A graph convolutional network for classification of resting-state fMRI data

Elena Pitsik
Samara State Medical University
Samara, Russia
0000-0003-1850-2394

Semen Kurkin
Samara State Medical University
Samara, Russia
0000-0002-3438-5717

Alexander Hramov
Institute of Cardiological Research
Saratov State Medical University
Saratov, Russia
0000-0003-2787-2530

Rositsa Paunova
Plovdiv Medical University
Plovdiv, Bulgaria

Denitsa Simeonova
Plovdiv Medical University
Plovdiv, Bulgaria

Sevdalina Kandilarova
Plovdiv Medical University
Plovdiv, Bulgaria

Drozdstoy Stoyanov
Plovdiv Medical University
Plovdiv, Bulgaria

***Abstract*—Machine learning methods have been widely applied in neurophysiological data studies for classification and clusterization purposes. However, analysis of connectivity data requires consideration it's graph-like structure to utilize it's structural and functional information. To address this issue, we propose a machine learning model based on graph convolutional network for classification of connectivity matrices obtained from fMRI data. We show that out relatively simple model has a good generalization ability and is able to achieve high performance on moderate amount of data.**

***Index Terms*—graph convolutional network, machine learning, fMRI, classification**

I. Introduction

The connectivity features of the brain evaluated via neurophysiological data such as MEG, EEG and fMRI, can be modelled as a graph with brain regions as the nodes and structural or functional relationships between them as the edges [1], [2]. Such representation allowed to gain an insight into the structural and functional organization of the brain by applying the mathematical methods of graph theory [3]–[5]. Besides, in medical studies, machine learning methods are widely used for processing the neuroimaging data [6], [7], among which the graph neural networks (GNN) draw the most attention in the context of analysis of graph-like data [8].

In this paper, we use GNN-based machine learning model for classification of resting state fMRI (rs-fMRI) data. Many studies are focusing on the rs-fMRI connectivity due to it's great potential in clinical applications. In particular, the differences between various network structures assessed via rs-fMRI were used in identification of mental disorders such as schizophrenia [9], [10], post-traumatic stress disorder [11], Alzheimer's disease [12], [13] and obsessive-compulsive disorder [14]. A bulk of studies is dedicated to machine learning methods, among which the convolutional neural networks (CNN) are recognized as the most appropriate [15]–[17]. In present study, we propose a model based on graph convolutional network (GCN) to classify rs-fMRI data. Unlike CNNs, that benefit from the grid-like structures of the images, GCN are able to operate directly on graphs by processing the node and edge features and taking into account the graph-like structure of the data [18]. Recently, GCNs were used in natural language processing [19], [20], chemistry [21], [22], computer vision [23] and social network analysis [24]. Here, we perform classification of rs-fMRI data of major depressive disorder patients using GCN-based model. We demonstrate that event the relatively simple model can achieve a good generalization ability on a moderate amount of data with a controllable risk of overfitting.

II. Methods

A. Experimental dataset

The performance of the proposed architecture was evaluated with rs-fMRI dataset containing 91 correlation matrices: 50 healthy controls and 41 major depressive disorder patients. The scanning procedure was performed on a GE Discovery 750w MRI system. We estimated the connectivity for 166 regions of interest by calculating an average BOLD time series across the voxels in each parcellation i and Pearson correlation coefficients for all pairs of mean parcellation activities. As a result, each connectivity graph was represented as connectivity matrix 166x166, each value representing the strength of the edge between two parcels:

$$r_{i,j} = \frac{\sum_{k=1}^{n}(x_{i,k} - \overline{x}_i)(x_{j,k} - \overline{x}_j)}{\sqrt{\sum_{k=1}^{n}(x_{i,k} - \overline{x}_i)^2}\sqrt{\sum_{k=1}^{n}(x_{j,k} - \overline{x}_j)^2}}, \quad (1)$$

where n is the length of the time series x, and $\overline{x}$ is the mean of the time series.

For GCN classification, a representation of each graph included a node feature matrix, edge data in coordinate format, a 1D vector of edge weights and label (see fig. 1A). Since each node of the correlation matrix represents a certain brain region, we emphasized their uniqueness by assigning a single feature to each of them, thus obtaining a 166x166 node feature matrix. The dataset was normalized and randomly shuffled before splitting into training, validation and testing subsets in the ratio $60/30/10\%$.

978-1-6654-6174-0/22/$31.00 ©2022 IEEE

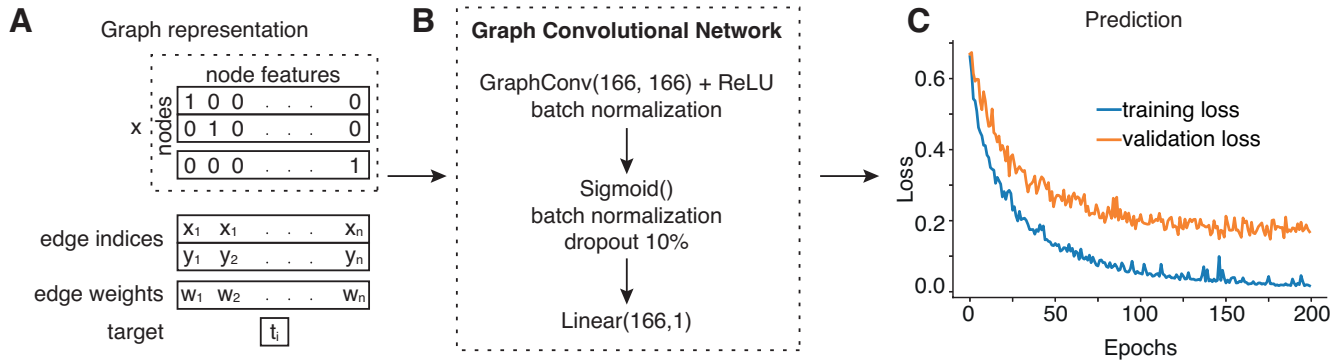

Fig. 1. **A** – a single graph representation in coordinate format; **B** – scheme of proposed GCN model; **C** – training and validation losses during 200 epochs of model training.

B. GCN architecture

Fig. 1B shows the scheme of the proposed classifier. The model included one k-dimensional graph convolutional layer (GraphConv) proposed in [25] with 166 input and 64 hidden neurons. The GraphConv layer computes the feature vector $f_k^{(t)}$ as follows:

$$f_k^{(t)}(s) = \sigma\left(f_k^{(t-1)}(s)W_1^{(t)} + W_2^{(t)}\sum_{u\in N_L(s)\cup N_G(s)} f(k)^{(t-1)}(u)\right), \quad (2)$$

where σ is an activation function (we used ReLU activation in proposed model), $W_1^{(t)}$ and $W_2^{(t)}$ are parameter matrices (sequences of weights), $N_L(s)$ and $N_G(s)$ are local and global neighborhoods of the node set s. For more details of the mathematical definition of GCN see [25]. The element-wise sigmoid function was applied to the feature vector before proceeding with fully-connected linear layer with one output neuron, which provides the prediction. Before each step, we applied the batch normalization [26], and before the output layer we used 10% dropout.

III. Results

The model was trained for 200 epochs using Adam optimizer [27] with learning rate 0.0001. We used binary cross entropy to calculate training, validation and testing loss. The data was fed to the model in batches with the batch size of 32. The results of training are presented on fig. 1C. One can see that although both training and validation loss continue to improve, there is a gap between the curves. Such pattern suggests the problem of unrepresentative validation set, i.e. the too small amount of validation data, which is rather expected considering a relatively small amount of data used to train the model. At the same time, the model was able to achieve training accuracy of 100% and validation accuracy of 98.89%. We also tested the model on a small amount of data that was never used in the training process and achieved 100% accuracy of classification. Therefore, the model demonstrated a good generalization ability.

However, this research has certain limitations. The most important one is a small dataset used to train GCN, which can lead to overfitting and unreliable results of classification even on testing dataset. To address this problem, several precaution steps were taken. The model was designed with only one graph convolutional layer to avoid possible problems of applying an overly deep model to insufficient data. Besides, we chose a small learning rate to avoid the instability of the training process, and adjusted the batches to the optimal size. As a result, the training and validation curves converge smoothly, and the gap between them suggests the insufficient amount of validation data rather than overfitting.

IV. Conclusion

In present research, we apply a graph convolutional network to classify rs-fMRI data from healthy controls and major depressive disorder patients. Despite the relatively small amount of initial dataset, the proposed model was able to achieve 100% of testing accuracy without the signs of strong overfitting.

Acknowledgment

The reported study was funded by RFBR and National Natural Science Foundation of China according to the research project 19-52-55001).

References

[1] D. S. Bassett and O. Sporns, "Network neuroscience," *Nature neuroscience*, vol. 20, no. 3, pp. 353–364, 2017.

[2] A. E. Hramov, N. S. Frolov, V. A. Maksimenko, S. A. Kurkin, V. B. Kazantsev, and A. N. Pisarchik, "Functional networks of the brain: from connectivity restoration to dynamic integration," *Physics-Uspekhi*, vol. 64, no. 6, p. 584, 2021.

[3] V. V. Makarov, M. O. Zhuravlev, A. E. Runnova, P. Protasov, V. A. Maksimenko, N. S. Frolov, A. N. Pisarchik, and A. E. Hramov, "Betweenness centrality in multiplex brain network during mental task evaluation," *Physical Review E*, vol. 98, no. 6, p. 062413, 2018.

[4] V. A. Maksimenko, N. S. Frolov, A. E. Hramov, A. E. Runnova, V. V. Grubov, J. Kurths, and A. N. Pisarchik, "Neural interactions in a spatially-distributed cortical network during perceptual decision-making," *Frontiers in behavioral neuroscience*, vol. 13, p. 220, 2019.

[5] W. Bao, Y. Gao, L. Cao, H. Li, J. Liu, K. Liang, X. Hu, L. Zhang, X. Hu, Q. Gong *et al.*, "Alterations in large-scale functional networks in adult posttraumatic stress disorder: a systematic review and meta-analysis of resting-state functional connectivity studies," *Neuroscience & Biobehavioral Reviews*, vol. 131, pp. 1027–1036, 2021.

[6] P. Rajpurkar, E. Chen, O. Banerjee, and E. J. Topol, "Ai in health and medicine," *Nature Medicine*, vol. 28, no. 1, pp. 31–38, 2022.

[7] E. N. Pitsik, N. S. Frolov, N. Shusharina, and A. E. Hramov, "Age-related changes in functional connectivity during the sensorimotor integration detected by artificial neural network," *Sensors*, vol. 22, no. 7, p. 2537, 2022.

[8] F. Scarselli, M. Gori, A. C. Tsoi, M. Hagenbuchner, and G. Monfardini, "The graph neural network model," *IEEE transactions on neural networks*, vol. 20, no. 1, pp. 61–80, 2008.

[9] B. Rashid, M. R. Arbabshirani, E. Damaraju, M. S. Cetin, R. Miller, G. D. Pearlson, and V. D. Calhoun, "Classification of schizophrenia and bipolar patients using static and dynamic resting-state fmri brain connectivity," *Neuroimage*, vol. 134, pp. 645–657, 2016.

[10] A. Anderson and M. S. Cohen, "Decreased small-world functional network connectivity and clustering across resting state networks in schizophrenia: an fmri classification tutorial," *Frontiers in human neuroscience*, vol. 7, p. 520, 2013.

[11] F. Liu, B. Xie, Y. Wang, W. Guo, J.-P. Fouche, Z. Long, W. Wang, H. Chen, M. Li, X. Duan *et al.*, "Characterization of post-traumatic stress disorder using resting-state fmri with a multi-level parametric classification approach," *Brain topography*, vol. 28, no. 2, pp. 221–237, 2015.

[12] A. Khazaee, A. Ebrahimzadeh, and A. Babajani-Feremi, "Application of advanced machine learning methods on resting-state fmri network for identification of mild cognitive impairment and alzheimer's disease," *Brain imaging and behavior*, vol. 10, no. 3, pp. 799–817, 2016.

[13] E. Challis, P. Hurley, L. Serra, M. Bozzali, S. Oliver, and M. Cercignani, "Gaussian process classification of alzheimer's disease and mild cognitive impairment from resting-state fmri," *NeuroImage*, vol. 112, pp. 232–243, 2015.

[14] B. Sen, G. A. Bernstein, T. Xu, B. A. Mueller, M. W. Schreiner, K. R. Cullen, and K. K. Parhi, "Classification of obsessive-compulsive disorder from resting-state fmri," in *2016 38th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC)*. IEEE, 2016, pp. 3606–3609.

[15] M. N. I. Qureshi, J. Oh, and B. Lee, "3d-cnn based discrimination of schizophrenia using resting-state fmri," *Artificial intelligence in medicine*, vol. 98, pp. 10–17, 2019.

[16] Y.-W. Niu, Q.-H. Lin, Y. Qiu, L.-D. Kuang, and V. D. Calhoun, "Sample augmentation for classification of schizophrenia patients and healthy controls using ica of fmri data and convolutional neural networks," in *2019 tenth international conference on intelligent control and information processing (ICICIP)*. IEEE, 2019, pp. 297–302.

[17] E. Canario, D. Chen, and B. Biswal, "A review of resting-state fmri and its use to examine psychiatric disorders," *Psychoradiology*, vol. 1, no. 1, pp. 42–53, 2021.

[18] S. Zhang, H. Tong, J. Xu, and R. Maciejewski, "Graph convolutional networks: a comprehensive review," *Computational Social Networks*, vol. 6, no. 1, pp. 1–23, 2019.

[19] A. Alhogail and A. Alsabih, "Applying machine learning and natural language processing to detect phishing email," *Computers & Security*, vol. 110, p. 102414, 2021.

[20] K. Sun, R. Zhang, S. Mensah, Y. Mao, and X. Liu, "Aspect-level sentiment analysis via convolution over dependency tree," in *Proceedings of the 2019 conference on empirical methods in natural language processing and the 9th international joint conference on natural language processing (EMNLP-IJCNLP)*, 2019, pp. 5679–5688.

[21] C. W. Coley, W. Jin, L. Rogers, T. F. Jamison, T. S. Jaakkola, W. H. Green, R. Barzilay, and K. F. Jensen, "A graph-convolutional neural network model for the prediction of chemical reactivity," *Chemical science*, vol. 10, no. 2, pp. 370–377, 2019.

[22] S. Ryu, Y. Kwon, and W. Y. Kim, "A bayesian graph convolutional network for reliable prediction of molecular properties with uncertainty quantification," *Chemical Science*, vol. 10, no. 36, pp. 8438–8446, 2019.

[23] H. Ren, W. Lu, Y. Xiao, X. Chang, X. Wang, Z. Dong, and D. Fang, "Graph convolutional networks in language and vision: A survey," *Knowledge-Based Systems*, p. 109250, 2022.

[24] J. Y. Chan, Z. Wang, Y. Xie, C. A. Meisel, J. D. Meisel, P. Solano, and H. Murillo, "Identifying potential managerial personnel using pagerank and social network analysis: The case study of a european it company," *Applied Sciences*, vol. 11, no. 15, p. 6985, 2021.

[25] C. Morris, M. Ritzert, M. Fey, W. L. Hamilton, J. E. Lenssen, G. Rattan, and M. Grohe, "Weisfeiler and leman go neural: Higher-order graph neural networks," in *Proceedings of the AAAI conference on artificial intelligence*, vol. 33, no. 01, 2019, pp. 4602–4609.

[26] S. Ioffe and C. Szegedy, "Batch normalization: Accelerating deep network training by reducing internal covariate shift," in *International conference on machine learning*. PMLR, 2015, pp. 448–456.

[27] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization," in *ICLR (Poster)*, 2015.