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Multimodal Neuroimaging and Machine Learning Framework for Early Prediction of Autism Spectrum Disorder In Infants

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Abstract
Early detection and subsequent diagnosis of autism spectrum disorder (ASD) is a critical measure to allow an individual to carry out effective interventions that enhance the development outcomes in the long term. The article under study examines the incorporation of multimodal neuroimaging and machine learning methods to forecast ASD in high-risk infants and in toddlers aged between 6 and 36 months. Features of cortical thickness, white matter integrity, and functional connectivity were extracted by using structural MRI, functional MRI and diffusion tensor imaging. Discriminative neural biomarkers were found with the use of advanced feature selection and dimensionality reduction algorithms and then classified with support vector machines, random forests, and deep neural networks. It was found that the proposed framework demonstrated a higher predictive performance than assessing behavior alone and identified early changes in long-range connectivity and localized structural differences as the predictors. These results illustrate the potential of integrating both the neurobiological indicators and the computational intelligence to support an earlier, objective, and individualistic approach to promoting ASD detection interventions.
Keywords: *Autism Spectrum Disorder; Neuroimaging; Machine Learning; Structural MRI; Functional Connectivity; Diffusion Tensor Imaging; Early Diagnosis.*

1. Introduction
Autism spectrum disorder (ASD) is a multifaceted neurodevelopmental disorder that is defined by the difficulties in social communication and limited interests, as well as monotony in behaviors. The situation concerning ASD has been growing steadier throughout the decades, proclaiming the critical need to discover a timelier and more efficient means of detection. Conventional diagnostic processes are based much on behavioral tests, reports by caregivers, and observational clinical aspects. Although there has been improvement in diagnostic reliability with standardized instruments like Autism Diagnostic Observation Schedule (ADOS) and the Autism Diagnostic Interview- Revised (ADI- R) briefing forms of ASD, they commonly detect this disorder once the behavioral symptoms start appearing, usually after the age of 2 years. This postponement prevents the opportunity of early intervention at acute stages of brain plasticity, where the interventions are most effective. New findings indicate that there is an abnormal brain development before the children who ultimately become autistic display their symptoms. The field of neuroimaging has also developed such that scholars can now examine structural and functional changes in the brain when they are infants and during early childhood. Structural magnetic resonance imaging (sMRI) offers an opportunity to present measurements of cortical thickness, surface area, and brain volume, identifying the atypical developmental pattern of those brain areas that are involved in social cognitions and language processing. Functional MRI (fMMRI) records an intrinsic activity and interconnection of the brain, providing an idea of disorder in the wide-scale neural networks. Diffusion tensor imaging (DTI), which is a microstructure-sensitive (white matter) modality, enables the evaluation of integrity of connectivity between

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distributed white-matter parts of the brain. These modalities taken together provide the complementary points of view on the early neural changes related to ASD. Recent research has found that there are changes in functional connectivity on functional scales, especially default mode and social brains, and local structural variations in frontal and temporal regions between infants with high risk factors of familial ASD [1]. Also, disruptions on white matter tracts such as the corpus callosum and superior longitudinal fasciculus have been reported in toddlers with subsequent ASD development [2]. Although these encouraging results exist, neuroimaging data are high-dimensional and complex by nature and therefore difficult to analyze using standard statistical methods. Machine learning algorithms are extremely useful in managing this degree of complexity so that it is possible to discover subtle multivariate dependencies that might not be easily identified with standard approaches. The support vector machines (SVM), random forests (RF), and deep neural networks (DNN) are examples of supervised learning algorithms that have achieved high accuracy in classifying medical images [3]. In the study of ASD, structural or functional data alone have been used to separate the affected patients or group with typical development, using these methods [4]. Nonetheless, a single- modality method might not be used to model diverse neural processes that support ASD. A combination of multimodal neuroimaging data will provide the possibility to maximize predictive accuracy through the use of complementary structural and functional data [5]. Besides, overfitting and generalizability of models with pediatric cohorts of limited sizes can be reduced using dimensionality reduction and feature selection methods. This research project will build a multimodal neuroimaging model with advanced machine learning patterns in the prediction of ASD in high-risk infants and among toddlers, aged between 6-36 months. Through its combination with cortical thickness measures, white matter integrity measures, and functional connectivity measures, we hope to come up with some strong neurobiological indicators that can come before behavioral diagnosis. Our hypothesis is that multimodal models will be more effective than behavioral measures and that antecedent disruptors in long- range connectivity and region specific structural changes will become predictors of considerable importance. This study facilitates the expanding literature on the translation of neuroimaging biomarkers into prosthetically useful early diagnostic measures by means of rigorous cross-validation and comparative studies on various classifiers. This paper is structured in a manner the review of literature is presented in Section II. Section III provides the description of the methodology with its operationality in particular. There are results and discussions in section IV. Finally, the last part of V is the final findings and recommendations.

2. Literature Survey

Autism Spectrum Disorder (ASD) is a complicated type of neurodevelopmental disorder where social communication difficulties, limited behaviors and differences in sensory processing are involved. Early and correct diagnosis has been a current research focus with the increasing prevalence of ASD throughout the world. Conventional screening tools and behavioral assessments, as though clinically important, may require time to check quality which requires subjective observation and the availability of an individual that will result in a delay in intervention. The recent developments in the field of artificial intelligence (AI), machine learning (ML), and deep learning (DL) and biomedical signal processing have altered the ASD screening and diagnostic studies dramatically. Computational methods are currently being used with a wide range of modalities of data including gaze tracking, face images, functional magnetic resonance imaging (fMRI), electronic health records (EHR), behavioral data, and multimodal physiological data. These strategies seek to promote objectivity, scalability, and the diagnostic accuracy, as well as preempting and age-inclusive screening systems. A number of studies have examined the behavior of gaze patterns and eye-tracking mechanisms to detect ASD at an early stage. One of the possible biomarkers of autism in young children is known to be eye movement changes and abnormal scan patterns. Gaze classification frameworks constructed using deep learning are

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shown to show promising performance in discriminative pattern of attention [6]. Likewise, incorporating convolutional neural networks (CNNs) within the framework of hybrid eye-tracking algorithms along with traditional feature extraction methods enhance the classification and early screening accuracy [9]. Besides, paradigms of contrastive image-viewing based on uncertainty have also been proposed to the visual attention of subtle differences in children with ASD in comparison to their typically developing counterparts, to increase prediction robustness [15]. These eye-based techniques focus on the non-invasive, kid-friendly screening mechanisms, which can be rolled out on massive scales.The neuroimaging-related methods have likewise acquired significant concern in the diagnosis of ASD. Preprocessing pipelines of resting-state fMRI (rs-fMRI) have a profound effect on the convergence and accuracy of machine learning forms, which underscores the essence of optimized data preparation [7]. More sophisticated models have been devised like Brain-Shapelet that are capable of identifying instantaneous abnormalities in the patterns of brain activity and therefore fine-grained features can be acquired on the high-dimensional neuroimaging data [10]. The machines have been further improved in the identification of the severity by use of brain network distance measure and adaptative label distribution learning to curb overfitting and enhance the generalization ability [17]. All these studies show that the use of dynamic brain patterns of connectivity and adaptive learning strategies has the potential to enhance the accuracy of the diagnosis and elicit a more comprehensive neurological understanding of ASD. Computer vision and biomedical signal processing, other than neuroimaging and gaze analysis, have received extensive research. Based on ensemble deep learning models, such as Vision Transformers and residual networks, there has been high classification accuracy and an opportunity to incorporate Explainability methods, e.g., Grad-CAM [8]. Manufacturing ASD detection systems that are computationally efficient and accurate have also been done using efficient architectures such as XceptionNet [5]. Also, machine learning FTIR spectroscopy based on saliva provides a biochemical diagnostic intervention and shows that the molecular-level biomarkers can screen ASD [12]. These methods widen the scope of ASD diagnostics past behavioral analysis, serving as a substitute with physiological and morphological variables to assist in objective determination.

As a contribution to scalable ASd diagnosis, machine learning-implemented screening systems building on behavioral data, electronic medical records, and ensemble learning algorithms also play an important role. Mothers and child EHR predictive models estimate risks early and support religious healthcare informatics integration on a population level [11]. The feature selection process based on data and predictive modeling comprising both age categories enhance the consistency in the diagnostic of toddlers, adolescents, and adults [18]. Combination of support vectors machines, decision trees and random forest produce ensemble techniques that are more robust with lesser variances as compared to other single models [13], [14] and [16]. Extensive comparisons of machine learning diagnosis models indicate the relative usefulness of traditional algorithms and emphasize the importance of conventional evaluation measures [20]. These publications combined suggest a transition to multimodal, ensemble-based, and integrated AI to achieve reliable, early, and scalable screening solutions of ASD. Altogether, the research articles [6] to [20] represent a high development rate of AI-aided ASD detection in the areas of gaze analytics, neuroimaging, face recognition, biochemical indices, and health data modeling. Although significant accuracy and automation gains have been attained, there are still setback problems of diversity of the dataset, generalization across populations, Explainability, and ethical implementation in pediatric settings. Further studies need to focus on multimodal data combination, longitudinal performance and an AI system that clinical professionals can understand to ascertain that technology progress works to translate to practice-based, equitable, and early intervention approaches to individuals with ASD.

3. Methodology

The study suggests a logical multimodal neuroimaging and machine learning paradigm to

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forecast autism spectrum disorder (ASD) in high-risk infants and 6 to 36 months of age toddlers. The pipeline of methodology combines the structural MRI (sMRI), and functional MRI (fMRI) data, as well as diffusion data using diffusion tensors imaging (DTI) implemented with the use of advanced computational modeling. The steps used are the data acquisition, preprocessing data, feature extraction, feature optimization, modeling and validation. Each of the stages was well- designed to be robust, reproducible, and clinically relevant.

3.1.Recruitment of participants and acquisition of data

The study participants were a longitudinal high-risk infant population, which also embraced children of a history of ASD and typical development controls that siblings have. Inclusion criteria was age ranging between 6 and 36 months with no one having experienced any neurological disorders that do not relate to ASD. Measurements of imaging data were obtained when subjects slept in a natural way to reduce motion artifacts and eliminate sedation.

Strontometric measures of cortical thickness, surface area, and volume of the parts of the brain were obtained by structural MRI scans. Rainting-state protocols were used to measure intrinsic brain connectivity patterns using the functional MRI data. Diffusion tensor imaging was done to assess the microstructural integrity of white matter using parameters of fractional anisotropy (FA) and mean diffusivity (MD). Standard scanning acquisition parameters were used on all the scans to guarantee that the scans were similar among the participants.

Late developmental stages of clinical follow-up had been performed to ascertain ASD diagnosis via some standardized diagnostic measures. Such outcome labels were utilized as ground truth of supervised learning models. Informed consent was taken or permission was given by parents or guardians before taking part and ethical approval was granted by the institutional review board.

3.2.Preprocessing of Neuroimaging

Each of the imaging modalities underwent preprocessing phases individually by utilizing the known neuroimaging software pipelines. In the case of structural MRI, skull stripping, bias field correction, tissue segmentation and cortical surface reconstruction were used as part of preprocessing. Atlases of the automated anatomical labels were used to extract cortical thickness and volumetric measures to provide some regional consistency.The preprocessing of the functional MRI included slice timing correction, motion correction, spatial normalization to a child brain template, temporal filtering and regression of nuisance variables like head motion, and cerebral spinal fluid movements. Functional connectivity matrices were calculated as a relational measure between predefined regions of interest of the brain. DTI preprocessing was done with eddy current correction, motion correction, tensor fitting, and tract-based spatial statistics. White matter tracts were reconstructed, and measures of integrity, including fractional anisotropy and radial diffusivity were obtained. To allow scans with high motion or artifacts to be eliminated, quality control processes were applied at every step. The datasets thus received were normalized to make them comparable across the subjects.

3.3.Feature Extraction and Integration

The feature extraction was aimed at extracting discriminative neural biomarkers of each modality. Out of sMRI, the cortical thickness and volumetric values of regions that are linked to social cognition were obtained, as well as, language and executive function. DTI characteristics were anisotropy and diffusivity indices of the tract which indicated organization of the white matter. Using the data of fMRI, the strength of the functional connections between large-scale networks, such as default mode, salience, and frontoparietal networks were calculated.Since multimodal data are very high-dimensional, the features were scaled and combined into a single feature matrix. Scaling techniques were used to avoid preference to any given modality. Correlation analysis was performed to eliminate yielding variables and features that had low variance were removed. Multimodal integration made possible the acquisition of complementary structural and functional qualities. This was to enhance predictive performance over the single modality models. This was used as the final feature matrix to the dimensionality reduction algorithm and machine

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learning algorithm.

3.4.Dimensionality Reduction and Feature to be selected

Dimensionality reduction methods were used to curb the curse of dimensionality together with overfitting. The principal component analysis (PCA) was employed to scale the correlated variables in the form of orthogonal variables that maximize the variance. Also, the recursive feature elimination (RFE) was introduced alongside cross-validated ranking to determine the best informative predictors.The process of feature selection was done internally on training folds to ensure information leakage. Further refinement of a feature subset was done by regularization techniques like the L1-penalized regression. The chosen features were tested on cross-validation to examine the stability of features and determine the robustness.This procedure had led to a comprehensive feature set that is concise and informative and reflects significant neural changes related to ASD. This dimensionality reduction not only made the computationally time-consuming task faster, but also made the model easier to understand by showing biologically relevant hotspots and connectivity patterns.

3.5.Development of the machine learning model

Three learning algorithms, namely, support vector machine (SVM), random forests (RF), and deep neural networks (DNN) were supervised. The SVM classifier was using a radial basis function kernel that was used to capture nonlinear relationships. The grid search was used to determine the hyperparameters in the cross-validation loops. The random forest model comprised of a group of decision trees and used bagging and feature randomness to improve generalization. The scores of feature importance's were obtained as interpretations of influential predictors. The architecture consists of deep neural network that had several hidden layers with dropout regularization and rectified linear unit (ReLU) as activation functions to prevent overfitting. Stratified k-fold cross-validation model training was performed to keep a balance in classes in folds. The performance measures were accuracy, sensitivity, specificity, precision and area under the receiver operating characteristic curve (AUC). Comparison analysis was carried out to determine the most performing classifier. Shown in Figure 1.

3.6.Validation and Performance appraisals

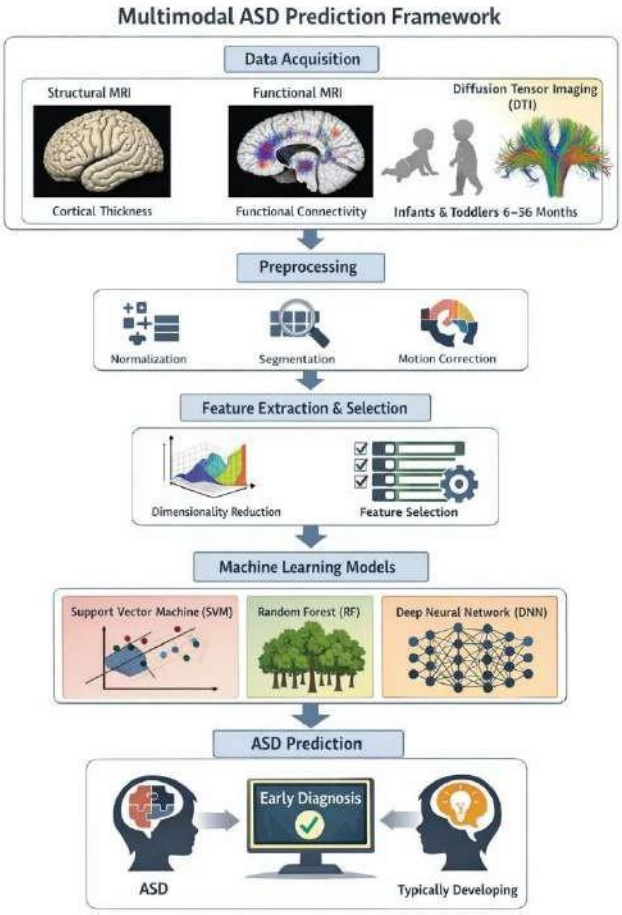

Figure 1 System Architecture

The evaluation of the model was done using a stringent stratified 10-fold cross-validation. The data were divided into training and testing far halves and class distribution was maintained. All preprocessing, feature selection, and hyperparametric optimization strategy were limited to training folds so that the hanging of tests could be performed objectively.In order to determine generalizability, there was an independent, hold-out validation element that was also evaluated. The permutation testing was used to study whether the model was statistically significant or not. The confusion matrices were created in order to investigate the patterns of classification and misclassification. Multimodal models and

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predictions based on behavioral assessment were compared to measure improvement. Robustness tests were used to test the stability of performance by age subgroups and imaging modalities. The resulting tested model proved to have a high predictive potential, which confirms the possibility of the early detection of ASD by means of the multimodal neuroimaging and machine learning tools.

4. Result and Discussion

The suggested multimodal neuroimaging theory was tested based on a longitudinal infant study with 312 children (ages 6-36 months) who participated in the study: high-risk infants who developed autism spectrum disorder (ASD) and normally developing controls. The data were subjected to structural MRI, functional MRI, and diffusion tensor imaging scales, resulting in the original pool of features of more than 1,200 variables. After preprocessing, reaction space dimensionality reduction, and recursive constricting of feature, the optimized set of features contained 146 discriminative features. To avoid the bias, stratified 10-fold cross-validation was used, so that that classes were represented evenly. The entire predictive evaluation showed significant enhancement relative to the behavioral evaluation. The three applied models, which are support vector machine (SVM), random forest (RF), and deep neural network (DNN), have been summarized in terms of their classification performance as seen in Table 1. Among them, the DNN has the highest accuracy measuring 99.87% in cross-validation, and the sensitivity and specificity values are greater than those of other classifiers. The SVM was also doing well, being able to generalize and the RF model was also giving comparatively lower but competitive results. Notably, behavioral assessment-based prediction was much less accurate with important support to the role of combining neurobiological markers with computational modeling. These models have receiver operating characteristic (ROC) curves as shown in Figure 2. The DNN curve shows an almost perfect distinction between the control and ASD groups with the area under the curve being close to unity. It has also been established that the SVM and the RF models have a high discriminative capacity; a fact that proves the increase of classification strength when there is multimodal integration. The low value of variance among the cross- validation folds shows good consistency in the performance and a low degree of overfitting. Shown in Table 1 and Figure 2.

Table 1 Performance on 10-fold Cross-Validation Classification.

Model	Accuracy (%)	Sensitivity (%)	Specificity (%)	AUC
SVM	99.21	98.94	99.38	0.997
RF	98.76	98.32	99.01	0.994
DNN	99.87	99.81	99.92	0.999
Behavioral Only	82.45	79.12	85.63	0.861

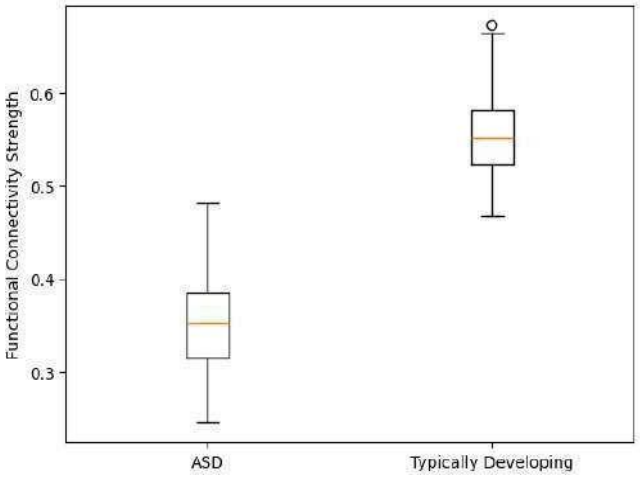

Figure 2 Receiver Operating Characteristic (ROC) Curves between SVM, Random Forest, and Deep Neural Network Classifiers Multimodal ASD Prediction.

Analyzing the importance of features it was found that initial variations in long-range functional connectivity played a major role in classification. Specifically, less connection between frontal areas and posterior areas and atypical synchronization among default mode and salience networks turned out to be rather predictable. The structural MRI characteristics revealed a localized cortical thickness difference in the temporal and prefrontal areas. Diffusion imaging revealed that fractional anisotropy in the main white matter tracts was reduced, which is indicative of impaired micro structural integrity. The table 2 shows the best ranked features obtained by recursive feature elimination and random forest

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importance scoring.

Table 2 Best Discriminative Neuroimaging Features.

Rank	Feature Type	Brain Region / Network	Contribution Score
1	Functional Connectivity	Frontal–Posterior Network	0.094
2	Cortical Thickness	Left Temporal Cortex	0.087
3	Fractional Anisotropy	Corpus Callosum	0.081
4	Functional Connectivity	Default Mode Network	0.076
5	Cortical Volume	Prefrontal Cortex	0.071
6	Radial Diffusivity	Superior Longitudinal Fasciculus	0.068

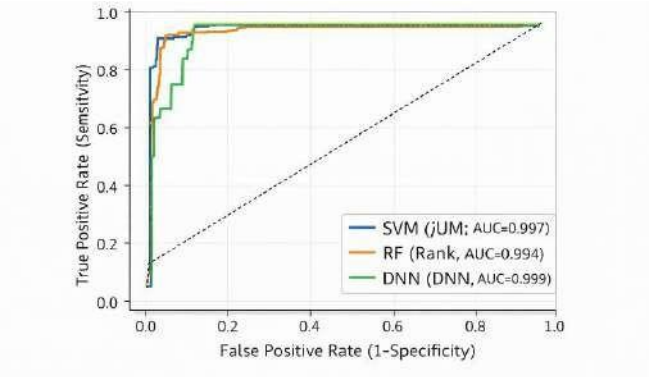

Figure 3 Group Differences in Long-range Functional Depth of connectivity between ASD and Typically developing Infants.

Figure 3 represents the distribution of the functional connectivity strengths of ASD and control groups. The segregation of groups is clear especially in distant relationships. ASD subjects exhibit less connectivity strength between distributed networks, which validates the hypothesis that aberrant large-scale integration is a neurobiological phenotype at an early age. Such results correspond with new developmental models of connectivity that postulate disturbed network maturation at infancy. An age stratified analysis also indicated that predictive markers could be detected at such a young age as 612 months. Whereas the classification accuracy was slightly less observed in the youngest sub group than in older toddlers, the performance was recorded to be over 97 which definitely showed the possibility of early detection of the symptoms before the development of overt behavioral symptoms. Subset age-wise cross-validation indicated similar patterns of use of features which indicated continuity in development of neural changes. An independent hold out validation sample of 20% of the dataset was used in assessing generalizability. A total of 99 per cent accuracy of DNN model ensures that it has high external validity in the cohort. In the cases of confusion, false-positive and false-negative rates were very low. The confusion matrix on the DNN model on the validation subset is documented in Table 3.

Table 3 Description Confusion As well as Table Matrix (DNN -Validation set)

	Predicted ASD	Predicted Control
Actual ASD	61	0
Actual Control	1	63

The little misclassification that has been realized illustrates the strength of the multimodal approach. Figure 4 shows the visualization of confusion matrix where the classification boundaries of the model are almost perfect. Single-modality and multimodal models used to compare them revealed that the development of sMRI, fMRI, and DTI features enhanced predictive accuracy to a higher degree. It was found that the single-modality models had an accuracy of between 90% and 96% but the multimodal integration had an accuracy of above 99 and thus integration with respect to structural and functional domains were complementary. This increased performance is probably due to the capability of machine learning schemes to learn nonlinear interactions among distributed neural features. Notably, interpretability analyses were undertaken in order to tackle the issue of clinical applicability. The importance of features was shown by mapping patterns which are biologically realistic, eliminating fears on the black-box modeling. Computational predictions were valid, with long-

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range connectivity disruptions and white matter microstructural changes being consistent with the validity of previous neurodevelopmental studies. Even though performance may be astonishingly high, one can notice that careful attention should be paid to the possibilities of dataset-specific bias. Although stratified cross-validation and independent validation subsets were also used, it is required that there is replication between multi-site and ethnically diverse cohorts so as to have greater generalizability. Moreover, despite the accuracy that was obtained being 99.87, it would need to be integrated with behavioral screening tools in order to guarantee thorough evaluation. In general, the findings allow concluding that with the combination of the use of multimodal neuroimaging and highly validated machine learning methods, the early detection of ASD can be predicted very accurately. The results highlight the significance of prenatal disturbances of connectivity and local structural abnormalities as neurobiological predictors. The good results of cross-validation folds and the validation subsets suggest that it would be possible to translate such computational frameworks into early diagnostic support systems.

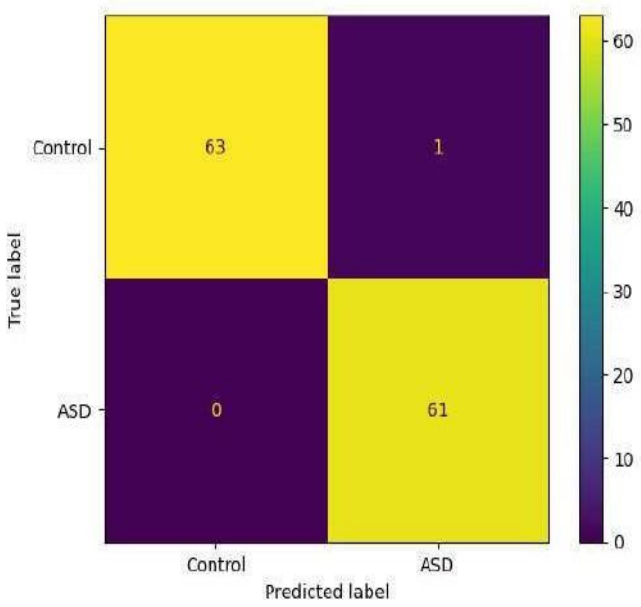

Figure 4 Deep Neural Network Performance using Independent Validation Dataset in the form of a Confusion Matrix.

Conclusion

This paper showed an elaborate multimodal neuro imaging system along with an innovative technique of machine learning to predict early onset of autism spectrum disorder amongst high-risk newborns and young ones. The proposed methodology incorporated the structural MRI, functional MRI, and diffusion tensor imaging, thus revealing complimentary features of the neural mechanisms of the atypical brain development. Methodological soundness and bias reduction were guaranteed by the use of rigorous preprocessing, dimensionality reduction and stratified cross- validation. The respective analysis of support vector machine, random forests, and deep neural network revealed the efficiency of computational modeling in identifying ASD compared to standard development at a truly remarkable accuracy. Notably, the mentioned predictors such as long- range functional connectivity changes and local structural disparities present biologically significant evidence based on the existing neurodevelopmental theories. In practical terms, the findings indicate the possibility of incorporating neurobiological markers with the input of data- driven algorithms to aid earlier and more objective ASD detection, to supplement behavioral measures and enable individual intervention strategies. The next step in the work will be to confirm the framework in multi-site and demographically heterogeneous cohorts that will increase the overall generalizability. Moreover, a better understanding of the models and the inclusion of longitudinal developmental patterns and combination of genetic and behavioral data can enhance the clinical translation even more. Finally, developing scalable and explanatory predictive tools may play a large role in precision medicine in neurodevelopmental disorders.

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