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Comparison of ensemble and correlation graphs in the task of classifying brain states based on fMRI data

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Abstract. The study of functional brain networks that support cognitive processes is one of the central goals of modern neuroscience. Functional magnetic resonance imaging (fMRI) is widely used to obtain data on brain activity. However, the high dimensionality and dynamic nature of fMRI data makes their processing challenging. Network-based methods of data representation offer a promising approach to describe the brain as a network, where nodes correspond to brain regions and edges correspond to functional connections between them. This allows us to further explore the topology of brain networks and their role in cognitive states. The *purpose* of this paper is to compare ensemble and correlation graphs in a brain state classification task based on functional magnetic resonance imaging (fMRI) data. *Methods.* This paper presents a novel method for representing fMRI data in graph form based on ensemble learning. To demonstrate the effectiveness of the data representation method, we compared it with correlated graphs by applying a graph neural network to classify brain states. *Results and Conclusion.* Our results showed that ensemble graphs lead to significantly more accurate and stable classification. The better classification performance suggests that using this method we are more efficient in identifying functional connections between brain regions during cognitive tasks.

Keywords: cognitive processes, functional magnetic resonance imaging, ensemble graphs, classification, machine learning.

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Introduction

One of the central goals of modern interdisciplinary science is to study the fundamental principles of human brain function. Currently, there is no general theory describing these principles. The primary approach is to study brain activity using various physical methods (electroencephalography, magnetoencephalography, functional magnetic resonance imaging, etc.) and, based on these data, to identify functional brain networks responsible for specific cognitive processes. Understanding how different brain regions interact and coordinate their activity during various cognitive tasks, and the ability to accurately classify brain states, can provide important insights into the nature of cognitive processes and facilitate the development of diagnostic and treatment methods for neurodegenerative diseases. In this context, functional magnetic resonance imaging (fMRI) [1,2] has become an important tool for obtaining data on brain activity [3–6].

Analyzing fMRI data is challenging due to its high-dimensional and dynamic nature. In recent years, increasing attention has been paid to the application of network-based methods of data representation to describe the functional connections between different brain regions [7–9]. These methods allow one to construct a model of the brain as a network, where nodes represent brain regions and edges represent the functional connections between them. This approach enables a deeper understanding of the nature of cognitive states by revealing both local and global connections in brain activity. Using network-based methods for fMRI data analysis allows one to study not only the characteristics of functional brain networks but also their topology using machine learning methods [6, 10–12].

Currently, there are several methods for representing fMRI data in network form in neuroscience. The simplest and most popular method is the correlation graph [6, 10, 13]. In general, any other metric, which may or may not be invariant with respect to time and spatial location of brain regions, can be used instead of Pearson correlation to calculate the functional connectivity between two brain regions [14–16].

In this paper, we propose a new approach to constructing connectivity graphs based on ensemble learning [17–19], which has not previously been used to represent cognitive data. It is designed for the task of binary classification of brain states and offers several significant advantages. First, ensemble learning allows us to effectively cope with noise, which is inevitably present in the data and is particularly characteristic of neuroimaging data, as well as with individual differences in cognitive processes among subjects. Second, preprocessing the data using machine learning methods before applying a complex classification model leads to improved classification accuracy. Third, our method for representing fMRI data allows us to use multimodal data and reflect in the graph the useful information carried by various connectivity metrics and time series characteristics of brain regions. In other words, our method combines the advantages of various metrics while constructing a single graph. This reduces the computer memory required for data storage and the computational time spent on subsequent network data analysis. Such graphs can be called ensemble or "synolitic"graphs, from the Greek word «synolo», meaning ensemble [20].

To verify the above statements, we constructed correlation graphs (as a relatively simple and most popular method for representing fMRI data) and ensemble graphs using HCP 1200 Subject Release data [21, 22]. Brain states were then classified using a graph neural network (GNN). The constructed correlation and ensemble graphs, as well as the entire code, are available for review on Zotero and GitHub [23].

1. Method

1.1. Data. To test the proposed method, fMRI data from 100 healthy individuals were selected from the HCP 1200 Subject Release [21,22]. The final sample consisted of 50 men and 50 women aged 22 to 35 years. We used data collected from subjects participating in one of six different experiments: working memory, gambling, limb movement, social perception, relational perception, and emotional perception [24]. For the binary classification task, we identified two brain states in each experiment (Table 1). Each brain state corresponded to a specific cognitive task performed by the subjects. Thus, each of the seven experiments contained 200 labeled data sets.

Table 1. Two brain states for each cognitive task, between which classification is made

	state 1	state 2
working memory	0-back	2-back
gambling	victory	loss
limb movement	left arm or leg	right arm or leg
social perception	random movement	mental interaction
relational perception	attitude	similarity
emotional perception	neutral	fear

The data were acquired at 3 T with a 208×180 mm field of view, 2.0 mm isotropic voxel size, 0.72 s repetition time (TR), 33.1 ms echo time (TE), and 52° flip angle. fMRI preprocessing was performed by HCP, including head motion correction, magnetic field distortion correction, spatial normalization, and spatial and temporal noise filtering. More details on the data acquisition and processing methods can be found in [24, 25]. Additionally, we removed the linear trend from the data, normalized the voxel time series, and parsed them into 379 regions using the [26] atlas. Time series within each region were spatially averaged such that each brain region corresponded to one time series.

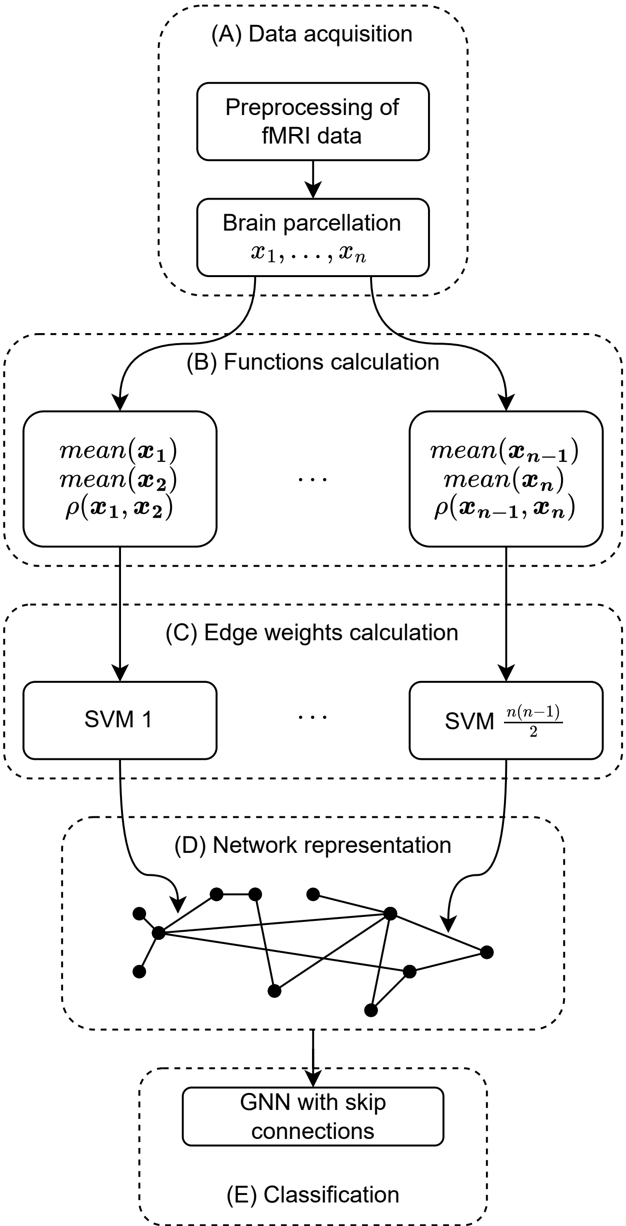

Fig. 1. An overview of representing fMRI, EEG/MEG data in graph form for classification of brain states. Initially, the data is preprocessed in the required way and time series are extracted from the data (A). Then, functions are calculated on the time series (B), the values of which are then fed to classifiers to calculate the edge weights of the graph (C). After that, the data is presented in graph form (D) and fed to a meta-classifier, e.g. a graph neural network, for the final classification (E)

1.2. Representation of fMRI data in graph form. Let us introduce the necessary notation. The graph $g = (V, E, H, W)$ consists of the set of vertices $V = \{i|i \in 1, \dots, n\}$, the set of undirected edges $E = \{ij|i \in V; j \in V; i \neq j\}$, the set of vertex values $H = \{h_i|i \in V\}$, and the set of edge values $W = \{w_{ij}|ij \in E\}$. Each vertex of the graph is associated with a brain region obtained by parcelling the fMRI data. The time series of brain region i will be denoted by $\boldsymbol{x_i}$.

For comparison with ensemble graphs, we used correlation graphs, well-known in the field of neuroimaging and easy to interpret. In such graphs, the value of vertex i is the average value of region $h_i = \overline{\boldsymbol{x_i}}$, and the value of edge ij is the Pearson correlation between the time series of the two regions $w_{ij} = \rho(\boldsymbol{x_i}, \boldsymbol{x_j})$. For each graph, we normalized the weights of its edges.

In the general case of ensemble graphs, the value of edge ij is calculated as the difference in the probabilities of two brain states given the values of some set of functions $f_1, \dots, f_k$ from the time series of brain regions i, j:

$$w_{ij} = P(2|f_1(\boldsymbol{x_i}, \boldsymbol{x_j}), \dots, f_k(\boldsymbol{x_i}, \boldsymbol{x_j})) - P(1|f_1(\boldsymbol{x_i}, \boldsymbol{x_j}), \dots, f_k(\boldsymbol{x_i}, \boldsymbol{x_j})). \tag{1}$$

For the functions $f_1, \dots, f_k$, we chose the same metrics as for the correlation graphs: the mean value of regions i and j and the Pearson correlation between them. Thus, to calculate the edge weights, we had to train an individual classifier for each edge. In particular, we used the support vector machine [27] with a radial basis kernel and a regularization parameter equal to one. From equation (1) it follows that the edge weight can take values from -1 to 1. Accordingly, if the edge weight w_{ij} is negative, then edge ij carries the information that brain state 1 is the most probable state. If the edge weight w_{ij} is positive, then edge ij carries the information that brain state 2 is the most probable state. The larger the absolute value of edge weight $|w_{ij}|$, the more information edge ij carries for classification. Since information about the average values of regional time series is already included in the edge weights, and the GNN requires vertex values, the value of each vertex i is one ($h_i = 1$). The entire process of constructing ensemble graphs and classification is shown in Fig. 1.

1.3. Graph neural network. To classify the graphs obtained in the previous step, we used a simple graph neural network with the following architecture. The graph to be classified was fed to a convolutional graph layer [28], after which ReLU [29] was applied. After the nonlinearity, Batch Normalization [30] and DropOut [31] layers were used to prevent overfitting of the neural network. Next, so-called «skip connections» [32] were used, when the output of the convolutional layer after nonlinearity is connected to the data at the layer input. Two more convolutional layers were applied in a similar manner. The result was vertex embeddings that take into account the influence of neighboring graph vertices. Global max Pooling was used to transition from vertex embeddings to full-graph embeddings. Next, after another Batch Normalization layer, the data was fed to a fully connected layer, after which class membership scores were calculated using the sigmoid function. Cross-entropy was used as the loss function.

1.4. Training and validation scheme. For the graph construction procedure, each dataset was split into training and test sets based on the number of subjects: 70 subjects in the training set (140 datasets) and 30 subjects in the test set (60 datasets). The training set was used to train graph construction models, which were then used to construct graphs on the test set.

Graph classification was performed using a deep neural network (GNN) with the same division into training and test sets as for the graph construction task. The test set was further split into a validation set of 20 subjects (40 labeled graphs), which was used to search for optimal GNN hyperparameters, and a test set of 10 subjects (20 graph sets), which was used to evaluate the classification metrics. After selecting the hyperparameters of the GNN on the validation set, the GNN was trained and tested 50 times with different random seeds, which made it possible to estimate the mean and standard deviation of the metrics.

Results and conclusion

The results of a comparison of the correlation and ensemble representation methods based on HCP fMRI data are presented in Table 2. It presents the average classification accuracy and F1 metric, along

Table 2. Comparison of correlation-based and ensemble-based representation methods on fMRI data of HCP. Classification accuracy and F1 metric in mean (standard deviation) format are presented

		Correlation graphs	Ensemble graphs
working memory	Accuracy (%)	71.7 (7.11)	79.4 (3.56)
	F1 (%)	72.78 (7.86)	74.37 (5.23)
gambling	Accuracy (%)	65.3 (6.12)	98.9 (2.07)
	F1 (%)	70.7 (5.82)	98.95 (1.97)
limb movement	Accuracy (%)	62.3 (6.34)	68.0 (4.36)
	F1 (%)	42.66 (12.36)	67.75 (4.55)
social perception	Accuracy (%)	80.6 (5.71)	98.2 (2.4)
	F1 (%)	82.57 (4.5)	98.11 (2.53)
relational perception	Accuracy (%)	85.3 (5.69)	95.0 (0.0)
	F1 (%)	85.46 (5.8)	95.24 (0.0)
emotional perception	Accuracy (%)	54.2 (5.23)	73.8 (6.37)
	F1 (%)	55.64 (6.34)	73.7 (5.18)

with their standard deviations. The ensemble method (on average) leads to more accurate and stable classification for each experiment type.

We hypothesize that our method outperforms the correlation method because correlation graphs contain noise generated by the following factors: instability of correlation coefficients due to short time series. When calculating correlation coefficients based on short time series, typical of fMRI data, a standard error arises, leading to unreliable correlation estimates. The shorter the time series, the higher the error and, consequently, the higher the noise level. It is also important to consider that time series from adjacent regions can influence each other due to the physical proximity of blood flow changes. This leads to distortion of the measured correlations. Furthermore, global signal changes, for example, due to a general change in activity level, can superimpose on local signals, creating spurious correlations. Due to the above issues, correlation graphs constructed from fMRI data require additional processing to filter out noise. In turn, the ensemble method, due to the nature of its computation, marks edges that are insignificant for classification with a weight close to zero in absolute value. This reduces the influence of information in the data that is irrelevant for classification.

As an example of visualizing the topology of graphs constructed using the ensemble method, we present the edge weight matrix averaged over the test sample in a working memory experiment (Fig. 2). Some edges are clearly highlighted, indicating their importance in classifying between two states.

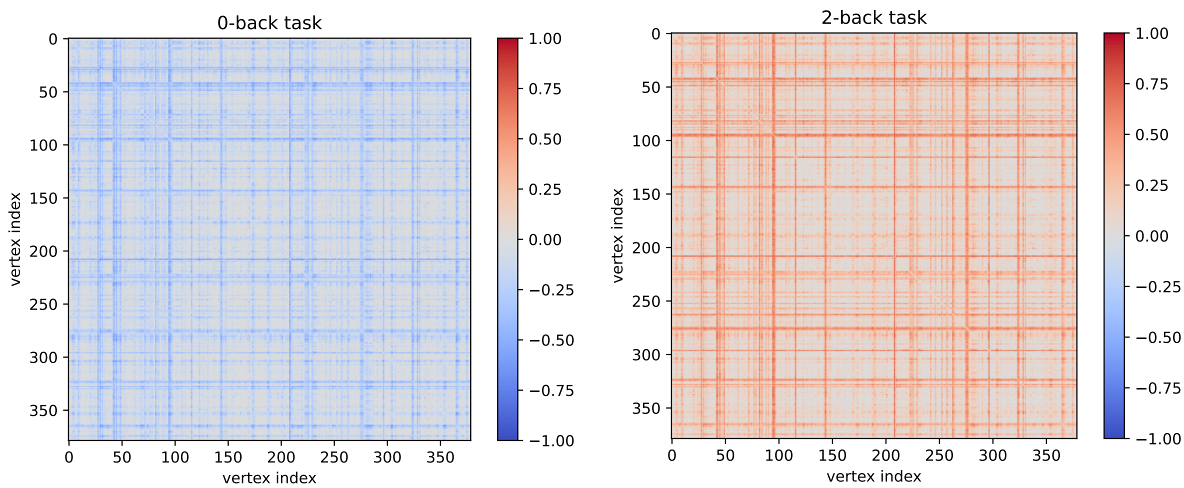

Fig. 2. Test sample averaged matrices of edge weights for ensemble graphs in the working memory experiment. Vertically and horizontally there are vertex indices, the color reflects the edge weight (color online)

It should be noted that the format in which we constructed ensemble graphs can also be interpreted as a transformation over correlation graphs using machine learning methods.

In conclusion, this paper presents a data representation method based on ensemble learning, which demonstrated superior performance across all tasks compared to the most widely used method, making it suitable for fMRI data analysis. This improved classification performance suggests that this method is more effective in identifying functional connections between brain regions during cognitive tasks. We hope that in the future, as such experimental data accumulates, our method will enable further advances in our understanding of brain processes.

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