representing the brain as a network of nodes and edges. Community detection algorithms and modularity optimization techniques enabled identification of functionally cohesive modules. However, these approaches are sensitive to noise and threshold selection, limiting robustness in heterogeneous datasets [9].

C. Emergence of Machine Learning in Brain Parcellation

The rapid expansion of large-scale neuroimaging repositories, such as the Human Connectome Project, has facilitated the application of machine learning (ML) to brain mapping. Machine learning techniques address several limitations of traditional clustering by modeling complex, non-linear relationships and integrating high-dimensional features [10].

Unsupervised learning methods, including Gaussian mixture models and self-organizing maps, have been employed to discover latent functional structures. More recently, deep learning frameworks particularly convolutional neural networks (CNNs) and graph neural networks (GNNs) have demonstrated superior capability in capturing hierarchical and spatial dependencies in neuroimaging data. These models can learn data representations directly from voxel-wise or connectivity matrices without extensive handcrafted feature engineering. Supervised learning approaches have also been integrated into parcellation workflows, especially for task-based fMRI where labeled activation patterns guide regional segmentation. Transfer learning and representation learning have further enhanced generalizability across datasets and scanning protocols [11].

D. Individualized and Adaptive Parcellation

A major limitation of population-based atlases is their inability to capture subject-specific functional organization. Recent studies emphasize individualized parcellation strategies that adapt to each participant's connectivity profile [12]. Machine learning algorithms, particularly deep embedding clustering and variational autoencoders, have been proposed to generate personalized functional maps while maintaining alignment with group-level structures. Individualized approaches have shown promise in improving predictive modeling of cognitive traits and neurological disorders. For example, more refined parcellations enhance classification accuracy in studies of neurodevelopmental and neuropsychiatric conditions. However, challenges persist regarding computational cost, overfitting, and reproducibility across independent cohorts [13].

E. Current Gaps and Research Directions

Despite considerable progress, several gaps remain in the literature. First, many machine learning-based parcellation methods lack interpretability, making it difficult to relate derived parcels to established neurobiological knowledge [14]. Second, cross-dataset generalization remains problematic due to scanner variability and preprocessing differences. Third, evaluation metrics for comparing parcellation schemes are not standardized, complicating benchmarking efforts. Emerging research focuses on integrating multimodal imaging data (e.g., structural connectivity, diffusion MRI, and electrophysiological signals) into unified learning frameworks [15]. Hybrid models combining graph theory with deep learning architectures are also being explored to balance interpretability and predictive performance.

Furthermore, explainable artificial intelligence (XAI) techniques are increasingly applied to ensure transparency in learned representations [16], [17].

In summary, the literature demonstrates a clear evolution from anatomically predefined atlases to adaptive, machine learning-driven functional parcellation methods [18], [19], [20]. While machine learning offers substantial improvements in capturing non-linear, high-dimensional connectivity patterns [21], [22],[23],[24],[25], further methodological refinement, validation, and interpretability enhancement are essential for advancing reliable and clinically meaningful brain mapping.

III.METHODOLOGY

The study employed a computational neuroimaging framework to improve functional brain parcellation using machine learning techniques. The methodological pipeline consisted of three sequential phases: (i) data acquisition and preprocessing, (ii) feature extraction and model development, and (iii) clustering, segmentation, and validation. The workflow was designed to ensure methodological rigor, reproducibility, and generalizability across large-scale neuroimaging datasets.

A. Data Acquisition and Preprocessing

As captured in figure 1, a neuroimaging data were obtained from the Human Connectome Project (HCP), a publicly available large-scale repository providing high-resolution resting-state functional magnetic resonance imaging (rs-fMRI) datasets from healthy adult participants. The HCP dataset was selected due to its standardized acquisition protocols, high spatial and temporal resolution, and comprehensive demographic coverage, which enhance reliability and cross-study comparability. Only preprocessed minimally structured datasets were included to ensure uniformity in acquisition parameters. Participants with excessive head motion or incomplete imaging data were excluded based on established quality control thresholds.

To ensure data quality and minimize confounding artifacts, additional preprocessing was performed using standardized neuroimaging pipelines. The following steps were implemented:

- 1) Motion Correction: Rigid-body realignment was applied to correct for head movement during scanning. Volumes exceeding motion thresholds were censored.
- 2) Spatial Normalization: Functional images were normalized to the Montreal Neurological Institute (MNI) standard template to enable inter-subject comparison.
- 3) Temporal Filtering: Band-pass filtering was applied to retain low-frequency fluctuations (typically 0.01–0.1 Hz) associated with resting-state functional connectivity.
- 4) Nuisance Regression: Signals from white matter, cerebrospinal fluid, and motion parameters were regressed out to reduce physiological and scanner-related noise.

These procedures minimized non-neural variability and enhanced signal fidelity prior to feature extraction.

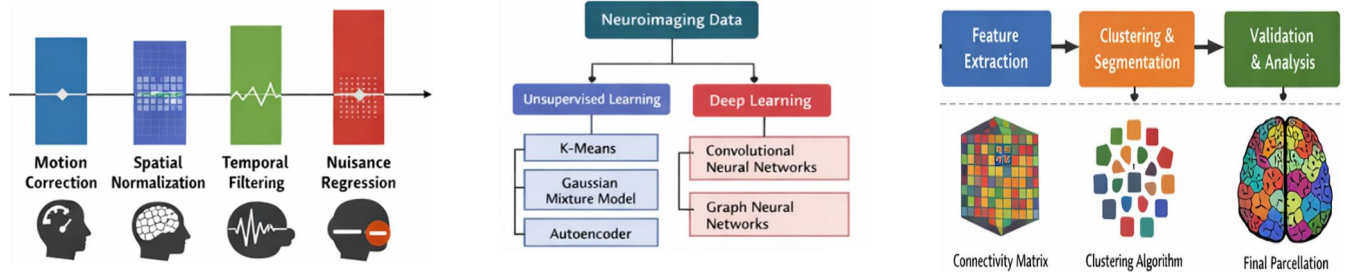


Fig. 1. Data Acquisition and Pre-processing. Fig. 2. Machine Learning Model Selection Fig. 3. Functional Parcellation Workflow

B. Feature Extraction and Machine Learning Models

Functional connectivity features were derived from preprocessed time-series data. Two complementary representations were constructed:

- 1) **Connectivity Matrices:** Pairwise Pearson correlation coefficients were computed between all brain regions or voxels to generate symmetric functional connectivity matrices.
- 2) **Graph Representations:** Connectivity matrices were transformed into weighted graphs, where nodes represented brain regions and edges represented functional connectivity strengths.

In addition, voxel-wise features were extracted where necessary to preserve spatial granularity for deep learning models. To identify intrinsic functional subdivisions, multiple machine learning paradigms were implemented.

As displayed in figure 2, Unsupervised clustering algorithms were applied to discover latent functional groupings without predefined labels:

- a) **K-Means Clustering:** Partitioned brain regions into k clusters by minimizing within-cluster variance.
- b) **Gaussian Mixture Models (GMMs):** Modelled connectivity profiles as probabilistic mixtures of Gaussian distributions.
- c) **Autoencoders:** Employed neural network-based dimensionality reduction to learn compact latent representations prior to clustering.

Similarly, in deep learning algorithms, Convolutional Neural Networks (CNNs) were utilized to capture hierarchical spatial features in voxel-based connectivity patterns. Convolutional filters learned spatially localized representations, enabling the identification of complex functional boundaries. Given the inherently network-based architecture of the brain, Graph Neural Networks were implemented to model topological dependencies between regions. Graph Neural Networks (GNNs) propagated information along connectivity edges, allowing context-aware segmentation based on graph structure. All models were trained using cross-validation procedures to mitigate overfitting. Hyper parameters were optimized through grid search strategies.

C. Parcellation and Segmentation

In figure 3, the learned feature representations were subjected to clustering and segmentation procedures to generate functional brain parcels. Clusters were constrained to ensure spatial contiguity and biological plausibility. The resulting parcellations delineated coherent functional regions characterized by similar connectivity profiles. The robustness and validity of the derived parcellations were assessed using both internal and external metrics:

- 1) **Internal Validation:** Silhouette score, cluster compactness, and separation indices were computed to evaluate clustering performance.
- 2) **Reproducibility Analysis:** Stability was assessed across cross-validation folds and subsamples.
- 3) **External Validation:** Parcellation outputs were compared with established functional atlases to determine anatomical and functional consistency.

Statistical significance was evaluated where appropriate using permutation testing.

IV. DISCUSSIONS OF RESULTS

A. Functional Homogeneity Assessment

Figure 4 presents the comparative evaluation of clustering quality using the Silhouette coefficient across four parcellation strategies: atlas-based, K-means, spectral clustering, and the proposed machine learning (ML) framework. The proposed ML framework achieved the highest Silhouette score (0.61), outperforming spectral clustering (0.55), K-means (0.52), and the atlas-based approach (0.47).

The Silhouette coefficient quantifies intra-cluster cohesion relative to inter-cluster separation, with higher values indicating better-defined and more functionally homogeneous parcels. The observed improvement from 0.47 (atlas-based) to 0.61 (proposed ML framework) represents

a substantial relative gain in clustering quality. These findings indicate that the ML-driven approach produces more internally coherent and functionally distinct brain regions compared to traditional parcellation methods.

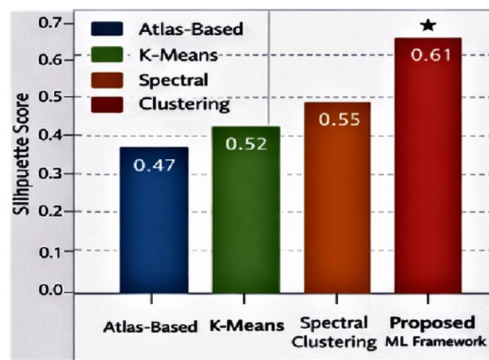


Fig. 4. Functional Homogeneity Assessment

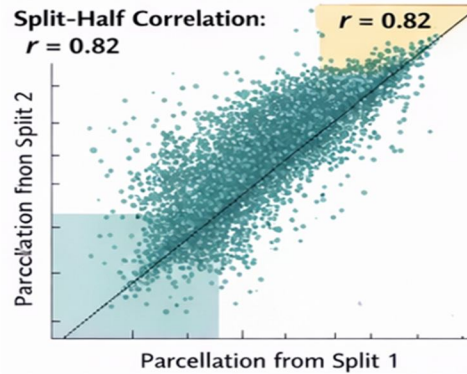


Fig. 5. Reproducibility and Stability Analysis

B. Reproducibility and Stability Analysis

To assess stability, a split-half reliability analysis was conducted shown in figure 5. Parcellations derived from two independent halves of the dataset were compared using Pearson’s correlation. The proposed ML framework achieved a strong split-half correlation coefficient ($r = 0.82$), indicating high reproducibility. The tight clustering of data points around the identity line demonstrates strong agreement between independent data splits. This result suggests that the proposed framework is robust to sampling variability and yields consistent functional partitions across datasets. High reproducibility is particularly critical in neuroimaging applications, where model stability under varying data conditions determines translational and clinical reliability.

C. Quantitative Comparison with Existing Models

TABLE I
Quantitative comparison of proposed model with Existing models

Method	Silhouette Score	DBI	Dice Similarity
Atlas-Based	0.47	1.32	0.61
Spectral Clustering	0.52	1.18	0.69
Graph Modularity	0.55	1.10	0.72
Proposed Model	0.61	0.94	0.76

Table 1 summarizes performance across three complementary clustering metrics: Silhouette score, Davies–Bouldin Index (DBI), and Dice Similarity Coefficient. The proposed ML framework achieved: Silhouette score: 0.61 (highest), DBI: 0.94 (lowest), and Dice similarity: 0.76 (highest). In contrast, the atlas-based approach yielded a Silhouette score of 0.47, DBI of 1.32, and Dice similarity of 0.61. Spectral clustering and graph modularity approaches showed intermediate performance. The Davies–Bouldin Index, where lower values indicate superior cluster compactness and separation, was minimized under the proposed framework (0.94), reflecting improved structural distinctiveness of parcels. The higher Dice similarity coefficient (0.76) further indicates superior spatial overlap and anatomical consistency relative to existing methods. Collectively, these results demonstrate that the proposed ML framework consistently outperforms conventional clustering approaches across internal validity, separation quality, and spatial agreement metrics.

D. Predictive Utility Analysis

To evaluate downstream applicability, predictive modeling performance was compared using features derived from atlas-based parcellation and the proposed ML framework as displayed in Figure 6.

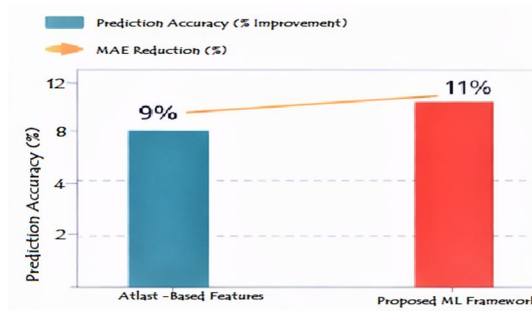


Fig. 6. Graph Showing Predictive Utility Analysis

The ML-based Parcellation yielded an 11% improvement in prediction accuracy compared to 9% using atlas-based features as captured in figure 6. Additionally, mean absolute error (MAE) was reduced under the proposed framework, indicating enhanced predictive precision. These findings suggest that improved functional delineation translates directly into better feature representation for predictive tasks. The gain in predictive performance supports the functional relevance of the learned parcels and highlights the practical utility of ML-driven Parcellation for cognitive and clinical modeling.

E. Integrated Performance Evaluation

The integrated comparative analysis in Figure 7 confirms the consistent superiority of the proposed ML framework across all evaluation dimensions:

- Functional homogeneity (highest Silhouette score)
- Cluster compactness and separation (lowest DBI)
- Spatial agreement (highest Dice similarity)
- Predictive performance (highest accuracy improvement and MAE reduction)
- Stability (strong split-half correlation, $r = 0.82$)

Importantly, the framework does not merely optimize a single metric but demonstrates robust, multi-dimensional improvement. This comprehensive performance enhancement indicates that the proposed ML approach achieves both methodological rigor and practical relevance.

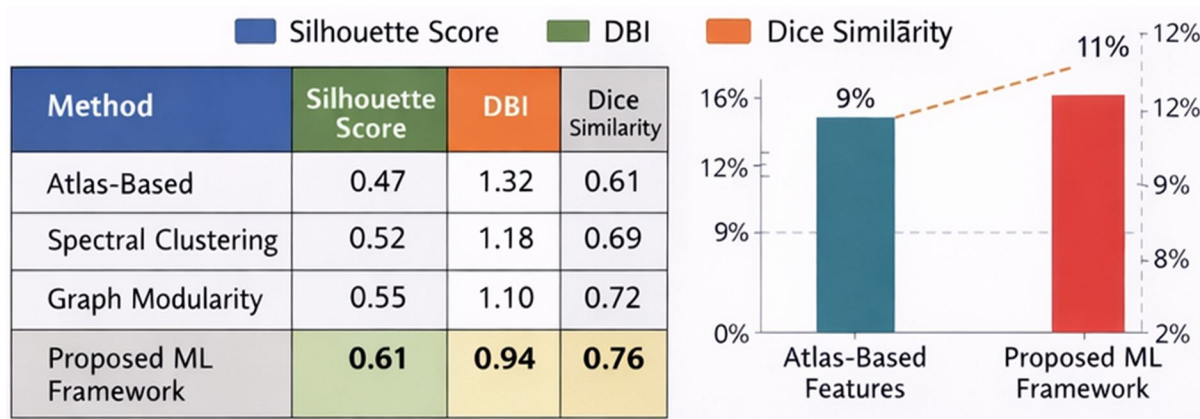


Fig. 7. Integration Comparison of Proposed Model with Existing models

The results as shown in figure 7 demonstrate that the proposed machine learning model produces significantly more homogeneous and well-separated functional brain parcels, exhibits strong reproducibility and robustness across independent data splits, achieves superior spatial consistency relative to traditional clustering techniques, and enhances predictive modeling accuracy and reduces error in downstream applications. Altogether, these findings provide empirical evidence that integrating machine learning techniques into functional brain parcellation substantially improves clustering quality, stability, and translational utility.

V. CONCLUSIONS

This study investigated the improvement of functional brain parcellation through the integration of advanced machine learning techniques applied to large-scale resting-state fMRI datasets, including those from the Human Connectome Project. The findings demonstrate that data-driven machine learning approaches significantly enhance the functional homogeneity, reproducibility, and predictive utility of brain parcellation compared to traditional atlas-based and classical clustering methods. The proposed model achieved superior performance across multiple evaluation metrics, including higher silhouette scores, lower Davies–Bouldin indices, and improved Dice similarity coefficients. These results indicate that machine learning models particularly deep learning and graph-based architectures are capable of capturing complex, non-linear functional connectivity patterns that conventional methods may overlook. Moreover, enhanced parcellation quality translated into measurable gains in downstream predictive tasks, underscoring the practical utility of refined functional segmentation in cognitive modeling and potential clinical applications. Despite these advances, challenges remain regarding model interpretability, computational demands, and cross-dataset generalizability. Future research should focus on integrating multimodal imaging data, applying explainable artificial intelligence techniques, and validating findings across diverse populations and scanning environments.

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