

## GCN based Bio-Inspired Classifier for Autism Spectrum Disorder

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Autism spectrum disorder is a diverse neurological state with long-lasting and in most instances lifetime implications for individuals. The early identification and intervention are crucial in mitigating the impact of this disorder, necessitating the development of an objective diagnostic method. This study proposes a novel diagnostic approach that utilizes the data extracted from resting state Functional Magnetic Resonance Imaging (rs-fMRI) and critical phenotypic data of each individual. Recursive feature elimination with Grey Wolf Optimization (GWO) is employed for identifying the optimal attributes from the fMRI data. The selected attributes are then inputted into a Graph Convolution Network (GCN) along with the demographic and basic clinical information for categorization purposes. By utilizing a bioinspired optimization algorithm, the likelihood of identifying the optimal feature subset is enhanced. The study compares the performance of the GCN obtained from the GWO feature selection using both the wrapper and filter approaches. The feature set selected through the GWO wrapper approach demonstrates improved accuracy, achieving 73.86%, along with an AUC of 0.817 when inputted into the Graph Convolution Network. These detections emphasise the significance of an objective and accurate ASD diagnosis method with a limited feature set.

**Keywords:** ASD diagnosis, Feature selection, Functional connectivity, Graph convolution networks, Pre-processed fMRI

### Introduction

Autism Spectrum Disorder (ASD) is a neural brain-based disorder that impairs the communicative coordinates and behavioural patterns that begin before birth or in early childhood. The symptoms usually include poor eye contact, difficulty in communication, restricted interests, monotonous actions, hyperactivity, attention deficit and also difficulty in learning.<sup>1</sup> Though it is a disorder which causes a longitudinal impact on the individual, early diagnosis, interventions and prognosis of the disease can have a long lasting positive effects on the skill development, symptoms and ability to function in an autistic person.<sup>2</sup> Individuals with ASD have several obstacles in their daily lives, and are highly perilous of inheriting comorbidities like epilepsy, anxiety and sleep complaints and attention deficiencies that complicates the process of calibrating the infirmities.<sup>3</sup> ASD causes significant impact on the higher-level functionality of the human brain making it very complex and challenging. Advancements in the

faculty of medical imaging of the brain & neural coordinates related technology have made it possible to evaluate the operational and constructure related alterations correlating with ASD in the last decade, which is a significant step forward.<sup>4</sup> Different sensing mechanisms like Electroencephalography (EEG), Event-Related-Potential (ERP), Functional Magnetic Resonance Imaging (fMRI) detects various patterns in the structure and connections of the brains. Among the many imaging techniques available, fMRI appears to be a promising field in analysing and capturing the interactions between the brain regions.

Over the past few years, machine learning, deep learning and neural networks have become increasingly significant in the field of medicine. Graph based machine learning algorithms are used in several applications specifically in the area of medical diagnosis<sup>5</sup> and signal processing in human brain.<sup>6</sup> Deep learning algorithms are being increasingly utilized in the diagnosis of several diseases including autism. Graphs provide a framework for representing the feature set of each individual patient as nodes and also to capture the interactions between them using the edges. Recently, Graph convolution network has

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been contemplated as a prospering model because of its intrinsic characteristics of dealing with non-Euclidean data.<sup>7</sup> With the advancements in the field of neuro imaging, terabytes of imaging data and other phenotypic data are available for research. The dataset used in this work to study the examination of neurological connectivity in the brain is the ABIDE dataset. Each individual subject has features from both the fMRI analysis of intervals of temporal successions of events and the phenotypic information such as age in months, gender, site acquisition details, Autism Diagnostic Observation Schedule (ADOS) score etc.

Development of several models to detect this disorder has been continuing, but the majority of these models fail to pick the features that form a critical part of the analysis in detecting the presence of autism in the subject leading to poor accuracy, hence feature selection algorithms can be used. The primary objective of any attribute selection method is to lessen the number of features at the same time enhance the performance of the classification.

Meta-heuristic algorithms are frequently used in feature selection and are broadly motivated by natural or biological phenomenon. Metaheuristic algorithms<sup>8</sup> usually take different approaches such as evolutionary<sup>9-12</sup>, physics-based<sup>13,14</sup>, swarm intelligence<sup>15-17</sup>, and human social behaviour.<sup>18</sup> Bio-inspired metaheuristic algorithms have been recognized as an effective optimization algorithm and is widely used in solving complex computational, scientific and medical problems.<sup>19,20</sup> These bio-inspired algorithms have also established a strong foothold in the field of feature selection and feature reduction techniques.

This work combines the benefits of both graph convolutional networks and a biologically inspired grey wolf optimization to improve the efficiency to diagnose ASD. The primary contributions of this work are use of hybrid architecture - combination of Recursive Feature Elimination (RFE) with grey wolf optimization to the GCN architecture in the diagnosis of ASD and efficient modelling of the adjacency matrix of the network based on the phenotypic similarity between the subjects.

The requirement for a more quantitative analysis in the diagnosis has propelled research towards analysing brain imaging data, such as MRI and fMRI. Recently, there has been a growing research focus to analyze the rs-fMRI<sup>21</sup> of the brain to comprehend the

Functional Connectivity (FC) thereby establishing neurological bio-markers which could help in computer aided diagnosis of the disease.

The following section describes the various methodologies that focus on developing a computer aided model for the classification and bio-inspired feature selection strategies that have proven to increase the classification efficiency.

### Deep Learning Models for ASD Diagnosis

Most of the neural network computations employed in the ASD diagnosis are autoencoders based and ConvNet. ConvNets are extensively used in the classification of images by exploiting the information from the image (such as intensity, contrast etc). Convolutional Neural Networks (CNN) is widely utilized in image partitioning, localization and classification as well as in the medical image analysis of brain, lungs and other organs.

Eslami *et al.*<sup>22</sup> proposed an architecture called ASDiag on the ABIDE dataset. The model used the autoencoders to lower the number of dimensions and the resulting data is inputted to the Single Layer Perceptron (SLP) for the classification of the individual subject. Ahmed *et al.*<sup>23</sup> developed an image synthesizer that generated a single volume image of the brain from the complete 4D NIFTI image. The generated image is provided as an input into a convolutional neural network with an ensemble framework. Heinsfeld *et al.*<sup>24</sup> proposed a two stacked denoising auto encoders to transfer 19900 features into a deep learning model and achieving 70% accuracy in ASD diagnosis. However, while the autoencoders were able to learn lower level dimensions in feature representations, they discarded the spatial data structure.

Brown *et al.*<sup>25</sup> proposed a custom-built CNN to leverage on the topological locality of the structural connectivity matrices to learn the cognitive and motor development score. Though CNNs are able to capture the spatial information it is required to modify the existing models to incorporate both the topological features and non-Euclidean data for better generalization.

### Neuroimaging and Graph Convolutional Networks

Though convolutional neural networks have proven highly efficient in understanding the images, there is a significant difference while dealing with medical images because of less discriminative features.<sup>26</sup>

Graph Convolutional neural network generalizes CNN and harnesses the power of the graph network for learning higher dimensional and non-Euclidean data making it more suitable for learning medical images.<sup>7,27</sup> Graph convolutional networks have been extensively used in the field of neuro imaging<sup>28-30</sup> because of the inherent characteristics of representing the human brain and to capture the interactions between the regions.

Bullmore & Sporns<sup>31</sup> studied the functional/structural connectivity in the human brain and it was depicted with the help of the graph networks to understand the structure and connectivity of the whole brain. Parikh *et al.*<sup>32</sup> used graph CNN to combine the power of imaging data as well as non-imaging data especially for medical analysis. Their work was validated against ABIDE dataset and ADNI dataset for Alzheimer. The method achieved 70.4% accuracy for classification with respect to ABIDE dataset.

Kazi *et al.*<sup>33</sup> considered the features of each individual in node and the similarity of two nodes in the edges and focused on the receptive fields of the GCN architecture to enhance its efficiency. Yao *et al.*<sup>34</sup> modelled each graph as a subject with the similarity or the correlation matrix indicating the edges of the graph. The work employed triplet GCN with one anchor, positive and negative sample to predict the disease. Ktena *et al.*<sup>35</sup> developed a model using siamese GCN to assess the similarity between two graphs, each representing brain network connectivity.

### Feature Selection and ABIDE

The process of selecting influential or discriminative features from the fMRI feature set is principal in building a robust classification model. Not all features are necessary in building the classification model. This often results in higher computational complexity, leading to longer training times as the number of features grows. It might not be beneficial to use all of the features adversely it might lead to overfitting the model. This makes it imperative to identify and feed the correct subset of features to the algorithm to enhance its performance. Feature selection algorithms broadly come under three flavours. They are filter methods, wrapper and embedded methods.

RFE, a most prominent wrapper method is used in literature for the feature selection of ASD.<sup>36</sup> Huang *et al.*<sup>37</sup> utilized a methodology based on graphs for

identifying the most discriminative features from pairwise functional connectivity of the ROIs. Graph based KNN algorithm is used to select the top k connections and then classified by a three-layer deep belief network with an accuracy of 0.764. Demirhan<sup>38</sup> used multivariate pattern analysis to primarily determine the significant features observed from brain MRI. Guruvammal *et al.*<sup>39</sup> employed a bio inspired feature selection technique that mimics the levi flight and the cub update behaviour of the lion for choosing the most discriminating features which are then input to the classification algorithm based on neural and deep belief network.

There are many Meta heuristic feature selection algorithms<sup>8-20</sup> such as swarm optimization, genetic algorithm, ant colony and simulated annealing algorithm. However, these metaheuristic algorithms are not much explored in the feature selection approaches for ABIDE. Hence in this work, a combination of recursive feature elimination and binarized grey wolf optimization is used to reduce the features extracted from the functional connectivity of the mean time series ROI. The resultant features of each individual patient and their corresponding phenotypic characteristics are given as input to the graph convolution network which has intrinsic properties to learn data from the individual subject and correlates the similarity between the subjects.

## Materials and Methods

### ABIDE Dataset

ABIDE dataset - Autism Brain Imaging Data Exchange initiative<sup>40</sup> was supported by the lead federal agency of United States named National Institute of Mental Health (NIMH). The institute researches on various mental disorders. They have gathered functional MRI from several laboratories as part of their research study in order to speed up and better understand the neurological foundation of autism. It is a collaborative effort between 16 international sites to share datasets that will aid in diagnosis and targeted treatment using a data-driven approach. The dataset gathered fMRI scan images from 1,112 individuals. Among them, 539 are people with ASD, while 573 were healthy or Typically Developed (TD) people. The dataset contained subjects from age 7 to 64 years with 14.7 years of age as median. The dataset used in the work is a previously pre-processed ABIDE dataset using the configurable pipeline for the analysis of connectomes.<sup>40</sup> The diversity of the data distribution is

elaborated in Table 1. The dataset has ensured diversity of data across different demographics including gender, age group, culturally and geographically different data. Apart from the fMRI features the dataset has also incorporated the phenotypic information of the subject which serves as a valuable input to correlate with the features extracted from the brain images.

#### Deep Bio-inspired Classifier for Autism Architecture

The proposed system uses a deep bio-inspired classifier for detection of autism. The proposed methodology uses the binarized grey wolf optimizer for the feature selection followed by the graph convolution neural network for the diagnosis of ASD. The overall system architecture of the proposed model is represented in Fig. 1.

The proposed architecture has three main phases - functional connectivity computation phase, feature selection phase and deep learning network which incorporates a graph convolution network which is illustrated in the below sections.

#### Functional Connectivity Computation Phase

Time series data can be analyzed as either individual voxel-data or region based data. In this work, the Regions of Interest (ROIs) based analysis is employed as they directly study and identify the network of regions that are more functionally correlated. The cluster of voxels forms an ROI and is marked based on the neuroanatomical atlas templates. The time-series data is extracted from ROI and the mean of the time series information for the ROI is computed. Functional connectivity matrix is derived using the Pearson correlation index amidst the mean time-series of two regions of interest. The correlation coefficient is calculated for two distinct regions' time series data using the Eq. (1), where,  $i_t$  and  $j_t$  represents the time-series information of  $i$  and  $j$  region at time  $t$  where,  $\bar{i}$  and  $\bar{j}$  are the respective mean time series.

$$P_{ij} = \frac{\sum_{t=1}^T (i_t - \bar{i})(j_t - \bar{j})}{\sqrt{\sum_{t=1}^T (i_t - \bar{i})^2} \sqrt{\sum_{t=1}^T (j_t - \bar{j})^2}} \quad \dots (1)$$

Table 1 — ASD/TD Data Distribution across demographic sites

Site	Avg_Age (years)	ASD_Male	ASD_Female	TD_Male	TD_Female
CALTECH	27.4	15	4	15	4
CMU	26.4	11	3	10	3
KKI	10	18	4	24	9
LEUVEN	17.8	26	3	30	5
MAX MUN	26.1	21	3	29	4
NYU	14.7	68	11	79	26
OHSU	11.4	13	0	15	0
OLIN	16.5	17	3	14	2
PITT	19	26	4	23	4
SBL	35	15	0	15	0
SDSU	14.7	13	1	16	6
STANFORD	10	16	4	16	4
TRINITY	16.8	24	0	25	0
UCLA	13	55	7	41	6
UM	13.2	58	10	59	18
USM	23.5	58	0	43	0
YALE	12.7	20	8	20	8

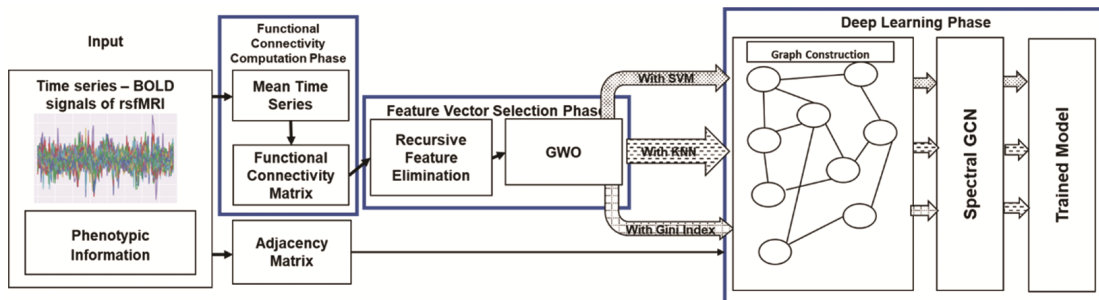


Fig. 1 — System architecture of the proposed model

Algorithm 1: Algorithm of the proposed model

**Input**

Timeseries data of the registered region obtained from Images

Phenotypic data of the corresponding individual

**Output**

Class Label – ASD or TD

**Algorithm**

# N ← Total Number of Subjects

# R ← Total Regions from Harvard\_ Oxford Atlas\_Image\_Registration

# rfe\_num ← Tot.No of Features selected from Recursive Feature Elimination

for each subject  $i \in N$

for each region  $r_j \in R$

$m_{r_j} \leftarrow \text{Mean}_{\text{Timeseries}(r_j)}$

Compute Functional Connectivity Matrix

$$FC_i = \begin{bmatrix} C_{11} & C_{12} & \dots & C_{1r} \\ C_{21} & C_{22} & \dots & C_{2r} \\ \dots & \dots & \dots & \dots \\ C_{r1} & C_{r2} & \dots & C_{rr} \end{bmatrix}$$

where  $C_{jk} \leftarrow \text{Pearson\_Corr\_Coef}(m_{r_j}, m_{r_k})$

Feature\_Vector<sub>i</sub> ← Upper\_Triangular\_Matrix (FC<sub>i</sub>)

Selected\_features ← Recursive Feature Elimination (Features, rfe\_num)

Optimum\_Features ← Binarized Grey wolf Optimization (Selected\_features)

for each feature vector<sub>i</sub>, construct a node  $n_i$  ( $i \leftarrow 1$  to N)

Compute adjacency matrix, A

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \dots & a_{2n} \\ a_{n1} & a_{n2} & \dots & \dots & a_{nn} \end{bmatrix}$$

$$a_{ij} = \text{Sim}_{FV}(n_i, n_j) \times \text{Sim}_{PM}(n_i, n_j)$$

where,  $\text{Sim}_{FV}(n_i, n_j) \leftarrow$  Similarity measure based on optimal feature vectors

$\text{Sim}_{PM}(n_i, n_j) \leftarrow$  Similarity between the nodes based on phenotypic information

Diagnostic Results ← Graph\_Convolution\_Network (n, A)

**Feature Vector Selection Phase**

To address a feature vector size N, the method employs a two-step feature selection process to systematically explore the extensive space of 2N for

optimal features. A total of 6105 features are derived from each subject's functional connectivity matrix. In the first step, 6105 features are given as an input to the recursive feature elimination algorithm and in the next step the output of the recursive feature elimination is given to the wrapper based Binarized Grey Wolf Optimization strategy (B-GWO) to further identify the most discriminative features.

**recursive feature elimination**

The feature vector extracted from the pairwise time series correlation of the ROIs is given as an input to the recursive feature elimination (RFE).<sup>41</sup> Each iteration of the RFE is trained based on the ridge classifier's coefficient. The feature count is reduced to 2000 using recursive feature elimination.

**binarized grey wolf optimization**

The binary variant of the GWO is implemented in the proposed method for the feature selection. The features extracted from the recursive feature elimination are then fed into the binarized grey-wolf optimization algorithm. GWO is an evolutionary computational technique proposed by Mirjalili *et al.*<sup>17</sup> which mimics the behaviour of grey wolves. They typically live in a pack of 5 to 12 wolves. Alpha ( $\alpha$ ) wolf is primarily responsible for making decisions and is considered as the chief of the pack of wolves. Beta ( $\beta$ ) or second in command level wolves assist the alpha in discerning their choices. The delta ( $\delta$ ) wolves occupy the third level and the least positioned grey wolf is omega ( $\omega$ ) and must follow the orders from the remaining wolves. The hunting behaviour of the wolf are searching the prey, tracking, chasing, encircling and attacking the prey.

**Problem formulation:** In this algorithm, the feature vectors are the values of the FC matrix obtained out of the timeseries data of the rs-fMRI. Initial State: The pack of wolves will be initialized. Each wolves take a position value initially which is the random assignment of ones and zeros for the 2000 features from the recursive feature elimination. The value of each wolf is updated using the BGWO algorithm. Goal Test: The algorithm runs until the fitness function converges. Final State: The optimal set of features selected that returns the best fitness value.

The feature representation of the grey wolf is indicated in Table 2. The population size of the wolves is N with the first three wolves representing

Table 2 — Feature representation as position of grey wolf

Wolf	F1	F2	F3	F4	F5	F6	...	F2000
1( $\alpha$ )	1	0	1	0	1	1	...	1
2( $\beta$ )	1	1	0	0	1	0	...	0
3( $\delta$ )	0	1	1	1	0	0	...	1
4( $\omega$ )	1	1	0	0	1	0	...	0
5( $\omega$ )	1	1	0	0	1	0	...	1
.	.	.	.	.	.	.	...	.
.	.	.	.	.	.	.	...	.
N( $\omega$ )	1	1	1	0	1	0	...	0

the optimal feature set at the end of each iteration. A value of one indicates the feature is chosen, whereas zero indicates it is not.

In the hunting process, grey wolves surround their prey and the corresponding expression of their hunting behaviour is formulated using  $\vec{D}$  which calculates the difference between the prey and the grey wolf in Eqs (2 & 3). The vectors  $\vec{A}$  and  $\vec{C}$  represents the coefficients and are calculated using Eqs (4 & 5)

$$\vec{D} = |\vec{C}\vec{X}_{ploc}(iter) - \vec{X}(iter)| \quad \dots (2)$$

$$\vec{X}(iter + 1) = \vec{X}_{ploc}(iter) - \vec{A}\vec{D} \quad \dots (3)$$

$$\vec{A} = 2a \cdot \vec{r}_1 - a \quad \dots (4)$$

The parameter ‘a’ mentioned in Eq. (4) is used to control the balance involving exploration and exploitation factor and is linearly decreased from [2, 0].

$$\vec{C} = 2\vec{r}_2 \quad \dots (5)$$

where,  $\vec{r}_1$  and  $\vec{r}_2$  are random vector [0,1].

where,  $\vec{X}(iter + 1)$  represents the location of the wolf and  $\vec{X}_{ploc}(iter)$  indicates the prey’s location.

After each iteration, the top performing wolves  $\alpha, \beta$  and  $\delta$  are chosen and the remaining wolves revise their position in line with the top wolves’ position based on Eqs (6 – 12)

$$\vec{D}_\alpha = |\vec{C}\vec{X}_\alpha(iter) - \vec{X}(iter)| \quad \dots (6)$$

$$\vec{D}_\beta = |\vec{C}\vec{X}_\beta(iter) - \vec{X}(iter)| \quad \dots (7)$$

$$\vec{D}_\delta = |\vec{C}\vec{X}_\delta(iter) - \vec{X}(iter)| \quad \dots (8)$$

The position of the first three wolves is updated using Eqs (9 – 11)

$$\vec{X}_1 = \vec{X}_\alpha(iter) - \vec{A}_1 \cdot \vec{D}_\alpha \quad \dots (9)$$

$$\vec{X}_2 = \vec{X}_\beta(iter) - \vec{A}_2 \cdot \vec{D}_\beta \quad \dots (10)$$

$$\vec{X}_3 = \vec{X}_\delta(iter) - \vec{A}_3 \cdot \vec{D}_\delta \quad \dots (11)$$

The position of the grey wolf is updated using Eq. (12) to maintain the binary state for the feature selection.

$$x_d^{t+1} = \begin{cases} 1 & \text{if } \text{sigmoid}\left(\frac{x_1+x_2+x_3}{3}\right) \geq \text{rand} \\ 0 & \text{otherwise} \end{cases} \quad \dots (12)$$

#### Algorithm 2: Binarized Grey Wolf Algorithm

##### Input:

Set  $N_{iter} \leftarrow$  No of Iterations

Set  $N \leftarrow$  No of grey wolves in the pack

##### Output:

Optimal Feature set,  $f(\alpha)$  best fitness value

##### Algorithm:

1. Initialize the position of the grey wolf population  $X_i$ ,  $i$  from 1 to 10
2. Initialize with random values for the  $\vec{X}_\alpha, \vec{X}_\beta$  and  $\vec{X}_\delta$  positions
3. Initialize  $a, A$  and  $C$  using the Eqs (4 & 5)
4. Calculate the fitness of each grey wolf using the Eq. (13)
5. Calculate the  $\alpha, \beta$  and  $\delta$  based on the fitness value
6. while ( $t <$  Max number of iterations)
7. for each wolf ( $\omega \in$  pack) do
8. Update the position of the wolves using Eq. (12)
9. Update  $a, \vec{A}, \vec{C}$  using the Eqs (3 & 4)
10. Calculate the fitness of all the wolves using the Eq. (13)
11. Update  $\vec{X}_\alpha, \vec{X}_\beta$  and  $\vec{X}_\delta$  positions using the Eqs (9 – 11).

The wrapper method uses a learning algorithm to assess the selected subset of the feature vector. The fitness functions used in the binarized grey wolf optimization are the classification accuracy of the K nearest neighbour and SVM in the wrapper method and gini-index in the filter method. The fitness function used is a combination of the classification accuracy and the ratio of the selected to the total features and is given in Eq. (13)

$$\text{Fitness Function} = \alpha \gamma_R + \beta \frac{|N-R|}{|N|} \quad \dots (13)$$

$$\gamma_R = \frac{TP+TN}{TP+FN+FP+TN} \quad \dots (14)$$

$\gamma_R$  in the Eq. (14) denotes the classification accuracy of KNN and SVM respectively.  $|N|$  indicates the count of the total features and  $|R|$

indicate the count of the nominated features. The classification accuracy is evaluated with the True Positive (TN), True Negative (TN), False Positive (FP), False Negative (FN). The algorithm stops running once the fitness function converges. The best wolf position at the end of the algorithm will be selected subset features.

#### Deep Learning Network Phase

Graph Convolution Network is a modified graph based neural network that does a convolution on a graph instead of a pixel image. Graphs are mathematical structure that captures the information about a node and the interactions between the nodes. The GCN runs a filter over the graph, searching for critical vertices and edges that can assist in classifying nodes within the graph. A graph  $G = (V, E)$  where  $V = \{v_i | i \in \{1, \dots, N\}\}$  and  $E = \{e_{ij} | \forall i, j \in \{1, \dots, N\}\}$  with the  $v_i$  indicating the feature vectors of the  $subject_i$  and  $E$  indicating the adjacency matrix. Constructing the population graph is critical for the method's success, as an inadequately constructed graph will hinder GCNs from reaching their full potential. Incorrect graph construction corresponds to performing image convolutions on unrelated data instead of the desired image patch.

The two key decisions that must be made in order to construct the population-graph model are 1) Formulation of the feature vector  $x(v)$  representing the characteristics of the individual subject in each graph node and 2) The adjacency matrix of the graph constituting the edges  $E$  and the corresponding weights  $W$ , which exhibits the correlation between the subjects and its associated features. The feature vector corresponds to the optimal feature set returned by the Binary GWO.

#### Adjacency Matrix Construction

The graph's adjacency matrix is constructed based on similarity of the subjects in terms of imaging features and its phenotypic similarity using the Eq. (15). The phenotypic information describes the similarities between various subjects in terms of Age, Gender, ADOS Score, etc. Adding these features<sup>42</sup> has proven to be advantageous in terms of increasing the accuracy. The phenotypic information taken into consideration for the adjacency matrix construction.

$P = \{Age, Sex, Handedness, Full IQ\}$ . The adjacency matrix,  $A$  is defined in Eq. (15).

$$A(v, w) = Sim(S_v, S_w) \sum_{p=1}^P \gamma(M_p(v), M_p(w)) \dots (15)$$

$Sim(S_v, S_w)$  is the similarity between the subjects in-terms of the feature vector.  $\gamma(M_p(v), M_p(w))$  denotes the similarity in terms of phenotypic measure as per the Eqs (16 & 17).

if  $p \in \{Sex, Handedness\}$

$$\gamma(M_p(v), M_p(w)) = \begin{cases} 1 & \text{if } M_p(v) = M_p(w) \\ 0 & \text{if } M_p(v) \neq M_p(w) \end{cases} \dots (16)$$

if  $p \in \{Age at Scan, Full IQ\}$

$$\gamma(M_p(v), M_p(w)) = \begin{cases} 1 & \text{if } |M_p(v) - M_p(w)| < \text{threshold} \\ 0 & \text{Otherwise} \end{cases} \dots (17)$$

#### Graph Convolution Networks

The first layer of the graph convolution is as follows

$$h^{(1)} = \sigma(A X W^0) \dots (18)$$

where,  $W^0$  indicates the weight matrix containing the trainable parameters at the first layer,  $A$  denotes the adjacency matrix and  $X$  denotes the feature description and, in this work, functional connectivity measure is used as an input feature. The activation function  $\sigma$  in Eq. (18) refers to the ReLU function.

The higher-order features are aggregated from the neighbours by stacking layers and is mathematically denoted as in Eq. (19)

$$h^{(l+1)} = \sigma(\hat{A} h^{(l)} W^{(l)}) \dots (19)$$

$h^{(l)}$  indicates the previous layer's output,  $l$  indicates the number of layers,  $W^{(l)}$  indicates the weight matrix of trainable parameters at the layer  $l$ .  $\hat{A}$  in Eq. (19) denotes the normalized adjacency matrix with self-loops. At each iteration, the hidden states of the nodes are updated by the weighted sum of the features of their neighbour.

$$\hat{A}_i h^{(l)} = \sum_{k=1}^n A_{i,k} h_k^{(l)} \dots (20)$$

Every node within the graph corresponds to the subject and the graph is partially labelled. After training the unlabelled nodes are labelled as either ASD or TD subject.

#### Results and Performance Analysis

The functional connectivity matrix of each individual node corresponds to 6105 features. The

Recursive feature elimination reduces features from 6105 to 2000 features. BGWO further reduces the feature set and the feature subset size using the different classifiers is given in Table 3.

The reduced feature set is given as input to the GCN along with the adjacency matrix. In GWO, the number of wolves is chosen to be ten after comparing the accuracy of GWO for different number of wolves as illustrated in Fig. 2.

The parameter settings for the graph convolution network are shown in Table 4. It is seen that the GCN produces an overall accuracy of 73.86% when combined with RFE and GWO using SVM as the classifier.

The existing work with the GCN using the ABIDE Dataset<sup>43</sup> has achieved an accuracy of 70%. The grey wolf optimization is applied to analyze the impact of bio-inspired optimization to the ABIDE dataset. The comparison of the performance of different feature selection approaches in conjunction with the GCN for the ABIDE dataset is illustrated in Table 5.

The training and validation accuracy over 100 epochs is depicted in Fig. 3 and it shows that validation accuracy is better than the training accuracy. The model’s results on the training and the validation datasets are close to each other suggesting that the model is well-trained and generalizes well to unseen data. It can also be inferred that the model has achieved a balance

between underfitting and overfitting. The results show an accuracy of 73.86% which demonstrates an increase of 3% accuracy from the plain GCN model. The fitness function, utilizing SVM as the wrapper function as in Eq. (13) converges to a feature subset size of 926.

**Scalability and Generalizability**

The proposed framework used GCN to capture the complex relationship between brain features. Each node of the graph comprises features extracted from an fMRI of a single subject. The edges between the nodes represent the similarity between the two nodes/subjects which is represented by using the adjacency matrix. The phenotypic information such as

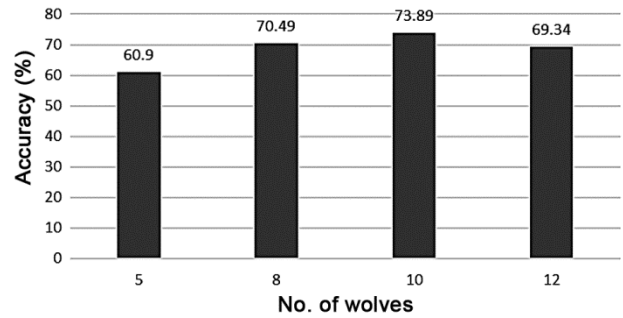


Fig. 2 — Accuracy of the model Vs number of wolves

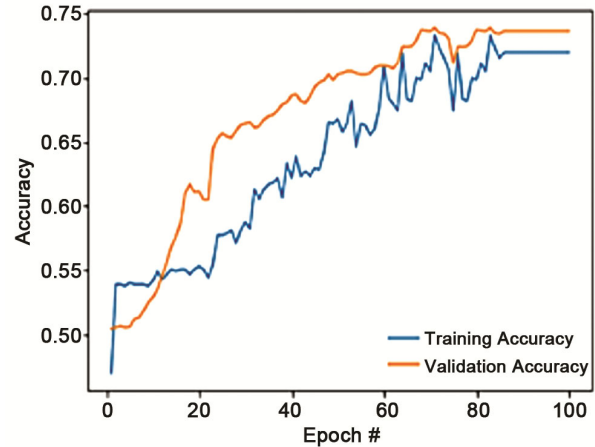


Fig. 3 — Accuracy of the model Vs epochs

Table 3 — Feature selection in BGWO

Fitness function	Method	Feature subset size
K-Nearest neighbor	Wrapper	555
Support vector machine	Wrapper	926
Gini index	Filter	553

Table 4 — GCN model parameters

Hyperparameter	Value
Learning rate	0.005
Dropout	0.3
Hidden layers	16
Activation function	Relu and SoftMax
Epochs	150

Table 5 — Comparison of ASD diagnosis using different fitness function

Measure	RFE+GCN	GWO+GCN (Wrapper method)		GWO+ GCN filter method Gini index
		Classifier	Classifier	
Accuracy	69.34	KNN 71.59	SVM 73.86	70.46
Area under curve	0.716	0.762	0.817	0.735
Precision	62.36	72.99	73.26	70.89
Recall	60.23	65.90	71.25	63.89
Specificity	63.64	75.00	73.92	73.87

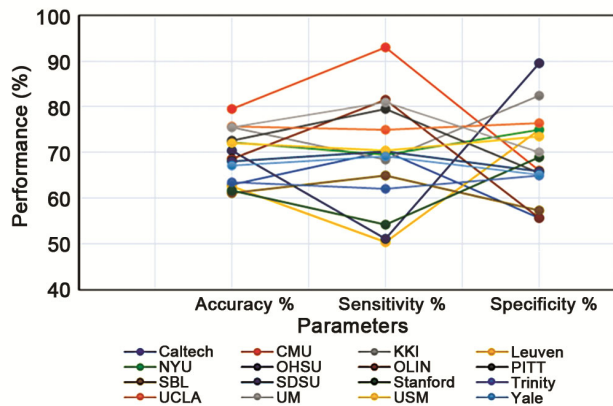


Fig. 4 — Site wise performance (Accuracy, Sensitivity and Specificity) analysis of the sites

Age, Gender, ADOS score and clinical information is used in computing the similarity between the nodes. The weight of the edge is assigned based on the similarity between two nodes' demographic and clinical data. When the nodes are not similar, the adjacency matrix will contain a value of zero. Thus, instead of using a fully connected graph, the approach uses a sparse connection based on the similarity matrix. The approach is scalable for larger datasets as new subjects can be added as a node. While there are no upper limits on the number of nodes in the graph, its performance varies with the computing resources and similarity between the nodes. To ensure that the framework generalizes well across different populations, the model is trained using the ABIDE dataset, which is the largest publicly available collection of fMRI images from individuals with diverse socio-cultural backgrounds, genders, and age groups.

#### Clinical Impact of fMRI-based ASD Diagnosis

In the proposed work, rs-fMRI images are leveraged to understand the correlations of the brain regions to the diagnosis of ASD. Rs-fMRI contains a multitude of features that can be challenging to analyze in their entirety proposed work uses hybrid architecture of GWO with RFE to extract the most informative features. This feature selection process helps reduce dimensionality and retain the most critical information for further analysis. These selected features along with their phenotypic features are given as input to the GCN for classification of the disease. Integrating non-invasive neuroimaging techniques such as fMRI-based analysis into the clinical practice helps avoiding misclassification due to the subjective

perception of the clinician and will help in more accurate and early diagnosis of the disease. Although this study is used in the diagnosis of autism, it can also be extended to investigate the functional and structural alterations in the brain of an autistic person, understand the prognosis of the condition over time. This makes the proposed work not only valuable for initial diagnosis but also a potential tool for long-term monitoring and understanding of the disorder.

The ABIDE dataset is a consortium of 16 sites and the site wise analysis is depicted in Fig. 4 as a line graph indicating the accuracy, sensitivity and specificity of data from each site. The accuracy across different research sites ranges from 61% to 76%. Sites such as KKI, UM, and UCLA, which have a more balanced distribution of ASD and TD participants, demonstrate higher accuracy (76%). This suggests that a more representative sample of both ASD and TD groups may lead to better generalization and improved model performance. On the other hand, sites like SBL and Stanford, with more uneven participant distributions (e.g., zero female participants in some categories), show lower accuracy scores (61% and 62%). This indicates that a more balanced representations of each class leads to better accuracy.

#### Conclusions

This study presents a GWO-GCN hybrid framework for diagnosing Autism Spectrum Disorder (ASD), achieving 73.86% accuracy by refining feature selection from fMRI data with RFE and BGWO, surpassing the baseline GCN model's 69.36% accuracy. The improved accuracy indicates that the well selected features substantially increase the performance. However, one limitation is that ASD subjects often struggle to remain still during scans, which affects data quality despite efforts for motion correction. The cross-sectional design based on single-scan fMRI data, limits longitudinal insights that could reveal brain changes over time. Future research aims to examine brain's region-specific features and correlate ASD severity with areas like the cerebral cortex, basal ganglia, and amygdala, which are essential for communication, motor skills, and social interaction. Mapping neural connectivity in these areas could enable more tailored diagnostics and treatments, while longitudinal studies may further enhance developmental outcomes by tracking brain development and therapy response in ASD individuals.

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