Representation Learning with Distance-Residualized Functional Connectivity for Cortical Parcellation from rs-fMRI

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Abstract. Functional parcellation of the cerebral cortex from resting-state functional magnetic resonance imaging (rs-fMRI) is a fundamental step for large-scale brain network analysis. Learning functional parcellation from rs-fMRI is essentially a dimensionality reduction of vertex-wise functional connectivity (FC), where previous studies have relied on linear dimensionality reduction techniques, failing to capture the non-linear nature of brain functional organization. In this work, we propose a self-supervised representation learning framework for whole-cortical, group-level parcellation to relax the linear constraints in feature extraction. Specifically, we first decouple FC strength from spatial proximity via distance-based residualization, enabling the learning of functionally meaningful features beyond geodesic constraints. A variational autoencoder (VAE) is then employed to learn compact and uncertainty-aware FC representations, augmented with a neighborhood-based contrastive objective to explicitly promote local functional coherence. Spatial continuity is further encouraged through Laplacian positional encoding prior to clustering. Experiments demonstrate that the proposed method achieves favorable average standardized scores among widely used cortical parcellations, reflecting a balanced performance across functional homogeneity, functional boundary alignment, clustering quality, and consistency with task-evoked activation patterns.

Keywords: Cortical parcellation · rs-fMRI · Representation learning.

1 Introduction

Functional parcellation of the cerebral cortex is a fundamental prerequisite for large-scale brain network analysis [3], providing meaningful functional units for studying intrinsic connectivity, task-evoked activation, and brain-behavior

relationships [4, 18]. Resting-state functional magnetic resonance imaging (rs-fMRI) captures spontaneous low-frequency neural fluctuations [5] and is therefore widely adopted for data-driven parcellation, as it reveals functional organization beyond anatomical boundaries [14]. By aggregating signals within functionally homogeneous regions, rs-fMRI-based parcellation reduces data dimensionality and improves the interpretability and reliability of functional connectivity (FC) analyses [21].

Most existing rs-fMRI-based parcellation methods follow classical data-driven paradigms, including clustering-based approaches [1, 16, 17], region-growing or gradient-based methods [8], and hybrid frameworks that integrate local gradients with global similarity [2, 9, 15, 22]. Despite their methodological diversity, these approaches largely rely on predefined similarity measures and linear feature transformations, which limits their ability to model the high dimensionality, noise heterogeneity, and nonlinear structure of fMRI data [25]. This has motivated increasing interest in deep learning as a means to introduce flexible objective design and nonlinear representation learning into parcellation pipelines.

To date, most deep learning-based parcellation studies focus on individual-level settings [11], typically relying on predefined group-level atlases. Unsupervised deep learning approaches for group-level parcellation remain limited. Existing efforts either apply deep models to subdivide specific brain regions [12], where reduced spatial scope alleviates high-dimensional challenges, or incorporate deep learning into the clustering stage of whole-brain parcellation [24], while still relying on linear dimensionality reduction beforehand. The limitation of linear compression still exists, suggesting that a central bottleneck of current pipelines lies in functional representation learning: vertex-wise FC profiles are inherently high-dimensional, nonlinear, and strongly confounded by spatial proximity, which cannot be adequately addressed by linear compression alone.

Motivated by this limitation, we revisit whole-cortical group-level parcellation from the perspective of functional representation learning. We propose a self-supervised framework that disentangles FC patterns from spatial proximity and learns nonlinear, uncertainty-aware representations directly from high-dimensional FC profiles. As illustrated in Figure 1, the pipeline combines distance-based residualization, variational representation learning, and neighborhood-level self-supervision to capture local functional structure, while spatial continuity is reintroduced in a controlled manner through graph-based positional encoding prior to clustering. This design enables a principled transition from vertex-wise representations to multi-resolution cortical parcellations.

2 Method

2.1 Parcellation Framework

Dataset We use minimally preprocessed rs-fMRI data provided by the Human Connectome Project (HCP) [20], which have been mapped onto the fs_LR_32k cortical surface. All time series are further band-pass filtered within 0.01–0.1 Hz

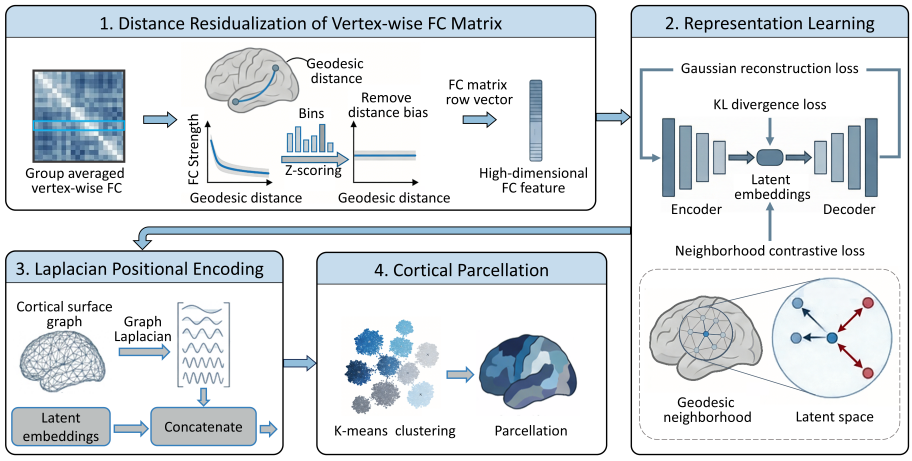

Fig. 1. Overview of the proposed parcellation method.

to preserve main neural activity-related components [19]. We randomly selected 500 subjects for training, 100 subjects for validation, and 400 subjects for testing, ensuring a reliable and unbiased evaluation.

Vertex-wise FC and Distance Residualization Let N denote the number of vertices on a single cortical hemisphere, with $i, j \in 1, \ldots, N$. We compute the group-average FC matrix $\mathbf{F} \in \mathbb{R}^{N \times N}$, where each connection is defined as the Pearson correlation between vertex-wise fMRI time series, computed for each training subject and then averaged across subjects. Geodesic distances between vertices are computed on the cortical surface using Dijkstra's algorithm. To balance computational efficiency and spatial coverage, the maximum distance is truncated at 50 mm, and distances are averaged across all subjects to obtain the group-level geodesic distance matrix $\mathbf{G} \in \mathbb{R}^{N \times N}$.

We perform distance-based residualization to decouple FC strength from spatial proximity. Specifically, distances within $[0, G_{\max}]$ (with $G_{\max} = 45$ mm) are discretized into bins of width Δd (set to 1 mm in this paper). For each bin b, we compute the mean μ_b and standard deviation σ_b of FC values. The residualized FC is defined as

$$\tilde{F}_{ij} = \begin{cases} \dfrac{\mathbf{F}_{ij} - \mu_b(i,j)}{\sigma_b(i,j)}, & \mathbf{G}_{ij} \leq G_{\max}, \\ \dfrac{\mathbf{F}_{ij} - \mu_{\text{glob}}}{\sigma_{\text{glob}}}, & \text{otherwise}, \end{cases} \tag{1}$$

where μ_{glob} and σ_{glob} denote the global mean and standard deviation of all the elements of $\mathbf{F}$. For each vertex i, its FC feature vector is defined as the i-th row of $\tilde{\mathbf{F}}$, i.e., $\mathbf{x}_i = \tilde{\mathbf{F}}_{i,:} \in \mathbb{R}^N$, representing its connectivity profile to full-cortex vertices. This procedure effectively removes distance-induced biases and facilitates the discovery of genuine functional boundaries.

FC Feature Learning

VAE with Gaussian Decoder. We adopt a VAE with a Gaussian decoder to learn compact FC representations [10], augmented with a neighborhood contrastive objective. The encoder is implemented as a multilayer perceptron (MLP) with two hidden layers of sizes 1024 and 512, each followed by ReLU activation and layer normalization. Two independent linear heads project the final hidden representation to the mean $\boldsymbol{\mu}_z$ and log-variance $\log \boldsymbol{\sigma}_z^2 \in \mathbb{R}^{d_z}$ of the approximate posterior distribution, where the latent dimension is set to $d_z = 32$. Latent variables are sampled using the reparameterization trick for end-to-end training.

The decoder mirrors the encoder with hidden layers of sizes 512 and 1024, followed by a linear output layer that predicts the mean $\boldsymbol{\mu}_x$ of the reconstruction distribution. Instead of using a simple mean-squared error, we explicitly assume a Gaussian likelihood for the observations and introduce a learnable global diagonal log-variance parameter $\log \boldsymbol{\sigma}_x^2 \in \mathbb{R}^N$ as part of the decoder. This design enables adaptive modeling of feature-wise uncertainty, which is particularly suitable for FC data with heterogeneous scales and noise levels.

The VAE training objective consists of a reconstruction term and a Kullback–Leibler (KL) divergence term. The reconstruction loss is given by the Gaussian negative log-likelihood:

$$\mathcal{L}_{\text{rec}} = -\mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x} \mid \mathbf{z})\right] = \frac{1}{2N} \sum_{n=1}^{N} \left(\frac{(x_n - \mu_{x,n})^2}{\sigma_{x,n}^2} + \log \sigma_{x,n}^2 \right), \tag{2}$$

while the KL divergence regularizes the latent distribution toward a standard normal prior:

$$\mathcal{L}_{\text{KL}} = KL(q(\mathbf{z} \mid \mathbf{x}) \parallel \mathcal{N}(\mathbf{0}, \mathbf{I})) = \frac{1}{2d_z} \sum_{d=1}^{d_z} \left(\mu_{z,d}^2 + \sigma_{z,d}^2 - \log \sigma_{z,d}^2 - 1 \right). \tag{3}$$

Neighborhood Contrastive Learning. Optimizing reconstruction alone primarily enforces similarity between FC patterns, without explicitly encouraging functional homogeneity among nearby vertices. To address this limitation, we introduce a neighborhood-based contrastive loss. The neighborhood of vertex i is defined as $\mathcal{N}_i = \{j \mid 0 < G_{ij} \leq G_{\max}\}$. Based on the distance-residualized FC values, we first identify candidate positive and negative sets by selecting the top 15% and bottom 25% of connections within $\mathcal{N}_i$, respectively. From these candidate sets, we randomly sample positive samples $\mathcal{P}_i$ and negative samples $\mathcal{N}_i^-$ for each anchor vertex. For an anchor vertex i, the InfoNCE loss is defined as

$$\mathcal{L}_{\text{NCE}}^{(i)} = -\log \frac{\sum_{j \in \mathcal{P}_i} \exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_j)/\tau)}{\sum_{j \in \mathcal{P}_i} \exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_j)/\tau) + \sum_{k \in \mathcal{N}_i^-} \exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_k)/\tau)}, \tag{4}$$

where $\mathrm{sim}(\cdot,\cdot)$ denotes cosine similarity and τ is a temperature parameter. The overall training objective is

$$\mathcal{L} = \mathcal{L}_{\mathrm{rec}} + \beta\mathcal{L}_{\mathrm{KL}} + \gamma\mathcal{L}_{\mathrm{NCE}}, \tag{5}$$

where β and γ balance latent regularization and contrastive learning, respectively.

Laplacian Positional Encoding and Vertex Clustering Since distance residualization removes spatial information from FC features, we explicitly introduce positional encoding to promote spatial continuity. Although this design may appear contradictory, it is intentional: spatial effects are first decoupled to prevent implicit spatial bias during representation learning, and are then reintroduced in a controlled manner to guide spatially coherent clustering.

From the cortical surface mesh, we construct a vertex adjacency graph with adjacency matrix $\mathbf{A}$ and compute the normalized graph Laplacian:

$$\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}, \tag{6}$$

where $\mathbf{D}$ is the degree matrix. We extract the smallest $k+1$ eigenvectors of $\mathbf{L}$ and discard the constant eigenvector, yielding positional embeddings:

$$\mathbf{P} = [\mathbf{u}_2, \ldots, \mathbf{u}_{k+1}] \in \mathbb{R}^{N\times k}, \tag{7}$$

with $k = 5$ in our experiments. Each Laplacian feature dimension is z-score normalized across vertices before concatenation. For each vertex, the final representation is obtained by concatenating latent features and positional encoding, $\tilde{\mathbf{z}}_i = [\mathbf{z}_i \| \mathbf{p}_i]$.

These representations are subsequently clustered using a K-means model to produce the final cortical parcellation. The number of clusters was set to 50, 100, 150, and 200 for each hemisphere, resulting in whole-brain parcellations comprising 100, 200, 300, and 400 regions, respectively. Figure 2 provides a visualization of the proposed parcellation.

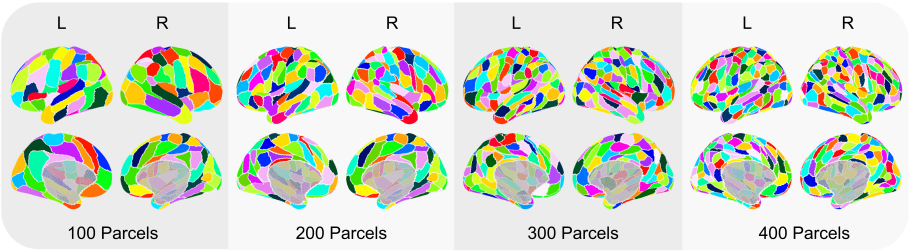

Fig. 2. Visualization of the Proposed DRFC Parcellation.

2.2 Implementation Details

All experiments were implemented in PyTorch 2.6.0 [13] and conducted on a single NVIDIA RTX 4090 GPU with 24 GB memory. Model optimization used the Adam optimizer with an initial learning rate of 1×10^{-4}. The model was trained for 200 epochs with a batch size of 32. The KL weight $\beta = 2.0$ was linearly warmed up over the first 50 epochs, and gradient norms were clipped to 5.0 for training stability.

For neighborhood contrastive learning, each anchor used 6 positive and 32 negative samples, with temperature $\tau = 0.1$. The contrastive loss was weighted by $\gamma = 0.1$ and activated after the first 50 epochs.

K-means clustering was performed using *scikit-learn* with default settings, where the number of clusters followed the target parcellation resolution. Other parameters remained unchanged, including *k-means++* initialization, 300 maximum iterations, and a convergence tolerance of 1×10^{-4}.

3 Experimental Results

3.1 Evaluation Protocol

Null-model-based Z-score Normalization Several evaluation metrics are sensitive to parcellation scale and the number of regions. To mitigate such confounding effects, we adopt a null-model-based z-score normalization. Null models are generated by randomly rotating parcellation labels on the inflated fs_LR_32k spherical surface, preserving topology and spatial continuity while breaking the correspondence between parcels and functional or task signals. For each parcellation, 1000 null models are generated. Metrics are computed on both the original parcellation and its null counterparts, and the z-score is calculated by standardizing the original metric value relative to the null-model distribution, enabling fair comparison across parcellations with different scales and numbers of regions [24].

Evaluation Metrics We evaluate the quality of parcellations using the following four metrics, where null-model-based z-score normalization is applied to Functional Homogeneity, Silhouette Coefficient, and Task Inhomogeneity to account for scale effects:

Functional Homogeneity (Func-Homo). Functional homogeneity measures the consistency of functional activity within parcels. Using rs-fMRI from the test set, we compute vertex-wise FC and average all pairwise FC values within each parcel, followed by a size-weighted average across parcels.

Distance-Controlled Boundary Coefficient (DCBC). DCBC [23] evaluates whether parcellation boundaries align with functional discontinuities while explicitly controlling for geodesic distance. Vertex pairs are binned by surface distance, and within-parcel and between-parcel FC similarities are compared within each bin. Higher values indicate better alignment with functional boundaries.

Silhouette Coefficient (SC). The SC assesses clustering quality in the functional feature space by jointly considering within-parcel compactness and between-parcel separability. Here, each vertex is represented by its FC profile, and pairwise distances are computed using cosine distance. The overall score is obtained by averaging vertex-wise silhouette values, which range from -1 to 1.

Task Inhomogeneity (Task-Inho). Task inhomogeneity measures the alignment between parcellations and task-evoked activations. We use HCP S1200 Group Average task fMRI data represented as Cohen's d maps across 86 task contrasts. For each contrast, we compute the within-parcel variance of activation values and then aggregate these variances across parcels and contrasts to obtain the final task inhomogeneity score. Lower values indicate more homogeneous task responses.

3.2 Comparison Results

We compare the proposed parcellation with a range of widely used and open-access cortical parcellation methods, including Baldassano [2], Fan [6], Glasser [7], Gordon [8], JOINT [1], Schaefer [15], Schaefer-homo [22], and Shen [16]. For Schaefer and Schaefer-homo, results with 100, 200, 300, and 400 parcels are reported to account for different parcellation granularities. Quantitative results are summarized in Table 1.

Table 1. Quantitative comparison of different parcellations. Methods are ranked by averaging the standardized scores of four evaluation metrics. DRFC is our proposed parcellation. Best and second-best results among parcellations are highlighted in bold and underline, respectively.

Method	$N_{parcels}$	Func-Homo (z)	DCBC ($\times 100$)	SC (z)	Task-Inho (z)↓
DRFC-200	200	2.43	2.79±0.72	5.70	-3.48
DRFC-100	100	3.18	2.58±0.77	<u>5.81</u>	-2.70
Schaefer-100	100	<u>3.33</u>	2.04±0.79	5.61	-3.01
Schaefer-200	200	1.98	1.93±0.75	**6.31**	-3.15
DRFC-400	400	1.96	1.66±0.61	4.78	**-4.31**
DRFC-300	300	2.27	1.91±0.64	4.47	-3.95
Glasser	360	-0.48	<u>2.97±0.83</u>	4.63	<u>-4.15</u>
Schaefer-300	300	1.72	0.95±0.85	5.03	-3.21
Gordon	333	-1.41	**3.80±1.02**	3.93	-2.61
Schaefer-400	400	1.33	0.87±0.84	5.02	-3.14
Baldassano	171	**3.61**	0.66±0.86	2.97	-3.19
Schaefer-homo300	300	1.15	1.17±0.80	3.83	-2.52
Schaefer-homo400	400	0.75	0.94±0.87	4.02	-2.48
JOINT	400	-1.04	1.75±0.59	4.39	-2.18
Schaefer-homo200	200	1.64	0.59±0.78	3.79	-1.78
Schaefer-homo100	100	2.05	0.94±0.59	2.24	-1.70
Fan	210	-1.69	2.34±0.56	2.90	-1.67
Shen	200	-2.28	2.87±0.71	2.48	-1.54

Overall, the proposed parcellations with 200 and 100 parcels achieve the highest average standardized scores among all compared methods. The variants

with 300 and 400 parcels also rank among the top performers according to the same averaged-score criterion. Although DRFC does not achieve the best value for every individual metric, it provides a balanced trade-off across functional homogeneity, functional boundary alignment as quantified by DCBC, clustering quality in the functional feature space, and consistency with task-evoked activation patterns. These results suggest that the proposed approach is competitive for cortical parcellation when multiple complementary evaluation criteria are considered jointly.

3.3 Ablation Study

We conduct an ablation study to assess the contributions of key components in the proposed framework, including distance residualization (w/o DR), Gaussian decoder (w/o GD), neighborhood contrastive learning (w/o NC), and Laplacian positional encoding (w/o LPE). All ablation experiments are performed with the number of parcels fixed to 200. In addition to standard quantitative metrics, spatial continuity is evaluated using the average number of connected components per parcel (Avg. CC), where lower values indicate better contiguity.

The results are summarized in Table 2. Removing distance residualization leads to a clear drop in DCBC and clustering quality, despite slightly improved task consistency. Excluding the Gaussian decoder results in reduced functional homogeneity and clustering quality. Without neighborhood contrastive learning, most functional metrics, including DCBC, clustering quality, and task consistency, degrade substantially, although spatial continuity is marginally improved. Removing Laplacian positional encoding increases the number of connected components per parcel, despite improved functional homogeneity. Overall, the full model achieves the best balance across functional homogeneity, functional boundary alignment, clustering quality, task-evoked activation consistency, and spatial continuity.

Table 2. Results of ablation study. Best and second-best results among parcellations are highlighted in bold and underline, respectively.

Method	Func-Homo (z)	DCBC ($\times 100$)	SC (z)	Task-Inho (z)↓	Avg. CC↓
DRFC	<u>2.43</u>	<u>2.79 ± 0.72</u>	**5.70**	<u>-3.48</u>	<u>1.10</u>
DRFC w/o DR	2.37	1.89 ± 0.81	1.90	**-3.58**	1.12
DRFC w/o GD	1.46	**2.97 ± 0.78**	<u>3.85</u>	-2.22	1.17
DRFC w/o NC	1.75	0.20 ± 0.82	1.08	-1.93	**1.06**
DRFC w/o LPE	**3.03**	2.62 ± 0.75	2.19	-3.21	1.44

4 Conclusion

We presented a self-supervised representation learning framework for group-level cortical parcellation from rs-fMRI. Our approach decouples vertex-wise FC

strength from spatial proximity. By integrating a VAE with a Gaussian decoder and neighborhood-based contrastive learning, the framework learns compact, uncertainty-aware, and functionally coherent representations, while Laplacian positional encoding preserves spatial continuity. Extensive experiments show that the proposed method obtains strong average standardized scores across multiple resolutions, offering competitive trade-offs among functional homogeneity, functional boundary alignment, clustering quality, and alignment with task-evoked activations. These findings underscore the value of principled representation learning for cortical parcellation and provide a flexible foundation for future extensions to individual-level or multimodal parcellation.

Acknowledgments. This study was funded by the National Key Research and Development Program (Grant 2024YFC3016400), the National Natural Science Foundation of China (Grant No. 62306083), the Postdoctoral Science Foundation of Heilongjiang Province of China (Grant No. LBHZ22175), and the Ministry of Industry and Information Technology of the People's Republic of China.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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