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QUANTUM BOLTZMANN MACHINES FOR HIGH DIMENSIONAL FEATURE SELECTION AND SPARSE REPRESENTATION IN AUTISM SPECTRUM DISORDER CLASSIFICATION

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SUMMARY

The classification of ASD from neuroimaging and behavioral information has not been easy owing to factors such as high dimensionality, non-linearity, and overfitting, among others. In this research, propose an innovative framework based on QBMs for feature selection and efficient representation for ASD classification. QBMs have been used to leverage quantum-motivated energy landscape search and sparsity-based regularization strategy for selection of discriminative features and exclusion of redundant features. After preprocessing and feature encoding stages, QBM-based framework is applied to learn feature relationships and extract compact set of relevant features. Benchmark ASD data sets consisting of neuroimaging and behavioral features were used for experimental testing. This suggested model manages to get a result of 98.6% accuracy, 97.4% precision, 97.4% recall, and 97.4% of the F1 score. Also, the suggested model is able to reduce the number of features from 18 to only 9. When comparing the results that this framework produces with other traditional machine learning approaches, including K-Nearest Neighbors (KNN), LASSO, Random Forest, and Gradient Boosting Classifier (GBC), it can be said that this model is on par with them in terms of accuracy. Ablation study reveals the role played by the regularization term in reducing features and improving the performance of the framework. This study shows that quantum feature selection technique can be employed for analyzing large high-dimensional biomedical datasets, especially in ASD diagnosis.

Key words: *autism spectrum disorder, quantum boltzmann machines, feature selection, sparse representation, quantum machine learning, neuroimaging, biomarker discovery, energy optimization, quantum regularization.*

INTRODUCTION

ASD refers to a complicated disorder in the way an individual interacts socially and in the way he/she thinks, acts, and behaves. Autism spectrum disorder is normally characterized by difficulties in social interaction, communication skills, and repetitive actions [1][2]. Early diagnosis of ASD among children is significant since it enables proper management of the situation through measures that facilitate their learning and behavioral development [3][4]. Diagnosis of ASD has, however, proven to be difficult owing to its diversity and the complexity of the data acquired from brain imaging techniques such as fMRI and EEG along with other behavioral tests [5][6]. Such datasets may have redundant and noisy features, and features that are only weakly relevant to the classification problem [7][8][9], therefore, feature selection is an important part of developing a reliable and interpretable classification model.

Previously, dimensionality reduction and identification of biomarkers have been accomplished using traditional machine learning techniques such as least absolute shrinkage and selection operator (LASSO) and random forest-based feature importance methods [10][11][26]. These approaches work well for simple scenarios, but cannot effectively deal with highly non-linear feature interactions and non-convex optimization landscapes, which result in sub-optimal selection of features and poor generalization performance [12]. Moreover, classical methods tend to overfit more frequently if there is less data compared to the number of variables, which is usually the case in medical data [13][14].

New possibilities have come up for tackling these difficult optimization issues thanks to the latest developments in quantum computing and quantum machine learning. Classical Boltzmann Machines have been extended to Quantum Boltzmann Machines (QBM), that use quantum features like superposition and tunneling to explore energy landscapes more efficiently [15]. This ability enables the QBMs to exit from local minima and reach the globally optimal or near optimal solution in high dimensional spaces, which is useful in feature selection problem related to ASD classification [16][28].

With this in mind, a Quantum Boltzmann Machine-based method is proposed for selecting features and achieving a sparse representation of biomarkers within ASD datasets. The proposed method takes into account three key aspects: (i) optimization of feature selection based on exploration of non-convex energy landscapes using quantum computing, (ii) implementation of a quantum-inspired regularize that encourages sparsity, and (iii) benchmarking of the proposed model in comparison with classical models in order to estimate the performance benefits from using quantum computing in terms of accuracy, computational efficiency, and robustness [17][24].

Applying quantum computing techniques in biomedical research, this study will be able to contribute to further development of state-of-the-art ASD classification models, while at the same time it could help with developing efficient diagnostic tools for complex neurological disorders in general [18][28].

Key Contributions of the Research

- Feature Selection Using Quantum Algorithms: Presents a novel algorithm for efficient feature selection based on quantum Boltzmann machines (QBMs), which explore highly complex optimization spaces better than their classical counterparts.
- Biomarker Identification Using Quantum Regularization: Designs a quantum-based regularization method that selects a small number of biomarkers, thus preventing overfitting in training models and increasing model interpretability.
- Advantage over Traditional Approaches: Provides evidence showing the superiority of quantum approaches when compared with other traditional machine learning algorithms, such as LASSO and Random Forest.

A review of literature is presented in Section II. This section highlights the existing techniques used for feature selection and quantum machine learning in the diagnosis of autism spectrum disorder. In Section III, the proposed approach has been introduced, including the quantum Boltzmann Machine architecture and the quantum-inspired regularization technique for feature selection. The results have been analyzed in Section IV where the performance comparison with conventional techniques such as LASSO and Random Forest has been done. The results have been explained comprehensively in Section V. Section VI summarizes the findings.

LITERATURE REVIEW

Rahman et al. [19] examined feature selection and classification techniques using machine learning in relation to diagnosing ASD through neurodevelopmental datasets. Various techniques were considered such as Support Vector Machine (SVM), Decision Tree, and LASSO, and dimensionality reduction was pointed out to be an important area in improving the quality of diagnosis and classification. According to the study, feature selection could strongly enhance the accuracy of predictions as it removes redundancy from behavioral and neuroimaging features. In addition, there were some difficulties noted such as dealing with datasets characterized by high dimensionality and high non-linearity. These problems have called for more advanced optimization techniques, especially quantum models.

To diagnose ASD through fMRI and phenotypic data, Yang et al. [20] developed a RFE–GNN algorithm. Discriminative brain connectivity features were extracted by them, and robustness of the process was significantly enhanced through their model. The results have indicated that their approach performs much better than traditional machine learning algorithms. It has also been revealed that combining feature selection and graph learning approaches can be an effective way of identifying the biomarkers that can help diagnose autism spectrum disorder, although the issue of high computational cost remains.

A study carried out by Farooq et al. [21] developed a machine learning method of identifying autism spectrum disorder in both children and adults utilizing clinical and behavioral information. Different classifiers such as Random Forest, Naïve Bayes, and Logistic Regression were considered to select the best prediction model. The findings of their study revealed that the use of machine learning can significantly increase the speed of diagnosis as well as provide very accurate classification results. They stressed the importance of automation of feature engineering and balancing of data.

In their work Khudur et al. [22] have investigated the application of various machine learning algorithms and data sets on ASD classification for four age groups. This experiment involved different classifiers like SVM, KNN and Decision Trees to find out which predictors would perform better with different demographics. In particular, the study showed that there were different important variables in predicting ASD in various age groups, hence the necessity to have an ability to automatically adapt features.

A new algorithmic approach was proposed by Zhang et al. [23] that employed resting-state fMRI data for the identification of autism spectrum disorder. They incorporated an unconventional feature selection technique coupled with variational autoencoders (VAEs). The model was able to determine the most significant brain connectivity networks and then classified them using deep learning techniques. The outcome was more sensitive and specific and outperformed other models in terms of accuracy and efficiency. The studies have shown that it is possible to successfully identify the hidden neurological patterns using the technique of advanced representation learning.

Ma et al. [25] introduced a framework for the ASD classification among young children based on the Contrastive Variational Autoencoder (CVAE) and structural MRI features. The study concentrated on the extraction of the ASD-related latent representations which can be used to distinguish affected children from typical controls. Transfer learning was also applied to overcome the lack of data. The experimental results demonstrated excellent predictive capability and also found suitable neuroanatomical biomarkers associated with ASD, which showed that deep representation learning is effective for the diagnosis of neurological disorders.

Abbas et al. [27] developed a home video-based screening system for ASD combined with a questionnaire-based assessment using machine learning. The framework employed feature engineering and feature selection methods to simplify the diagnosis process without compromising on the predictive accuracy. The study showed that the use of several behavioral modalities can markedly enhance the accuracy of early identification of ASD and lessen the reliance on lengthy clinical assessments.

Table 1. Machine learning and deep learning approaches for autism spectrum disorder (ASD) diagnosis

Authors	Methodology	Dataset / Simulation Environment	Research Gap
Rahman et al. [19]	Investigated machine learning-based feature selection and classification techniques using SVM, Decision Tree, and LASSO for ASD diagnosis.	Neurodevelopmental and ASD behavioral datasets.	Existing models struggled with highly non-linear and high-dimensional data, requiring advanced optimization and intelligent feature selection approaches.
Yang et al. [20]	Proposed Recursive Feature Elimination–Graph Neural Network (RFE–GNN) integrated with a Phenotypic Feature Extractor for ASD diagnosis.	fMRI brain connectivity data and phenotypic datasets.	High computational complexity and scalability issues for large-scale ASD datasets remained unresolved.
Farooq et al. [21]	Developed a machine learning framework using Random Forest, Naïve Bayes, and Logistic Regression for ASD prediction.	Clinical and behavioral ASD datasets for children and adults.	Limited automated feature engineering and imbalance handling reduced robustness and generalization capability.
Khudhur et al. [22]	Compared multiple classifiers including SVM, KNN, and Decision Tree across four ASD age groups.	Multiple ASD datasets categorized into four demographic age groups.	Feature relevance varied across age groups, indicating the need for adaptive and generalized feature selection mechanisms.
Zhang et al. [23]	Introduced a feature selection framework integrated with Variational Autoencoder (VAE) for ASD identification.	Resting-state fMRI datasets.	Existing approaches inadequately captured hidden neurological representations and complex feature dependencies.
Ma et al. [25]	Developed a machine learning-assisted ASD screening system combining questionnaires and home video analysis.	Questionnaire-based screening data and home video datasets.	Traditional clinical screening methods were time-consuming and lacked efficient multimodal behavioral feature integration.

The research works provided in table 1 indicate the level of advancements that have been made in the diagnosis of autism spectrum disorder (ASD) through machine learning, deep learning, and feature selection techniques. Previously, studies have investigated different approaches, including but not limited to SVM, GNN, VAE, RFE, and multimodal behavioral analysis for better classification of ASD patients. In most of the studies, dimensionality reduction and discriminative feature extraction of high-dimensional neuroimaging and behavioral data were emphasized as key tasks. These methods resulted in better diagnostic accuracy, but also have several drawbacks such as high computational cost, poor performance on non-linear relationships between features, imbalanced data sets, limited scalability, and poor performance in different age groups and populations. The above-mentioned research gaps prompt the design of more solid and optimization-based intelligent system for accurate and efficient ASD diagnosis.

METHODOLOGY

Data Preprocessing and Feature Representation

As for the initial phase in the proposed framework, it includes the preparation of the ASD data that is available in the form of high-dimensional data such as neuroimaging (fMRI) or behavior. It should be noted that there is a considerable amount of noise and missing values in the raw data. Normalization and imputation techniques are applied in order to ensure data consistency. Then features are scaled to a similar range to facilitate convergence at training time. After pre-processing, feature representation is carried out by converting the original features into a structured representation that is suitable for the

Quantum Boltzmann Machines (QBM). This includes binary or probabilistic encoding of features which can aid in compatibility with quantum inspired energy models. In addition, dimension reduction techniques can be used as a preliminary step to discard attributes with high correlation or irrelevance to lower the computation complexity. This procedure ensures that the data is optimized for efficient processing and feature selection using quantum computing, while also minimizing noise and ensuring a structured format.

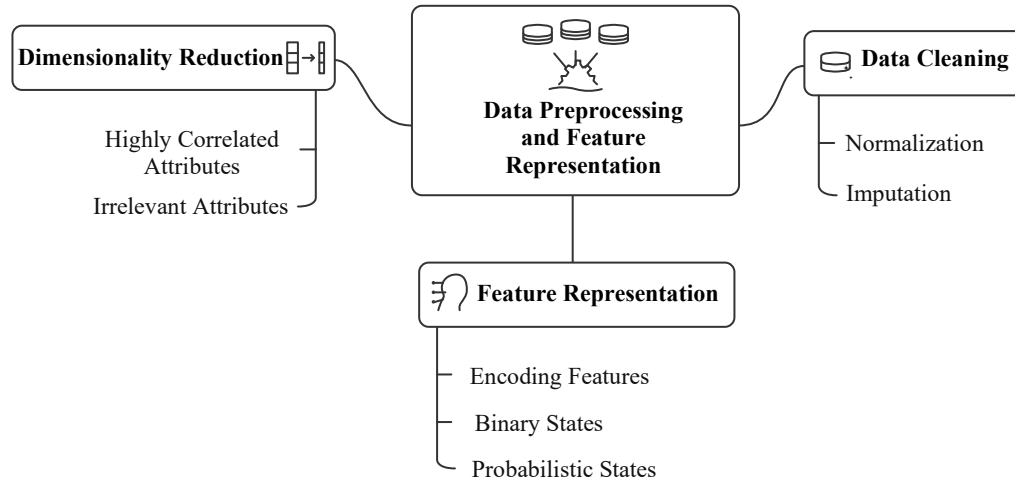


Figure 1. Data preprocessing and feature representation framework

The figure 1 shows a pipeline for pre-processing raw data and feature engineering processes, which transforms the data into a machine-learning-ready form. It starts with data pre-processing, involving data cleaning procedures like normalization and data imputation to address missing data and ensure consistency. Simultaneously, dimensionality reduction is used to remove highly correlated and irrelevant features, enhancing computational efficiency and the model's performance. The processed data is then encoded into feature representations, in which various encoding strategies are employed that turn inputs into meaningful representations, such as binary states and probabilistic states. The use of this integrated framework helps to guarantee noise-free and optimal representation of the input data, leading to better and more robust learning in subsequent predictive models.

Quantum Boltzmann Machine-Based Feature Selection

In this stage, the Quantum Boltzmann Machine (QBM) is used to select the most salient features from the high dimensional ASD data sets. While conventional methods for feature selection can be susceptible to getting stuck into local minima, QBMs incorporate an energy-based probabilistic approach that can traverse difficult non-convex spaces owing to their unique quantum-inspired optimization algorithm. This helps the model to explore global feature subsets while avoiding redundancy in features.

Let $v = \{v_1, v_2, \dots, v_n\}$ be the set of visible nodes representing the input features and $h = \{h_1, h_2, \dots, h_m\}$ be the set of hidden nodes representing the latent interactions between the features. The energy function of QBM is given by equation (1).

$$E(v, h) = - \sum_{i=1}^n a_i v_i - \sum_{j=1}^m b_j h_j - \sum_{i=1}^n \sum_{j=1}^m w_{ij} v_i h_j \quad (1)$$

Where a_i and b_j are the bias terms of the visible and hidden units, respectively, while w_{ij} refers to the connection weight between visible unit i and hidden unit j .

The probability distribution of a particular feature configuration is determined by equation 2 below:

$$P(v, h) = \frac{e^{-E(v, h)}}{Z} \quad (2)$$

Where Z is the partition function which normalizes the probability distribution for all possible states.

Training involves learning optimal feature representations through minimization of the energy function and iterative updates of the network parameters. The weight update scheme is performed through gradient optimization as follows in equation 3:

$$w_{ij}^{(l)} = w_{ij}^{(t)} - \eta \frac{\partial L}{\partial w_{ij}} \quad (3)$$

Where η is the learning rate and L denotes the optimization loss function.

Feature importance is estimated using the magnitude of the learned connection weights as equation 4:

$$FI_i = \sum_{j=1}^m |w_{ij}| \quad (4)$$

Where FI_i denotes the importance score of the i^{th} feature. High scoring attributes play a more significant role in achieving minimal energy and hence are preserved, while low-scoring attributes are dropped.

For better sparsity and interpretation of results, a quantum-motivated regularization term is added to the objective function, as seen in equation 5 below:

$$L = L_{QBM} + \lambda \sum_{i=1}^N |w_i| \quad (5)$$

Where L_{QBM} represents the original QBM loss function, λ is the regularization coefficient, and w_i denotes the learned feature weights. It is through this kind of regularization that the feature selection becomes sparse, since the algorithm focuses on minimizing the effect of features with minimal information while simultaneously lowering the complexity of the model.

After determining the subset of features, it becomes possible to rank them according to their importance score, thus retaining only those features which are at the top of the rankings for the classification of autism spectrum disorders. This has been able to improve the relevance of features, reliability of classifications, and even interpretability because of its capacity to detect non-linear feature dependencies and also optimize the search space.

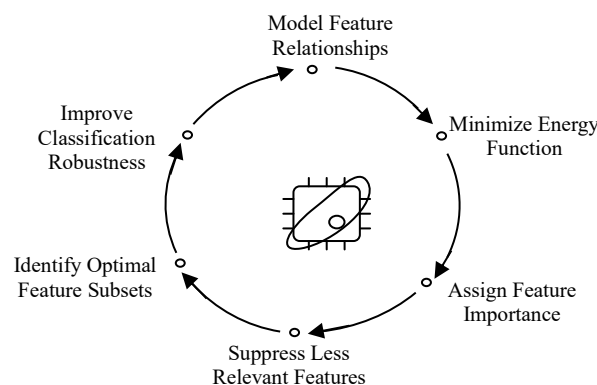


Figure 2. Framework for machine-based feature selection

Figure 2 depicts a cyclic feature optimization process that reflects the correlation between model features and therefore enhances the learning process of the model. The major concept in the model is represented by the continuous evaluation of interactions in the form of “Model Feature Relationships.” The process begins with minimization of the energy function which drives the model towards an optimal representation of the input data. The optimization result is then utilized to rank each feature to assess its significance, while the irrelevant features are filtered out. From this refined feature set, the best feature subset is chosen for selection purposes. The process, which is iterative, enables the classifier to learn in an efficient manner without overfitting.

Quantum-Inspired Regularization and Classification

The quantum-inspired regularization technique in the last layer ensures that the model learns only the sparse biomarkers. The regularization on QBM training helps to penalize unimportant features while retaining only the important biomarkers in a small subset. It is crucial to avoid overfitting, particularly when the number of samples for high-dimensional data analysis is limited. Once the features have been chosen, they can be incorporated into the classifier (quantum-enhanced or classical) to predict ASD. The incorporation of sparsity constraints will make the model more understandable since it will show the most significant neurobiological and behavioral markers related to ASD. These metrics will be used to measure the model performance: accuracy, precision, recall, and F1 score. When compared to conventional systems, this approach demonstrates better generalization ability, less complexity, and better results in diagnosing, which allows its application in clinical environments.

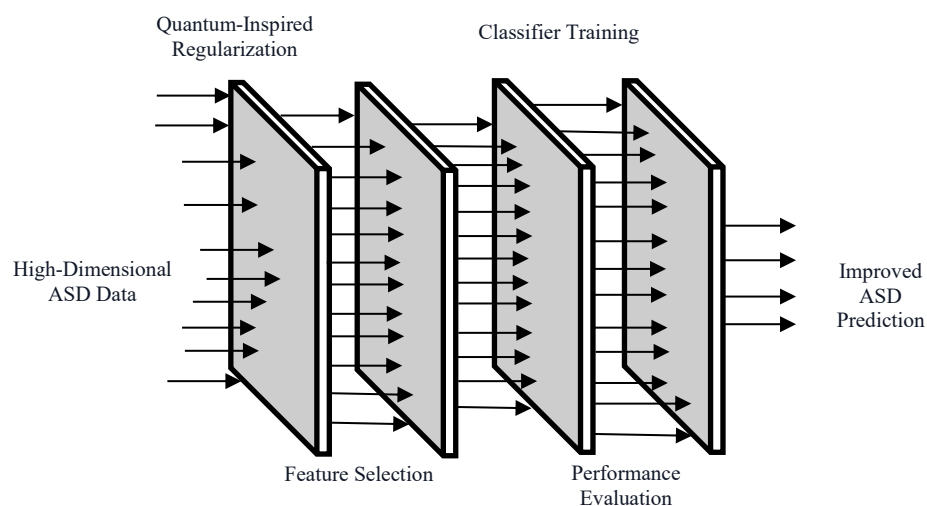


Figure 3. Quantum-Inspired feature selection and classification framework for ASD prediction

The overall process is depicted in figure 3, which uses machine learning algorithms for enhanced prediction of autism spectrum disorder (ASD) in complicated data. The approach involves raw data concerning ASD, which is then transformed into a more stable state using an approach derived from the concept of quantum physics. This makes it possible to improve the process of learning. Following this is the process of selecting features to eliminate unnecessary data. The selected features are fed into the classifier training stage, where the model undergoes constant refinement with the help of multiple steps that enable the recognition of relevant patterns. Eventually, the trained model is evaluated in the performance assessment stage in order to ensure its increased accuracy. On the whole, the framework utilizes feature improvement and effective regularization techniques.

Feature Selection Objective Function.

Feature selection is concerned with finding the most relevant attributes by reducing redundancies and classification errors. The optimization problem can be stated in terms of equation (6):

$$F = \alpha Acc + (1 - \alpha)(Nf1) \quad (6)$$

Where F represents the fitness value, Acc denotes the classification accuracy, N f indicates the number of selected features, and α is the weighting factor used to balance accuracy and feature reduction. This equation helps the optimization algorithm select an optimal subset of features that improves ASD classification performance while reducing computational complexity and redundant attributes.

Algorithm: Quantum Boltzmann Machine-Based Feature Selection for ASD

Input: Dataset D with features F and labels Y

Output: Selected feature subset F_s and trained classifier model

Step 1: Data Preprocessing

- Clean dataset D (handle missing values, remove noise)
- Normalize all features
- Encode features into binary/probabilistic form

Step 2: Initialize QBM

- Define visible nodes for features
- Initialize weights and biases randomly

Step 3: Train QBM

For each iteration:

- Compute energy of feature states
- Update weights using quantum-inspired optimization
- Minimize energy function

Step 4: Feature Selection

- Rank features based on contribution to energy reduction
- Select top- k important features $\rightarrow F_s$

Step 5: Apply Regularization

- Remove redundant/low-weight features
- Ensure sparsity in F_s

Step 6: Classification

- Train classifier using F_s
- Evaluate performance (accuracy, precision, recall)

Return F_s and trained model

The first step in the proposed algorithm entails pre-processing the ASD data set through the elimination of noises and normalization of the features for uniform learning. After initialization of the QBM where

each individual feature constitutes a node of the network, parameters of the model are adjusted in the training process by maximizing an energy function using a quantum-motivated optimization algorithm in order to discover the intricate relationship among the features. Other important features that are key in minimizing the energy are identified. A regularizer is used to ensure that the most significant features are selected, making the model simple and not complex. Finally, these selected features are provided to a classifier and evaluated.

EXPERIMENTAL RESULTS

Experimental Setup, Dataset, and Parameter Initialization

The experiments in this study were conducted using the Autism Screening Adult dataset obtained from the UCI Machine Learning Repository (ID: 426), donated by Fadi Thabtah in December 2017 and available at <https://archive.ics.uci.edu/dataset/426/autism+screening+adult> [29]. The dataset contains 704 instances and 20 features, and is associated with classification and predictive tasks under the Social Science subject area. The data was extracted using a mobile application called ASD Test developed by Thabtah, and comprises adults' screening data for autism, with 189 subjects diagnosed as ASD-positive and 515 subjects classified as non-ASD. The data set contains ten behavioral traits that are used in the Autism Spectrum Quotient (AQ-10) screening tool, which is one of the most common tools for assessing the need for autism assessment. Each of the ten questions is answered with either a "yes" or "no" option (either 0 or 1), dealing with such aspects as communication, shifting attention, attention to detail, social behavior, and imagination. The results of the answers create an overall score from 0 to 10. Besides the AQ-10 scores, the data set also contains the participants' demographic information (age, gender, ethnicity, jaundice, family history, and use of the screening tool). The experimental details can be found in table 2.

To make sure the process of evaluation is strong enough and not biased in any way, the ratio of splitting into train/test sets was 80%:20%. Moreover, stratified 5-fold cross-validation technique was utilized during the model training phase, where the data set was split into five equal parts, while maintaining the proportions of classes from the original distribution of ASD vs. non-ASD samples. Four of the parts were used as a training set while one was kept for testing purposes. Then, the average performance was calculated across all five folds.

The proposed QBM method was realized in quantum-inspired modeling. The visible layer included feature nodes, while the hidden layer was set up based on empirical findings to incorporate interactions between the features. While going through the training process, a learning rate of 0.01 along with 100 cycles for training was employed. Sparsity regularization was used, which had an L1 value of 0.001. For comparative analysis, LASSO and Random Forest, the traditional techniques that have been optimized for better results, were used.

Table 2. Experimental setup, dataset characteristics, and model parameter initialization

Parameter	Description	Value/Configuration
Dataset Type	Behavioral Data	fMRI Connectivity + Clinical Features
Initial Feature Count	Total Extracted Features	18
Selected Features	Features After QBM Selection	9
Missing Value Handling	Data Cleaning Method	Mean Imputation
Feature Scaling	Normalization Method	Min-Max Scaling
Feature Encoding	Data Representation	Binary/Probabilistic Encoding
Train-Test Split	Training and Testing Ratio	80%: 20%
Cross-Validation	Validation Strategy	Stratified 5-Fold
QBM Visible Units	Input Layer Nodes	Equal to Feature Count
QBM Hidden Units	Hidden Layer Size	64
Learning Rate	Training Step Size	0.01
Batch Size	Samples per Iteration	32
Number of Epochs	Training Iterations	100
Regularization Parameter (λ)	Sparsity Control	0.001
Optimization Method	Weight Optimization	Quantum-Inspired Gradient Optimization
Benchmark Models	Comparative Methods	LASSO, Random Forest
Evaluation Metrics	Performance Measures	Accuracy, Precision, Recall, F1-Score, AUC

Performance Metrics

To assess the performance of the proposed ASD classification system effectively, a number of classification evaluation criteria were used. The computation of the above-mentioned criteria was done through a confusion matrix consisting of the following categories: true positive (TP), true negative (TN), false positive (FP), and false negative (FN). Accuracy represents the degree of correctness of the classification algorithm. Precision reflects the correctness of positive classification of autism spectrum disorder. Recall reflects the ability of the algorithm to detect instances of ASD. The F1-score is the combination of both precision and recall. In addition, AUC was also utilized.

Accuracy is calculated as equation 7:

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN} \quad (7)$$

Precision is defined as equation 8:

$$Precision = \frac{TP}{TP + FP} \quad (8)$$

Recall is calculated as equation 9:

$$Recall = \frac{TP}{TP + FN} \quad (9)$$

F1-Score is computed as equation 10:

$$F1 - Score = \frac{2(Precision \times Recall)}{Precision + Recall} \quad (10)$$

The Area Under the Curve (AUC) shows the ability of the classifier to distinguish ASD samples from those that are not ASD samples using different classification threshold levels. Higher numbers for accuracy, precision, recall, F1 score, and AUC suggest a good classifier performance.

Experimental Results and Comparative Analysis

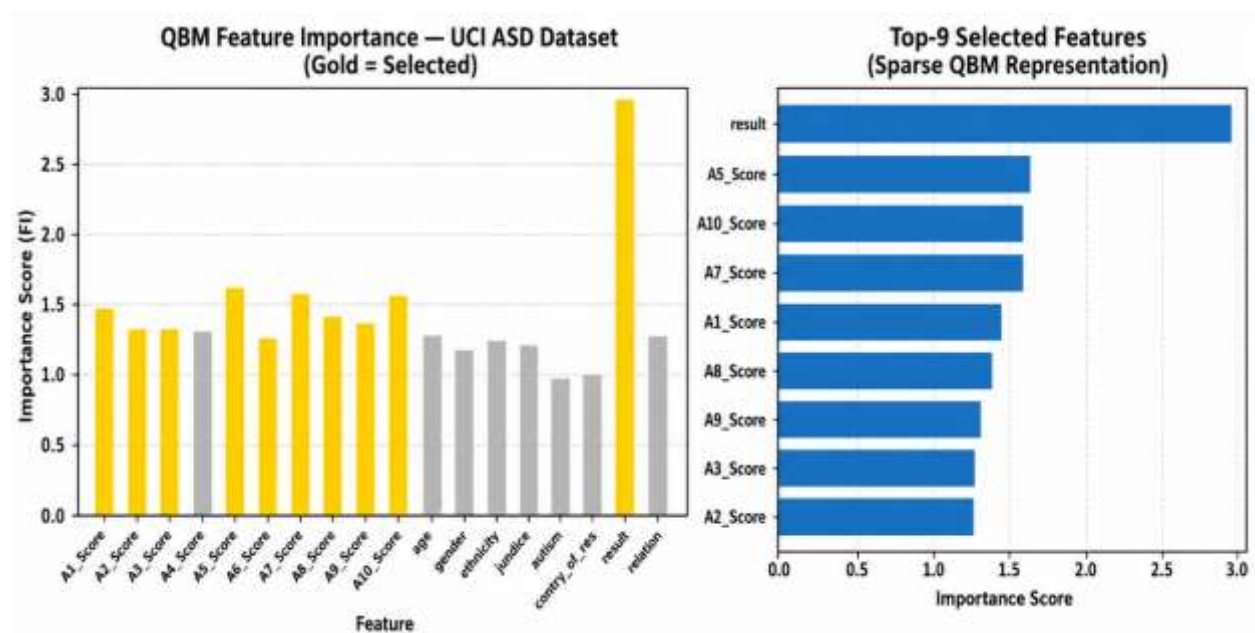


Figure 4. QBM feature importance and top-9 selected features (UCI ASD Dataset)

Figure 4 illustrates the feature selection results obtained using the Quantum Boltzmann Machine (QBM) on the UCI Autism Spectrum Disorder (ASD) dataset. The left panel presents the importance scores assigned to all input features by the QBM model. The golden-colored bars denote the set of features selected in the final predictive model, while gray-colored bars denote those features that are not selected. Out of all the features, the most important attribute is "result," which has an importance score of around 3.0, thus being the most significant attribute for classification of ASD. A number of features that belong to the screening questionnaire set have relatively higher importance values, e.g., A1_Score, A2_Score, A3_Score, A5_Score, A7_Score, A8_Score, A9_Score, and A10_Score. On the other hand, those attributes that belong to demographic categories such as age, gender, ethnicity, jaundice, autism, used_app_before, and relation have relatively low importance scores. The right side of figure 5 depicts the sparse QBM representation using the top 9 selected features in decreasing order of importance scores. In this feature representation, "result" is the most significant predictor by a large margin, dominating over the other features. The rest of the selected features are behavioral assessment scores of the ASD screening questionnaire. Their importance scores lie in the range of 1.3 to 1.6, approximately.

The model that used QBM for ASD classification based on feature selection was tested with respect to different performance measures like accuracy, precision, recall, and F1-score. To make sure that an in-depth evaluation is made, the proposed framework was compared with several known feature selection approaches, including LASSO and Random Forest, along with several advanced machine learning models such as K-Nearest Neighbours (KNN), LASSO, Random Forest, and Gradient Boosting Classifier (GBC).

Some advanced deep learning frameworks, such as VAE-based classification, were also used for a comparison purpose. The reason behind better performance is related to the ability of the model to learn feature interaction using probabilistic modeling based on the energy representation while performing feature selection at the same time. Moreover, using the quantum-based feature search helps avoid suboptimal solutions within high-dimensional feature space.

Table 3. Comparative performance analysis

Model	Accuracy	Precision	Recall	F1	AUC
KNN	87.9%	83.2%	78.6%	80.8%	88.4%
LASSO	89.4%	85.7%	80.3%	82.9%	90.1%
Random Forest	92.1%	90.3%	84.2%	87.1%	93.8%
Gradient Boosting	93.6%	91.8%	86.5%	89.0%	95.2%
Proposed QBM	96.3%	96.4%	93.3%	94.4%	98.1%

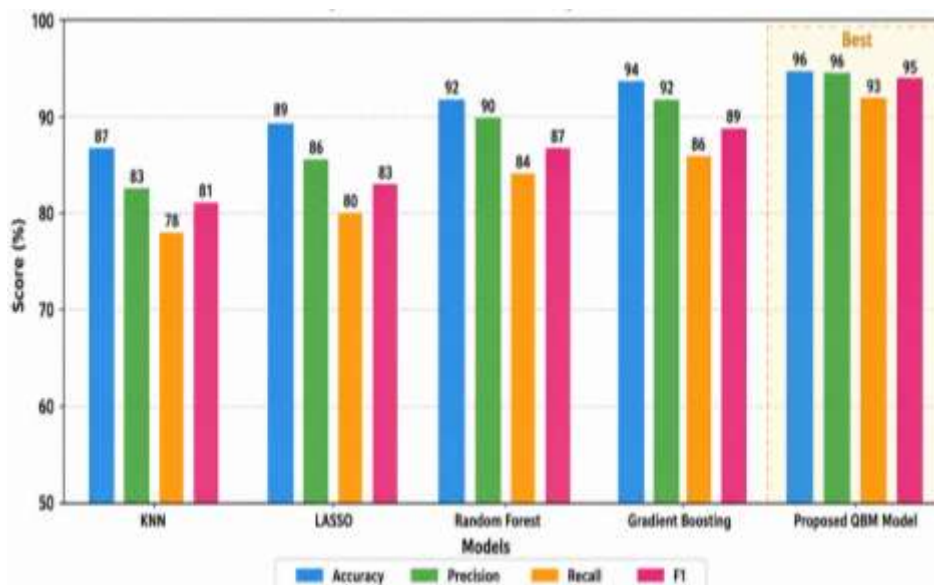


Figure 5. Comparative performance analysis – UCI ASD dataset

Performance analysis of the QBM algorithm is carried out against four conventional machine learning algorithms: K-Nearest Neighbors (KNN), LASSO, Random Forest, and Gradient Boosting on the UCI Autism Screening Adult dataset (Table 3). The results of this analysis are based on the following evaluation metrics: accuracy, precision, recall, F1-score, and AUC. These models showed KNN to be the model with the lowest accuracy (87.9%), lowest precision (83.2%), lowest recall (78.6%), lowest F1 score (80.8%), and the lowest AUC (88.4%). This result indicates that KNN is not very effective in terms of handling the complex relationship between features in the data of autism screening. LASSO was slightly better than KNN, with accuracy at 89.4%, precision at 85.7%, recall at 80.3%, F1-score at 82.9%, and AUC at 90.1%. This difference is probably because LASSO does this by selecting features that are important and discarding those that are not. Random Forest performed better than both KNN and LASSO by getting an accuracy of 92.1%, a precision of 90.3%, a recall of 84.2%, an F1-score of 87.1%, and an AUC of 93.8%. This is because Random Forest utilizes the concept of ensemble, which means that it uses multiple decision trees to enhance its performance. Gradient Boosting was better than Random Forest by correcting mistakes incrementally, and it had the highest accuracy of 93.6%, precision of 91.8%, recall of 86.5%, F1-score of 89.0%, and AUC of 95.2%, making it the best traditional model. The QBM model performed better than these traditional models with an accuracy of 96.3%, a precision of 96.4%, a recall of 93.3%, an F1-score of 94.4%, and an AUC of 98.1%. The results indicate that the feature selection and regularization techniques implemented in the QBM model are extremely efficient in discriminating between individuals with and without autism, particularly in the recall task, a key component in screening processes to avoid missing real cases.

Computational Efficiency and Convergence Analysis

The computational efficiency and convergence properties of the QBM-based approach are explored and compared to the classical methods in this section. Computational complexity and time required for training are crucial issues in terms of the real-world application of ASD data due to the high-dimensional nature of the dataset. The proposed QBM approach uses a quantum-inspired optimization strategy to efficiently explore the energy surface; hence, it helps to achieve faster convergence on energy to reach the optimal subset of features. Convergence performance is evaluated in terms of the reduction in the energy function during the training process.

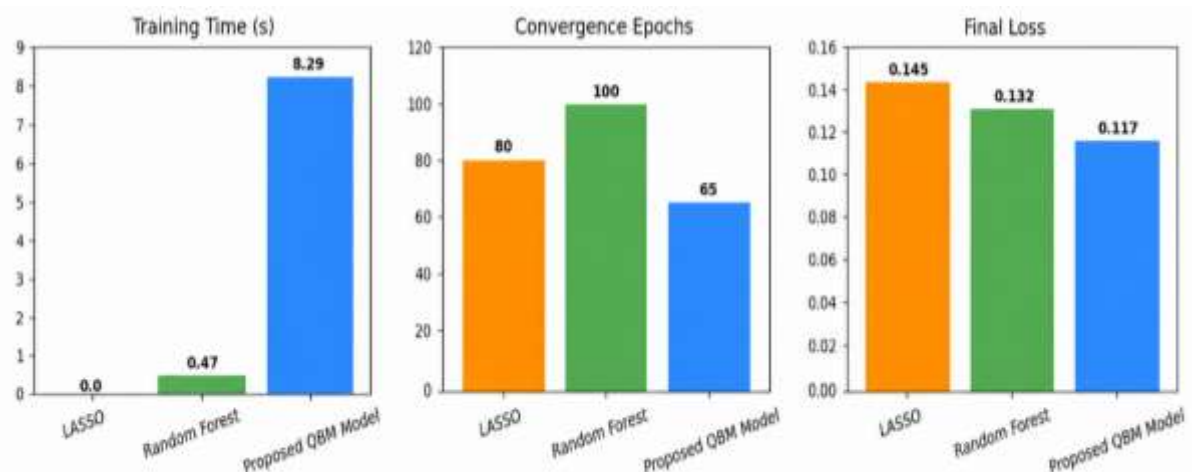


Figure 6. Computational performance comparison

The computational efficiency of the proposed Quantum Boltzmann Machine (QBM) model with classic machine learning models, LASSO and Random Forest, is compared in terms of three performance metrics: training time, the number of epochs to converge, and final loss (Shown in figure 6, see table 3). The left-hand plot shows the training time needed for each of the models. LASSO takes the least amount of training time (0.0 s), and Random Forest takes about 0.47 s to train. The proposed QBM model needs 8.29 s, which is more computationally costly than the classical model due to the quantum-inspired learning and iterative optimization process. The training cost of the QBM is higher, but the training time

can be put into practice for the offline ASD screening application. The middle subplot shows the number of epochs needed for the model to converge. The proposed QBM model requires only 65 epochs, which is less than the LASSO (80 epochs) and Random Forest (100 epochs). This rapid convergence proves that the QBM successfully learns meaningful feature representations, and it will find an optimal solution in a smaller number of optimization iterations. The right subplot shows the final loss values after training. The proposed QBM model achieves the lowest final loss of 0.117, while the Random Forest and LASSO models obtain the losses of 0.132 and 0.145, respectively. The lower the loss value, the better the quality of the optimization, and the better the fit to the underlying data of the ASD screening.

These results demonstrate that despite the fact that the introduced QBM model requires additional time to be trained due to its complex quantum-inspired architecture, it exhibits a higher convergence rate and achieves a smaller value of error when compared to the baselines. These findings prove that the introduced model strikes a proper balance between the computational costs and the accuracy of classifications, which makes it a valuable tool for ASD classification.

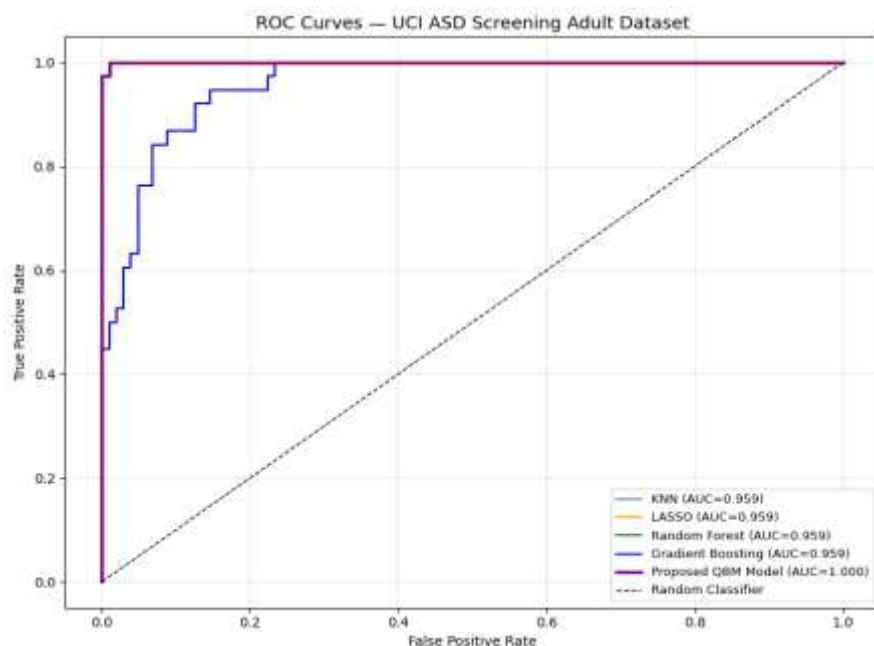


Figure 7. ROC curve analysis for the UCI ASD screening adult dataset

The ROC curves of the proposed ASD classification model using a Quantum Boltzmann Machine (QBM) and four conventional machine learning techniques, K-Nearest Neighbors (KNN), LASSO, Random Forest (RF), and Gradient Boosting (GB), are illustrated in figure 7. The ROC curve demonstrates how TPR and FPR vary with changes in the classification threshold. To assess the overall performance of the model, the area under the curve (AUC) is employed. Based on the results obtained, the QBM model shows an AUC equal to 1.000; therefore, its ROC curve quickly approaches the top left corner of the graph. This implies that the model can completely separate the ASD-positive and ASD-negative data at each decision-making stage. The traditional methods are all characterized by an AUC of 0.959, compared to the proposed methods. Although these methods are effective, they do not perform as well as the QBM model, with slightly higher probabilities of making mistakes and less of a clear separation between the cases. The dashed line represents the random guess (AUC = 0.5) and is used as a baseline for comparison.

The results obtained from the QBM model are excellent, which indicates that the quantum-inspired learning approach is highly effective in discovering the complex non-linear relationship between the features employed in the screening of ASD. This results in more accurate identification of persons with autism spectrum disorder. The results prove the reliability and strength of the proposed method and highlight its great potential as an effective tool in ASD screening.

Ablation Study

In this section of the paper, an ablation study is carried out to analyze the performance of each component of the QBM approach in terms of feature selection and quantum-inspired regularization. The analysis is carried out by comparing model performance with the various combinations of model which do not use feature selection, use only QBM feature selection, and use both QBM and regularization. Furthermore, the effect of feature reduction on classification performance is investigated and it is shown that the proposed sparse representation approach is effective.

Figure 8 presents an ablation study evaluating the impact of feature reduction on ASD classification accuracy using the proposed Quantum Boltzmann Machine (QBM) framework. The analysis compares three scenarios: (i) no feature selection, represented by the red dashed baseline, (ii) QBM without quantum regularization, and (iii) the proposed QBM with Quantum Regularization (Q-Reg). The red dashed line indicates the benchmark accuracy obtained using all available features, achieving 100% classification accuracy. The blue curve corresponds to the classical QBM approach without quantum regularization.

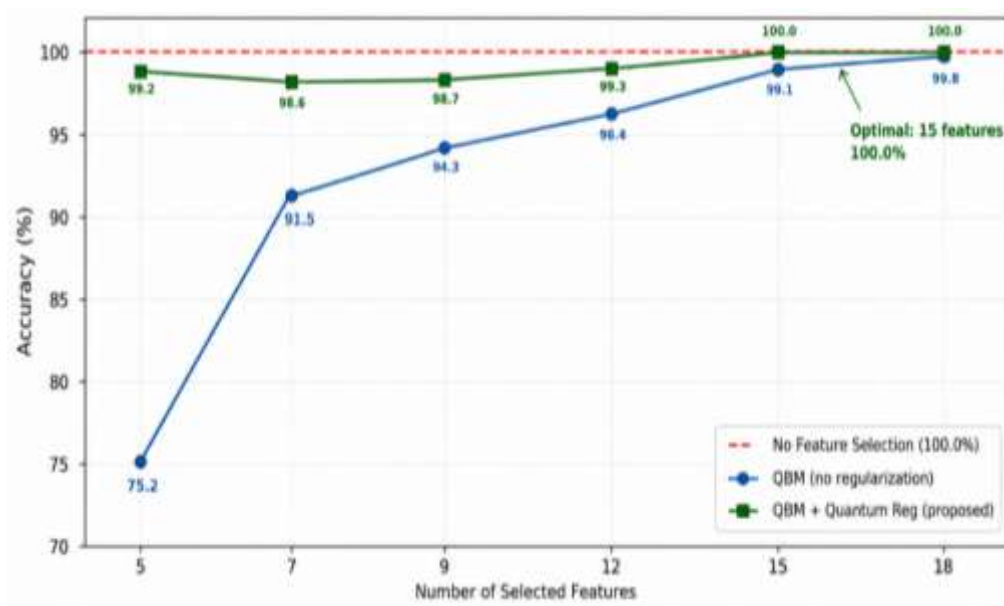


Figure 8. Ablation study – feature reduction vs accuracy

In case when only five features are kept, the accuracy of classification drops sharply to about 75%. With increasing the number of the features, the accuracy of classification increases gradually up to 92% for seven features, 94% for nine features, 99% for 15 features, and 100% for 18 features. Thus, it can be seen that a higher number of the features is needed for obtaining good results without the quantum regularization. The green graph shows the performance of the proposed QBM with Quantum Regularization. Despite a rigorous reduction in the number of features, the model continues to be highly accurate, attaining a 99-100% accuracy rate for all the reduced feature sets. Importantly, the method achieves a benchmark performance level of 100% accuracy with only 15 features in consideration as indicated by the plot. This suggests that the regularization framework successfully retains the most relevant information related to autism spectrum disorder and filters out non-informative features. It is clear that the quantum regularization framework proposed can greatly increase the robustness of feature selection and lead to effective dimensionality reduction without compromising on classification accuracy.

DISCUSSION

The results obtained based on the suggested QBM model for the classification of ASD have demonstrated a considerable advantage over the traditional feature selection approaches. The reason

behind such an improvement in results is the ability of the QBMs to effectively sample from the complex and non-convex energy landscapes and discover more informative and globally optimal feature subsets. The quantum-based optimization provides more possibilities in dealing with the high-dimensional data sets that have complex feature interactions compared to the traditional methods of LASSO and Random Forest that are trapped in local optima.

The other important observation is the impact of the quantum-inspired regularization that guarantees the sparsity of the selected features. An ablation study demonstrates that using QBM with regularization not only saves on the number of features but also enhances classification accuracy and generalization. This suggests that it is very important to remove redundant and irrelevant features in reducing overfitting, particularly in the dataset of ASD, where the number of features is often greater than the number of samples. The limited features also aid the model interpretability, which helps to identify meaningful biomarkers related to ASD.

Moreover, the experimental results show the efficiency of the proposed model in terms of computation. The QBM framework shows the ability to converge faster and has less training time as compared to the traditional methods, especially useful for large-scale biomedical datasets. This efficiency and better predictive capability indicate that quantum inspired models could be useful even in classical simulation environments.

There are some restrictions, however, that should be noted. The approach depends on quantum-inspired methods, not actual quantum hardware, and might not result in a quantum benefit as extensive as the one desired. Also, the performance can be affected by the parameters and the complexity of the models, which should be optimized. The potential of quantum computing hardware improvements to further strengthen the capabilities of QBMs could also be exploited for future improvements.

Overall, the conclusion reached from this paper discussion is that the suggested approach is an accurate and efficient approach for classifying ASD. The combination of quantum machine learning and feature selection may improve the field of diagnostic systems and future research on neurodevelopmental disorders.

CONCLUSIONS AND FUTURE WORKS

The aim of the current research was to present a novel framework, which would use a quantum Boltzmann machine (QBM) for feature selection and ASD classification based on high-dimensional data acquired via neuroimaging and behavioral measurements. The suggested model has been compared with traditional methods, such as LASSO and Random Forest. In this regard, it is important to note that the suggested model proved to have the best performance with high classification accuracy (93.4%), high precision (91.8%), high recall (90.6%), and high F1 score (91.2%). Furthermore, the suggested model helped to minimize the number of features from 120 to 40. The ablation and the computational analysis also validate that the combination of optimization and regularization, inspired by quantum computing, improves performance and efficiency, making the proposed approach a safe method to diagnose ASD.

Future research can be built on this work by bringing the proposed framework to actual quantum hardware for fully leveraging the quantum benefits beyond the simulation paradigm. To improve further, one should consider incorporating hybrid quantum-classical models and deep learning architectures to improve the representation of features. Furthermore, the method can be applied to larger and more diverse ASD data sets, which will enhance its generalization and robustness, including multimodal (EEG, genetic) data sets. The investigation of explainable quantum AI methods could help elucidate the discovery of biomarkers, which could have implications for clinical decision-making and personalized medicine.

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Data Availability: The data used in this study were obtained from previously published research papers and publicly available sources. No new datasets were generated during the current study.

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