Research on children's autism recognition based on graph neural network

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ABSTRACT

Autism spectrum disorder has become a global public health problem. Accurate diagnosis and prediction of autism are of great significance to determine the appropriate diagnosis and treatment plan. Based on the ABIDE autism data, this study uses a graph neural network to conduct a research on autism identification in children. Our main process includes preliminary data preparation processing, diagnostic model design and experimental result validation. The preliminary data mainly includes four steps: (1) extraction of blood oxygenation level dependent signal (BOLD signal for short) in brain regions; (2) generation of brain function network connection matrix; (3) matrix binarization and (4) brain map topology storage. Our initial data has 884 fMRI brain maps (two labels are ASD and HC). After data processing, it can be displayed as data in Euclidean space and data in non-Euclidean space. For the former, we use the method based on machine learning for model architecture; for the latter, we start from the graph classification model and establish Various graph neural network models. We have performed some evaluation and analysis for each model. At the same time, we take into account the scale of the data volume and use a data augmentation model to further process the original data. After the enhancement, the amount of data has been expanded by three times. Our graph classification model GAT can achieve 68.9% accuracy, 57.1% recall and 80.0% true negative rate, and the GAT model with data enhancement can achieve 72.3% accuracy, 58.3% Recall and 82.4% true negative rate.

Keywords: Autism, Graph Neural Network, ABIDE, Graph Classification

INTRODUCTION

In our lives, the number of people with autism is increasing year by year, and it has attracted widespread attention from all walks of life. Autism spectrum disorder is an early-onset neurodevelopmental disorder characterized by social interaction impairment, communication impairment, and stereotyped and repetitive behavior patterns, which seriously affect the daily life of patients. However, the current clinical diagnosis of autism is mainly through questionnaires to patients. In this way, the authenticity of the patient's answer needs to be considered and is affected by factors such as the doctor's experience and level, and the diagnosis results are subjective and prone to misdiagnosis. In recent years, there have been a lot of studies looking for biological diagnostic indicators of autism from the perspective of brain medical imaging.

In recent years, many scholars have conducted related research on the working principle of graph neural network and its possible medical applications.

In the graph neural network, GCN is a method often used for graph classification in recent years [10]. [8] proposes a scalable method for semi-supervised learning on graph-structured data based on an efficient variant of convolutional neural networks that operate directly on graphs. It motivates the

choice of convolutional architectures through local first-order approximations of spectral graph convolutions. Our model scales linearly in the number of graph edges and learns hidden layer representations that encode local graph structure and node features. Through this paper, we have learned the relevant basic GCN model knowledge, and have a preliminary understanding of the graph-based model classification method. However, the disadvantage of this paper is that GCN needs to put the entire graph into memory and video memory, which will consume a lot of memory and video memory and cannot handle large graphs; second, GCN needs to know the structural information of the entire graph during training (including the to-be-predicted nodes), which cannot be achieved in some real tasks (such as predicting tomorrow's data with a graph model trained today, then tomorrow's nodes will not be available); third, the use of this model is related to our depression. There are certain discrepancies and needs to be further improved.

In the past, there have also been studies using graph neural networks to judge depression. This report proposes a computer-aided diagnosis method for depression using a CNN-based graph convolution model. In terms of model method, this paper extracts the topology of brain network (brain map) from functional MRI images as input features, and performs feature extraction and depression diagnosis and classification based on graph convolutional neural network. In the diagnosis of depression, this paper studies the difference between the brain subregions of drug-effective RD and drug-ineffective NRD, and the auxiliary physician provides an appropriate diagnosis and treatment plan based on the prediction of drug response of each MDD patient, that is, efficacy prediction. The model is used to determine whether the subject suffers from depression. If it is determined to be non-diseased, it will be classified into the normal category; if it is determined to be suffering from the disease, it will be further judged whether the patient can be treated by taking antidepressant drugs (efficacy prediction) , which can be subdivided into two types: drug-effective depression and drug-ineffective depression. However, the data set used in this report comes from 132 patients in city hospitals, and there is a lot of room for improvement in generalizability and data scale.

We have paid attention to some methods for autism classification research using the ABIDE dataset[7][13][16], but the problem with most models is that the amount of data is small and not convincing. Or the model is relatively simple and does not have good generalization.

Our dataset uses ABIDE data collected by the NeuroBureau preprocessing program, giving us access to robust neuroimaging findings[1][9]. The data provided by this program included two fMRI preprocessing pipelines and gray matter density maps for voxel-based morphometry, but since the amount of data was not sufficient to fully support our model training process, we used data augmentation to further the model Process[2].

The main contributions of this paper can be summarized as follows:

1. In this paper, We focus on learning deep representations of brain connectivity networks from fMRI, where each brain network represents a subject-specific pattern of brain activity. We propose a GAT-based data augmentation method MixUp GAT (M-GAT) model, which can extract the most useful spatial features and capture the most important coherently embedded features from the perspective of graph classification

2. ASD is an early-onset neurodevelopmental disorder characterized primarily by impairments in social interaction, communication obstacles and stereotyped behaviors seriously affect children's daily life. Different from the clinical diagnosis method in which doctors inquire subjects with scales according to

general standards ,we provide a more effective auxiliary diagnosis method for potential patients with ASD by trying the graph neural network method.

3. Experiments on a total of 884 sets of data on the ABIDE dataset: diagnosis of ASD, show the effectiveness of our proposed model. The experimental results show that the prediction accuracy of ASD diagnosis can be improved by introducing the MixUp data augmentation method.

RELATED WORK

Methods used in this paper:

MLP MLP[17] (Multilayer perceptron) is the simplest forward propagation network in deep learning, and the input used is the flattened functional connection network. It consists of three network layers: input layer, hidden layer, and output layer. The MLP network learns based on data samples and consists of an m-dimensional input vector v1 and an n-dimensional output vector v2. By introducing an adaptive weight w, the input vector v1 is processed to generate an output y(v1,w).

The following models we use are all graph classification models.
In the graph classification model, each graph represents an individual, each node represents a brain area, and the edges between nodes are calculated based on the Pearson correlation coefficient matrix calculated from the BOLD signal of each brain area[11].

GCN GCN applies the convolution operation in image processing to graph structure data processing for the first time, and its authors gives a detailed derivation[5][6]. The most important one is the update equation of each node, which aggregates the features of neighbor nodes and then performs linear transformation. In order to enable GCN to capture the information of the k-hop neighbor nodes, multiple layers of GCN layers can be stacked, the matrix form of which is expressed as follows:

$$H^{(l+1)} = \sigma\left(D^{-\frac{1}{2}}\tilde{A}D^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

Where $D^{-\frac{1}{2}}\tilde{A}D^{-\frac{1}{2}}$ is the adjacency matrix after normalization, $H^{(l)}W^{(l)}$ is equivalent to doing a linear transformation to the embeddings of all nodes in the l layer, which is represented by the left multiplication by the adjacency matrix. For each node, the feature of the node is expressed as the result of adding the neighbor nodes. In this way, the GCN can encode the structural information of the graph and thus learn better node representations.

GraphSAGE GraphSAGE [4] is a general inductive framework that learns a function that generates node embeddings by sampling and aggregating features from a node's local neighborhood, i.e., it can leverage node feature information to efficiently generate previously unseen The data generation node embeddings. GraphSAGE was proposed to deal with some shortcomings of GCN. In the specific implementation, it only retains edge between training samples during training, and includes two steps, Sampling and Aggregating. Sample refers to selecting some nodes from neighbors, and Aggregate means to aggregate the embeddings of sampled neighbor nodes to update their own embedding information.

GAT In order to solve the problem that the importance of different neighbor nodes is not considered when GNN aggregates neighbor nodes, GAT draws on the idea from Transformer and introduces the masked self-attention mechanism[12]. When calculating the representation of each node in the graph, it will be based on the different characteristics of neighbor nodes are used to assign different weights to them. In order to improve the fitting ability of the model, multi-head self-attention mechanism is also introduced. That is, multiple W^k are used to calculate self-attention at the same time, and then the calculated results are combined (connected or summed). By operating on graph-structured data, GAT networks assign different weights to different nodes in the neighborhood by stacking layers where nodes are able to focus on the characteristics of their neighborhood, without requiring any kind of costly matrix operations or relying on knowledge of the graph early structure.

Data Augmentation Data Augmentation[14] methods are widely used in the field of image classification. It does not require ground-truth, instead, it incorporates prior knowledge to expand the training distribution by constructing virtual training samples across all categories, i.e., interpolation of features should lead to interpolation of relevant targets.

METHOD

Through comparative experiments, we found that the GAT model achieved the best results. We decided to select it as the baseline, and introduced data enhancement methods, incorporating the idea of MixUp.

For the GAT model, its input layer is N groups of F-dimensional node feature vectors h , where N is the number of nodes. This layer produces a new set of F'-dimensional vectors as output. By converting the input features into higher-dimensional features to obtain better expressiveness, it introduces linear changes, by applying a shared weight matrix W to each node, and then introducing a shared attention mechanism a to calculate the coefficient e_{ij} , It represents the importance of the feature of node j to node i. We then normalize the coefficients using a softmax function in order to make the coefficients of different nodes easier to compare.

$$\alpha_{ij} = softmax_j\left(e_{ij}\right) = \frac{exp\left(e_{ij}\right)}{\sum_{k\in\mathcal{N}_i} exp\left(e_{ik}\right)}$$

Data Augmentation plays a central role in training neural networks. It operates on the input data and improves the performance significantly. The sample size of the ABIDE dataset is 884. Compared with the general deep learning dataset, the sample size is small. It may fall into overfitting to the data and underfitting to the task, and the model generalization ability is not enough. From this we decided to try to introduce data augmentation methods.

Mixup is an advanced data augmentation method for training neural network based image classifiers, which interpolates both features and labels of a pair of images to produce synthetic samples. Drawing on the method in the Mixup for Node and Graph Classification[14] paper, the idea of Mix the Paired Graphs in Semantic Space is mainly used. We map the node attributes and topology of the paired graphs to the vector space representation through multi-layer convolutional layers, and then fuse the

graph representation and labels through the linear layer. We define a graph as G = (V, E), where V denotes the set of nodes, and E is the set of edges. For a given graph G_1 and G_2 , $\hbar_{G_1}$, $\hbar_{G_2}$ represent the embedding of the graph, y_{G_1}, y_{G_2} represent the label of the graph, we Fusion is done by:

$$\hat{\hbar}_{G_1G_2} = (\lambda)\hbar_{G_1} + (1-\lambda)\hbar_{G_2}$$

$$\hat{y}_{G_1G_2} = (\lambda)y_{G_1} + (1-\lambda)y_{G_2}$$

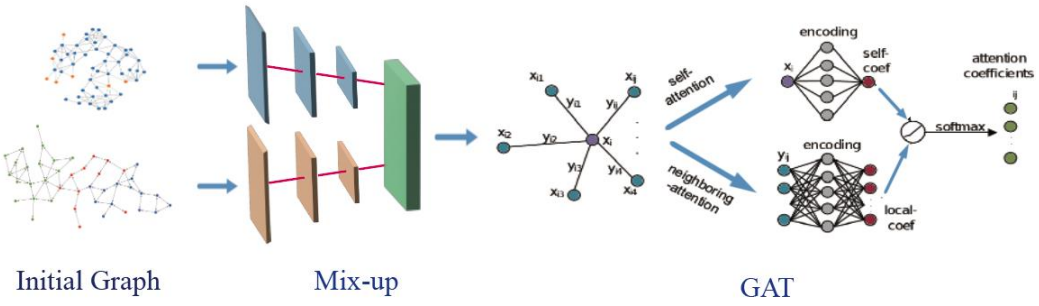

Figure 1. M-GAT Model Architecture

where $\lambda \in [0,1]$. Finally, the interpolated graph-level embedding $\hat{h}_{G_1G_2}$ will be passed to a multi-layer perception followed by a softmax layer to produce the predicted distribution for the targeted classes. We perform self-attention on the graphs by a shared attentional mechanism a to computes attention coefficients:

$$e_{G1G2} = a(W\vec{h}_{G_1}, W\vec{h}_{G_2})$$

Then we normalize them across all choices of j using the softmax function:

$$\alpha_{G1G2} = \text{softmax}_j\,(e_{G1G2}) = \frac{\exp(e_{G1G2})}{\sum_{k\in\mathcal{G}_i}\exp\,(e_{G1Gk})}$$

After obtaining the normalized attention coefficient, calculate the linear combination of the corresponding features as the final output feature of each graph.

$$\vec{y}_{Gi} = \sigma\left(\sum_{j\in\mathcal{G}_i}\alpha_{GiGj}W\vec{h}_{Gj}\right)$$

EXPERIMENT

Dataset

Our initial data had 884 fMRI scans, 618 of which were obtained after data cleaning. For the non-Euclidean space models, after data preprocessing, each image contains 90 brain regions, and each brain region have 266 features. All of our models are trained on these 618 scans with ten-fold cross-validation (train: val: test=8: 1: 1).

Data Processing

Here we use [1] to preprocess the data. The obtained data is a sampling of the blood oxygen level-dependent signal (BOLD) intensity of each brain region over a period of time. In order to obtain the functional connectivity network, we use this set of data to calculate the Pearson correlation coefficient between each brain region, where each brain region is a node, and the correlation coefficient between brain regions is the weight of its edge, thus constructing a functional connection network. The network constructed at this time is a fully connected network, and some models in our experiment do not support the existence of coefficients on the edges.

Therefore, for this part of the model, we threshold the network, only keep the edges whose weights are greater than the threshold. In addition, each node also needs its feature vector. There are also two solutions here, one is to directly use the BOLD signal strength sequence, and the other is to obtain the mean, variance, skewness and kurtosis of the sequence as features[3][15]. The former has a problem because the sequence lengths of the data collected by different organizations are different, and the graph neural network requires the feature vector length of each node to be consistent, so all sequences need to be truncated to the length of the shortest sequence. The data processing mentioned above is for the graph neural network. For comparison, we also conducted experiments on ordinary neural networks and other machine learning models in this project. These models do not support non-Euclidean data models such as graphs, so it is necessary to flatten the adjacency matrix of the functional connection network, specifically, taking the upper triangle of the matrix and splicing each row of the upper triangle.

Model setup

We conducted experiments on each of the above models separately, and Table 1 and Table 2 show all the hyperparameters of the model . We adjust the parameters according to the experimental data, and the final parameter selection results are shown in the table below.

Table 1. Graph Neural Network Parameter Settings

Model	GCN	GAT	GraphSAGE
Parameter	GraphConv(266, 128) GraphConv(128, 128) GraphConv(128, 128) Linear(128, 2)	GATConv(266,16, heads=16) GATConv(256,4, heads=4) Linear(4, 2, bias=True)	SAGEConv(266, 32) SAGEConv(32, 32) SAGEConv(32, 32) Linear(96, 32) Linear(32, 2)
Other	lr=0.001, bs=64	lr=0.0005,bs=64	lr=0.001, bs=64

Table 2. Neural Network Parameter Settings

Model	MLP
Parameter	Linear(208, 20) Linear(20, 10)

	Linear(10, 1)
Other	lr=0.01,bs=64,activation=LeakyReLu

Model results

Table 3 and Table 4 show the accuracy of each model. It can be seen from the table that under the original data composed of graphs constructed with Pearson coefficients, we directly use traditional machine learning methods SAE, MLP and graph neural networks GCN, GAT to classify and predict graphs. It can be seen that the effect of MLP The worst, the prediction results of GCN and GAT reached about 67%.

After experiments, we designed a 2-layer graph convolution layer for the data enhancement Mixup of the GAT model, and achieved a 3-5% improvement.It has been greatly improved, reaching an accuracy of 72.3%, and it has the best classification ability among all models. It can be seen that the data enhancement method of Mixup is indeed useful for improving the model's performance. The effect is helpful and the generalization ability of the model is improved.

Table 3. The training accuracy rate under the optimal parameters of each model

Graph Classification Model	**Raw Data**			
Model	GCN	GAT	Graph -SAGE	MLP
Accuracy	65.6%	68.9%	63.9%	59.1%
Recall	62.1%	57.1%	33.3%	30.8%
Specificity	68.8%	80.0%	88.2%	88.7%

Table 4. GAT model comparison

Graph Classification Model	**Model comparision**	
Model	GAT	M-GAT
Accuracy	68.9%	72.3%
Recall	57.1%	58.1%
Specificity	80.0%	82.4%

CONCLUSION

This method provides a novel and objective solution for the clinical diagnosis of ASD. Different from the clinical diagnosis method in which doctors inquire subjects with scales according to general standards, this paper innovatively uses fMRI, which is a highly objective medical imaging data, as the basis for diagnosis and treatment, and extracts the functional differences between brain regions of subjects. Sexual connection features are used as the input of the classification diagnosis network model, and are sent to the classification diagnosis model based on graph convolutional neural network proposed in this paper for feature learning and classification diagnosis. The problem of the small number of samples in the dataset is made up for by introducing a data augmentation method, and the accuracy of the improved model is further improved.

But there are still many problems at this stage.Because the ABIDE dataset integrates data collected from 17 organizations, the processes and instruments used by these organizations vary, and the data processing methods vary. Therefore, we will train different models for different sites in the future.

The data sample is rather limited. The sample size of our data set is 618. Compared with the general deep learning data set, the sample size is small. It may fall into the overfitting of the data and the underfitting of the task, and the generalization ability of the model is not enough. We will continue to try in the future. Other data augmentation models.

For the model, by replacing the more advanced convolution kernel, we will get a better graph neural network model, and further train it for our task, so as to improve our work in the model.

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东南大学 SOUTHEAST UNIVERSITY | 东南大学大学生创新创业成果展示

基于图神经网络的儿童自闭症辅助诊断研究

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项目简介

项目根据受试样本的功能性磁共振成像（fMRI）提取出反映大脑拓扑连接结构特征的脑图信号。将图信号以结构化的形式存储并输入GCN中进行参数学习，最终实现训练模型对测试样本的有效分类。具体分为三个步骤：（1）脑区信号提取（2）脑拓扑图构建（3）Graph-CNN得到最终的自闭症分类诊断结果。考虑数据集样本数量远小于传统深度学习数据集样本数，引入数据增强方法GAUG-M和MixUp方法，进一步提高模型精度，为解决自闭症辅助诊断问题提供基于图神经网络模型的深度学习思路方案

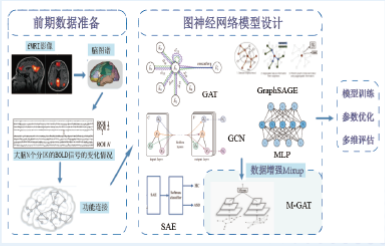

图1 框架流程说明图

研究成果

提出基于图神经网络GAT模型和MixUp数据增强方法的M-GAT模型，对比传统机器学习方法在模型精度上获得显著提升

创新点

（1）辅助诊断。传统自闭症临床诊断中，易受到外界多种因素影响，容易导致误诊。在我们的项目中，我们利用可靠的生物标志物量化为特征，有助于实现更精确的诊断
（2）医学信号的选取。现有自闭症诊断多从脑电信号中提取，空间分辨率有限且信号噪声大。我们选择了核磁共振成像的变体 fMRI，可以较好地捕捉抑郁症患者大脑功能性连接的不规律性
（3）对成像信息的充分利用。主流的自动编码器无法很好的表示空间拓扑信息。我们则使用了功能连接网络，通过图结构充分利用全脑空间信息
（4）使用图卷积神经网络。目前为止的自闭症诊断模型大多采用线性分类器或支持向量机等简单的模型进行训练，我们希望使用图卷积解决模型单一的问题，以达到更高的精确度