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ORIGINAL ARTICLE

Graph Alignment Exploiting the Spatial Organisation Improves the Similarity of Brain Networks

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Every brain is unique, having its structural and functional organisation shaped by both genetic and environmental factors over the course of its development. Brain image studies tend to produce results by averaging across a group of subjects, under a common assumption that it is possible to subdivide the cortex into homogeneous areas while maintaining a correspondence across subjects. This paper questions such assumption: can the structural and functional properties of a specific region of an atlas be assumed to be the same across subjects? This question is addressed by looking at the network representation of the brain, with nodes corresponding to brain regions and edges to their structural relationships. We perform graph matching on a set of control patients and on parcellations of different granularity to understand which is the connectivity misalignment between regions. The graph matching is unsupervised and reveals interesting insight on local misalignment of brain regions across subjects.

KEYWORDS

Structural Parcellation, network alignment, Unlabelled Graphs

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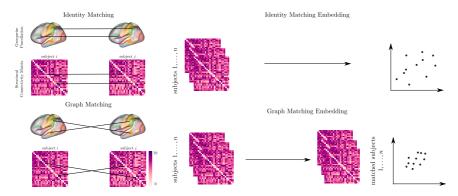


FIGURE 1 Left: Conceptual visualization of identity matching and graph matching in the context of structural brain connectivity. Right: Conceptual visualization of graph embedding in the context of identity matching and graph matching.

1 | INTRODUCTION

Every brain is unique, having its structural and functional organisation shaped by both genetic and environmental factors over the course of its development. This uniqueness directly translates into inter-subject variability in the location and extent of functional brain areas, the network organisation of structural connectivity, and the structure–function relationship. In imaging studies, which tend to produce results by averaging across a group of subjects, this variability introduces temporal and spatial variance in the localisation of specialized brain areas and their network connectivity. In particular, this variability undermines the common assumption that it is possible to subdivide the cortex into homogeneous areas while maintaining a correspondence across subjects. In other words, can the structural and functional properties of a specific region of an atlas be assumed to be the same across subjects? This question is of particular interest to studies that represent the brain as a network, with nodes corresponding to brain regions and edges to their structural or functional relationship. If there is a spatial variability across subject, then the nodes of the network may not be matched, and the networks of distinct subjects should not be compared directly.

A possible solution to this problem is to make no assumption on the correspondence between the nodes of the network and instead try to derive it using a data driven approach. This problem, whose solution results in a mapping between the nodes of two networks, is referred to in other domains as *graph matching* or *network alignment* (Conte et al., 2004). Given two networks, network alignment corresponds to finding a permutation of the nodes of one graph which minimizes a cost function - usually a dissimilarity measure between the graphs. As the problem is np-hard, many different techniques have been proposed in the literature, from exact matching to inexact matching (see Conte et al. (2004); Emmert-Streib et al. (2016) for exhaustive reviews on the topic). Notice that network alignment differs from the fingerprint matching and from the parcel matching problem (Mars et al., 2016; Gallardo et al., 2018a) as it only relies on the intrinsic properties of the network, for example edge weights, instead of node specific features. The network alignment problem gained attention in the context of neuroscience, aiming at understanding the heterogeneity across-subjects brain connectivity networks. However, current approaches where designed for the alignment of general networks, for example social networks, and do not typically impose spatial constraints on the node permutations. In the context of brain networks, arbitrary permutation may result in the large spatial displacement of brain areas which is highly improbable. Therefore, while local permutation explaining inter–subject variability is expected, permutation resulting in large displacement, for example permuting regions in the occipital and frontal lobes, should be discouraged.

Therefore, a graph alignment strategy promoting or enforcing local permutation may be more appropriate to brain network alignment. In Figure 1, we illustrate the different between the identity matching, where the parcels across patients are considered as the same nodes, and the graph matching, where we search for a better matching of parcels across patients. Both different similarity measures as well as different matching strategies can be defined, creating a wide range of papers in this literature (Frigo et al., 2021; Deslauriers-Gauthier et al.; Rasero et al., 2017; Frost et al., 2014; Takerkart et al., 2014; Becker et al., 2018).

In this work, we aimed at exploring the stability of group-wise parcellations when performing intra-subject analysis by looking at network alignment performances and characteristics on a set of control patients. Given a set of structural connectivity matrices built using the Gallardo Parcellation Gallardo et al. (2018b), we study the network alignment results on such matrices. Among the different alignment strategies, we choose the Fast Quadratic Assignment (FAQ) algorithm proposed by (Vogelstein et al., 2015), as it represents a state of the art in the network alignment literature and it shows to be well tailored for the analysis of brain connectivity networks Glaser and Kording (2016); Vogelstein et al. (2015). The analysis is conducted on the different prior of the matching procedure, by imposing different initial condition regarding the most probable matching, and at different parcels granularity. The proposed approach allows for the identification of the most stable and most unstable brain area in brain matching across patients.

2 | MATERIALS AND METHODS

2.1 | Brain Graph Matching

A graph is a mathematical object $\mathcal{G}_i = (N, E_i, w_i)$ with a set of nodes $N = \{1, ..., n\}$, a set of edges $E = \{(j, k) \in \{0, 1\}, j, k \in N\}$ and a weight function $w_i : E \to \mathbb{R}$. In matrix term, a graph can be represented as a weighted adjacency matrix $G_i \in \mathbb{R}^{n \times n}$. In the context of brain networks, the number of nodes n corresponds to the number of parcels per hemisphere and w encodes the connectivity, either structural or functional, between parcels. Given the matrix representation, different metrics can be defined to compare graphs (see Donnat and Holmes (2018) for a review and Frigo et al. (2021); Bassett and Bullmore (2017); Pandit et al. (2013)). In this work, we are using the Frobenious norm as it associates with a quick graph matching procedure:

$$d_F(G_1, G_2) = ||G_1 - G_2||^2$$

The Frobenious norm, like many others, is not invariant under node permutations, thus it allows for an analysis of the suggested nodes' permutations. Graph matching corresponds in finding an injective map from the parcels of the graph G_i to the parcels of the graph G_j . In geometrical terms, the nodes (parcels in this context) permutation is expressed using the matrix representation of the permutation group $\mathcal{P} = \{P \in \{0,1\}^{n \times n} : P^T 1 = P1 = 1\}$. Given an adjacency matrix G_i , it can be permuted into potentially n! different adjacency matrices by applying the permutation action. The results is an equivalence class of graphs $[G_i] = \{P^T G_i P : P \in \mathcal{P}\}$, obtained by permuting the rows and the columns of the adjacency matrices by matrix multiplication. If we are using the metric as the alignment cost function and the permutation matrix representation, aligning two networks G_i and G_j corresponds in finding the permutation matrix P_{ij} minimizing:

$$d([G_i], [G_j]) = \min_{P \in \mathcal{P}} d_F(G_i, P^T G_j P)$$
(1)

This minimization problem corresponds to the graph matching problem. In addition, $d([G_i], [G_i])$ is an induced metric

on on the quotient space $\mathbf{R}^{n\times n}/\mathcal{P}$ obtained by applying the permutation action to the space of adjacency matrices. This space is often called graph spaces and it is extensively described in Jain and Obermayer (2009) and Calissano et al. (2020).

In the context of brain network analysis, graph matching represents a way to understand if there is a misalignment between subjects and provides a way to correct it. In particular, a misalignment is detected when the optimal permutation matrix obtained by equation (1) is not the identity. In this situation, the similarity between subjects can be improved by permuting the labels of one subject, implying that the initial labels do not match. The optimal permutation matrix P to apply to the labels of subject j is also produced by equation (1) and can thus be applied as preprocessing step before further analysis or comparison of the networks.

2.1.1 | FAQ algorithm for graph matching

Among the different graph matching algorithms, we selected the Fast Quadratic Assignment method proposed by Vogelstein et al. (2015) as it represents the state of the art method proven to be effective in the context of brain network alignment. The FAQ matching is a fast method for inexact graph matching based on the Frobenious norm between adjacency matrices and it allows to select an initialization (a prior) to the matching procedure, which is important in this context where not all the parcels permutations are meaningful.

The idea behind the methodology is to relax the domain of permutation matrices from the discrete set \mathcal{P} to the continuous convex hull of doubly stochastic matrices $\mathcal{D} = \{P \in \mathbb{R}^{n \times n} : P^T 1 = P1 = 1, P \ge 0\}$. Starting from the minimization of the Frobenious norm between two adjacency matrices $G_i, G_j \in \mathbb{R}^{n \times n}$, the problem is manipulated into the following minimization:

minimizing
$$f(P) = -\text{trace}(G_i P G_i^T P^T)$$
 (2)

subject to
$$P \in \mathcal{D} = \{P \in \mathbb{R}^{n \times n} : P^T | 1 = P | 1 = 1, P \ge 0\}$$

The local solution in found by gradient descend in the space \mathcal{D} . To obtain a permutation matrix as output, the solution is then projected onto \mathcal{P} . As many optimization problems, the FAQ algorithm relies on an initialization P_0 , which could be interpreted as a prior knowledge on the parcels' matching. The main idea of the current work is to study how graph matching behaves in comparing healthy patients' brain structural graphs. By analysing the graph matching results at different parcellations, we can infer which areas of the brain most suffer from misalignment errors in the parcellation strategy.

2.1.2 | Graph matching initializations

A key parameter of the FAQ matching is the algorithm initialization matrix P_0 . In such context, the initialization matrix represents a prior about the misalignment, i.e., a guess on how the parcels should be aligned. We are proposing four different initializations:

 Barycenter: starting from a non informative permutation matrix, where all the parcels' permutations are equally probable;

2. Random: starting from a random doubly stochastic matrix, where we pick some parcels permutation at random;

- 3. Identity: starting from the identity matrix, suggesting that the current parcels' labelling is the correct one;
- **4.** Neighbours: starting from the neighbouring structure of the parcels, suggesting a permutation with the spatial neighbours of every parcel.

To evaluate all the experiments, we use the ratio between the objective function obtained graph matching (via FAQ network alignment) F_{opt} and the objective function obtained with the identity matching F_{id} (i.e., leaving the graphs with the current node labels).

$$F_{opt}^{ij}(P) = \operatorname{trace}(G_i P G_i^T P^T) \qquad F_{id}^{ij} = \operatorname{trace}(G_i I^T G_j I)$$
(3)

Given $\hat{P} \in \mathcal{P}$, the permutation matrix estimated via FAQ and $I \in \mathbb{R}^{n \times n}$ the identity matrix of the original alignment,

$$\frac{F_{opt}^{ij}(\hat{P})}{F_{id}^{ij}}$$

If the ratio is lower then 1, the observations are better aligned with the identity matching. If the ration is above 1, the observations are better aligned if a permutation is applied.

2.2 | Structural brain networks

Our dataset consists of 100 healthy young adults from the Human Connectome project, (U100 subject group) (Van Essen et al., 2012; Glasser et al., 2013). For each subject, a five-tissue-type image (Smith et al., 2012) was obtained using the Freesurfer pipeline (Fischl, 2012) invoked through Mrtrix3 (Tournier et al., 2019). A response function was estimated for the white matter, gray matter, and cerebrospinal fluid using a maximal spherial harmonic order of 8 for all tissues (Jeurissen et al., 2014). The fiber orientation distribution functions (fODFs) were then computed using the multi-shell multi-tissue constrained spherical deconvolution algorithm (Jeurissen et al., 2014). Finally, the fODFs were used as input for probabilistic anatomically constrained tractography performed with the iFOD2 algorithm (Smith et al., 2012) seeding from the gray matter - white matter interface and obtaining a total of five million streamlines per subject.

The structural brain connectivity network are built from the parcellation introduced in Gallardo et al. (2018b), as we are interested in group-wise parcellation. This parcellation is built based on 138 tractograms built from coregistered cortical surfaces from Human Connectome Project (Van Essen et al., 2012). Each tractogram is fit-transformed with a logit model and the parcels are obtained using a Hierarchical Clustering method on the average tractogram. Such clustering procedure offers different parcels granularity by sequentially aggregating parcels with similar connectivity structure. Thus, we study the parcellation at different granularities from 25 up to 500 nodes per hemisphere, to assess the threshold where the original alignment across patients is inexact.

2.3 | Comparing different initializations

For all the parcellations and hemispheres, we are aligning all the graphs G_i with all the other graphs G_j , i, j = 1, ..., 100 computing via FAQ the optimal permutation matrix \hat{P}_{ij} . The goal of the experiment is to see if the graph matching decreases the distance between structural brains with different initializations and parcellations. Thus, the ratio between

the graph matching and the identity matching $F_{opt}^{ij}(\hat{P}_{ij})/F_{id}^{ij}$ is computed. The choice of aligning all the patient with every other patients rather then with a reference subject allows us to study the variability of the misalignment across subjects.

2.4 Comparing different permutations

Once the graph matching is performed, we are interested in understanding how the parcels are matched by looking at the optimal permutation matrices \hat{P}_{ij} . We divide the type of permutations into three categories: Self Matching when the parcel is permuted with itself, Neighbours Matching - when the parcel is permuted with a neighbouring parcel, and Others - when the parcels are permuted with other parcels rather then the closer ones and themselves. In Figure 2, we provide a conceptual visualization of the meaning of permutations between parcels. Understanding how the initialization of the algorithm relates with the type of permutations selected allows us to understand the type of misalignment error, answering questions about the locality or not of the matching.

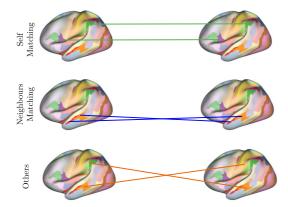


FIGURE 2 Types of parcels matching: (Top) Self Matching representing regions which are permuted with themselves; (Middle) Neighbours Matching representing regions permuted with their spatial neighbours on the brain; (Bottom) Others permutations with other regions rather then themselves or neighbours.

2.5 | Spatial distribution of permutations

The matching results can be also illustrated on cortical surface, allowing us to visualize the areas which are more often matched. Specifically, for each region we computed its permutation rate as a function of pair distance. We denote r_p^n the rate of permutation with an n^{th} neighbor. The symbol r_p^0 therefore corresponds to the rate of "no permutation" or self permutation, r_p^1 the rate of permutation with a direct neighbor, etc. This visualization provides insight on the spatial misalignment across patients and if certain regions are more permuted than other. It is also possible to visualise individual matching results by computing the rate of permutation of one region with all others across all subjects. This provides a region by region view of the stability of regions and the most likely permutations.

3 | RESULTS

3.1 | Comparing different initialization strategies

In Figure 3, we illustrate the distribution of the ratio for every parcellation and every initialization. The barycentric and random initialization are systematically outperformed by the original parcels matching, indicating that it is preferable to perform no matching rather than use these initialisation strategies. Contrarily, the identity and the neighbouring initialization outperformed by the original parcels matching for every atlas with a number of regions at or above 100, indicating that it is better to perform a cross subjects alignment. Furthermore, the improvement increases with the number of parcels. For example, at 100 parcels with the barycenter initialization the percentage of permuted parcels is 21% and it doubles at 1000 parcels, reaching 58.5%. The results are in line with the expectations, as the most significant priors on the brain parcels matching are the identity and the neighbouring rather then the random and the barycenter, as it is more plausible to have either none or only local misalignment between parcels in the brain. The plot shows how the alignment with identity or neighbouring initialization can decrease the misalignment error across-subjects.

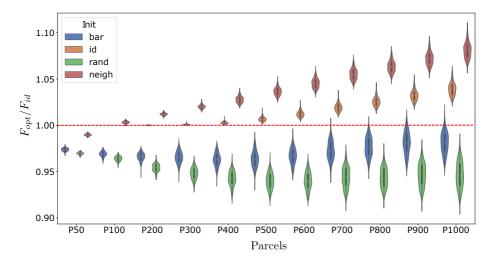


FIGURE 3 Distribution of the objective functions ratio for each parcellation and for each initialization.

3.2 | Comparing different permutations

The percentage of parcels which belong to Self Matching, Neighbours Matching, and Others is illustrated in Figure 4. When the graph matching was outperformed on average by the identity matching, indicating a poor matching, we report the results with a dashed line. For all four initialization strategies, as the number of parcels increases, the percentage of permuted nodes increases. For the identity and the neighbours initialization, the percentage of Self Matched nodes is higher then the percentage of matched nodes. Among the matched nodes, the percentage of nodes matched with Neighbours is predominant with respect to parcels permuted with others. These are plausible results,

as we expect the parcels to be permuted with neighbours due to local misalignment during the parcellation procedure. In addition, the identity initialization show an higher percentage of self permuted parcels while the neighbours initialization an higher percentage of neighbours matched parcels.

3.3 | Spatial organisation of the permutations

To understand the spatial distribution of the Stable, Unstable, and Neighbour parcels, we represent the permutations on the cortex. Figure 5 illustrates the permutation rates r_p^0 , r_p^1 , and r_p^2 , for atlases with a 100, 300, and 1000 regions. In agreement with the results of Figure 4, the majority of permutation are local, with their rate quickly decreasing with increased pair distance. No spatial organisation is noticeable, indicating that all regions have the same permutation distribution.

Examples of permutation for specific regions are illustrated in Figure 6 for 2 similarly located regions across the atlases with 100, 300, and 1000 regions. We observe a high locality of permutation, with the rate of permutation rapidly decreasing with increased distance from the region of interest. However, some long range permutations still occur, although with a low permutation rate (green arrow). Noticeably, as the number of regions of the atlas is increased, the permutations become more local and stable around the region of interest.

4 | DISCUSSION

Studies representing the brain as a network often implicitly assume a correspondence between the nodes across the subjects. However, due to inter–subject variability affecting the structural and functional organisation of the cortex, the labels of the nodes may not be matched leading to incorrect comparisons. In this work, we proposed a network alignment strategy that exploits the spatial organisation of the cortical surface and thus promotes local permutation of node labels. When applied to the structural connectivity matrix of healthy young adults, our proposed alignment reduced inter–subject variance.

In more detail, we considered the structural brain networks of 100 healthy subjects from the HCP, obtained from a state-of-the-art diffusion MRI tractography pipeline. The nodes of the network corresponded to the regions of a groupwise structural parcellation of the cortex with the number of regions varied from 50 to 500 per hemisphere. Among the different available network alignment techniques, we selected the FAQ matching as it allowed us to include priors on the spatial organisation of the cortex. We did so via the algorithm initialization, that is the parcels permutation matrix used as a starting point which we set to the adjacency matrix of the parcellation. Compared to other initialization strategies, using the adjacency matrix as a starting point systematically increased the similarity between subjects for atlases with more than 50 regions, as illustrated in Figure 3. On the other hand, using a random or mean initialisation lead to a decrease of inter–subject similarity. Note that our baseline for similarity is the identity matrix, which corresponds to the assumption that the atlas is matched across subject made in current studies. Therefore, by using either the identity or adjacency matrices as starting points, the alignment improves the correspondence between structural networks when compared to the implicitly selected alignment of current studies. Our results suggest that, for a healthy cohort, network alignment should be performed before any comparison of the networks across subjects.

The importance of exploiting the spatial organisation of the cortex when performing network alignment is further explored by looking at the individual permutations. Specifically, we considered the distance between permuted regions, in terms of the neighborhood. As illustrated in Figure 4, most permutation are either with the same label (no

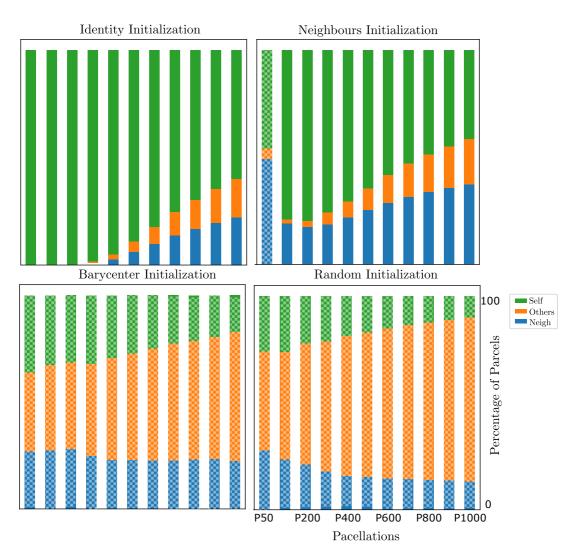


FIGURE 4 Type of permutations for both hemispheres. For each parcellation, the proportion of self permuted, unstable nodes and nodes permuted with neighbouring nodes is reported.

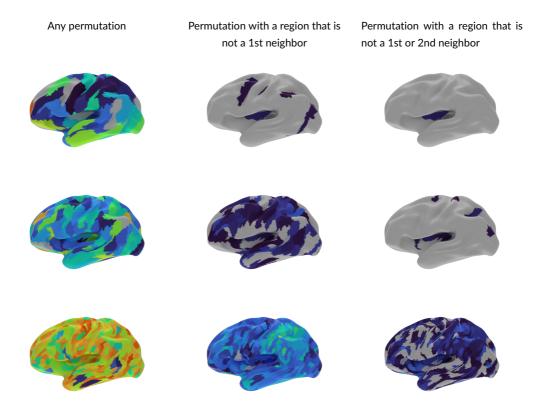


FIGURE 5 Surface visualization of the permutation type. For each regions, we considered the rate at which a regions was permuted with any other region (i.e. not a self permutation), with a region that is not a 1st degree neighbor, and with a region that is not a 1st or 2nd degree neighbor. Warmer and colder colors indicate a higher and lower permutation rates, respectively. Gray indicates no permutation. The three rows correspond to a brain parcellation with 100, 300, and 1000 regions.

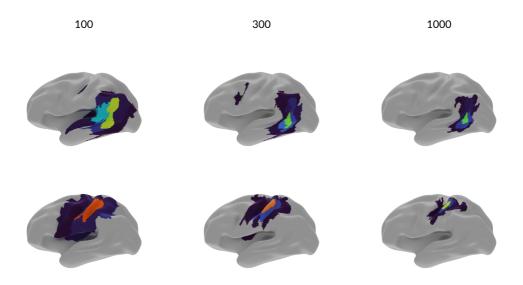


FIGURE 6 Comparison of the rate of permutations for 2 similarly located regions across the parcellations with 100, 300, and 1000 regions. Warmer and colder colors indicate a higher and lower permutation rate, respectively. Gray indicates no permutation.

permutation r_p^0) or with a direct neighbor (r_p^1) . As the number of parcels increase, there is an increase in the rate of long range permutation (r_p^n) with n > 1, reaching X% for 1000 parcels. This phenomenon can be explained by the size of the regions of the atlas which decreases as the number of parcel increases. In other words, r_p^1 and r_p^2 may correspond to the same cortical distance on two different atlases. In hindsight, these results suggest that a better notion of neighborhood could have been the distance between cortical regions rather than their adjacency in terms of cortical mesh. However, this approach would require the selection of an arbitrary distance threshold.

To understand the spatial distribution, the permutation frequencies for each region of the brain were illustrated in Figure 5. Overall, no specific patterns where identified and all regions presented a similar permutation distribution. From the inter–subject variability point of view, this supports the idea that the variance is not region specific and is instead uniform over the cortex. As illustrated in Figure 6, the permutation patterns were also consistent over different resolutions of the atlas. Regions were in general permuted with close neighbors, again highlighting the importance of the neighborhood information in the graph matching problem. While our proposed strategy favors local permutations, it does not forbid long range one and they were observed in some cases. Because we considered structural connectivity, the permutation of these nodes can indicate that they fulfil similar roles in terms of structural network organisation, or at least that they have similar connectivity to the rest of the brain. This could occur, for example, in tightly interconnected subnetworks with few connections to other subnetworks.

Our results show that brain network alignment increases the inter–subject similarity of structural connectivity. In the context of our healthy cohorts, this reduction in variability is advantageous as we expect all subjects to have normal, and therefore similar, connectivity. However, it is not trivial to extend these results to pathology as the intersubject variance may be a feature of the disease and should not be corrected explicitly. A possible solution would be to apply network alignment using a different alignment targets per class, as is common in registration. Finally, our

results considered only structural connectivity and may not generalize to functional connectivity or scenarios where both are considered simultaneously, e.g. structure–function mapping. In such cases, the alignment strategy should be modified to consider all available data to ensure a consistent permutation across the different networks.

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5 | APPENDIX

Firstly, we decompose the results across patients. In Figure 7, we look at all the permutations obtained across patients, to check if there are any subject anomalies. As the patients are control patients, we expect a consistent behaviour for each parcellation. As shown in the figure, the pattern is indeed consistent across patients and by increasing the number of parcels the FAQ suggests a matching procedure rather then leaving the nodes labels stable.

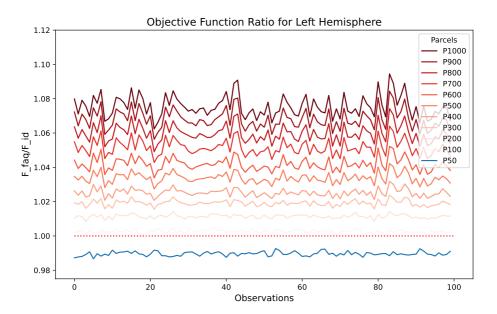


FIGURE 7 Left Hemisphere: Visualization of the ration between objective functions for each parcellations and each patients.

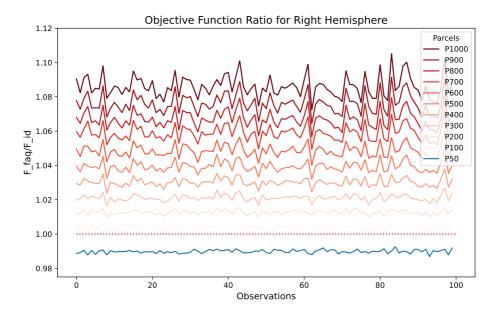


FIGURE 8 Right Hemisphere: Visualization of the ration between objective functions for each parcellations and each patients.