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Machine Learning-Based Exploration of Structural MRI for Autism Spectrum Disorder Detection

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Identifying reliable biomarkers for Autism Spectrum Disorder (ASD) is crucial for improving early diagnosis and intervention strategies. This study explores structural Magnetic Resonance Imaging (sMRI) as a biomarker for ASD using advanced machine learning techniques. Linear models (SVM, LR) and non-linear algorithms (Deep MLP, DenseNet-201) analyzed sMRI data from the ABIDE II dataset, which includes ASD and neurotypical controls (TC). The preprocessing pipeline included skull stripping, realignment, normalization, smoothing, Harvard-Oxford segmentation, and feature extraction of cortical thickness and volume. Feature vectors from the segmented sMRI served as inputs for classification models, with 10-fold cross-validation ensuring robust evaluation. Despite rigorous preprocessing and optimization, classification performance was modest. Deep MLP achieved the highest accuracy at 57.42%, with a validation accuracy of 58.29%, while SVM and LR showed modest accuracy around 56.3%, with challenges in precision and recall. These findings underscore the potential of cortical attributes of sMRI as ASD biomarkers and emphasize the need for further refinement in preprocessing, feature exploration, and model architecture to enhance predictive accuracy. This study highlights the exploration, promise and challenges of integrating structural MRI with machine learning for ASD detection.

Keywords: autism detection, sMRI, machine learning.

1. Introduction

Understanding the diverse and complex presentations within the neuropsychiatric continuum of Autism Spectrum Disorder (ASD) underscores the critical need for advancing detection methods, aiming to improve early intervention strategies and outcomes for individuals across the spectrum. Efforts to study ASD detection are driven by the variability in its presentation and the profound impact early intervention can have on long-term outcomes. By developing reliable detection methods, we can identify ASD earlier, allowing for tailored interventions that target specific needs during critical developmental stages. This approach not only enhances individual outcomes but also contributes to a deeper understanding of ASD's neurobiological underpinnings, paving the way for more effective therapeutic strategies.

Individuals within the ASD spectrum often exhibits persistent deficits in social communication, which can manifest as challenges in understanding nonverbal cues, maintaining reciprocal conversations, and developing meaningful relationships. These difficulties in social interaction may lead to feelings of isolation and exclusion, affecting their overall well-being and quality of life. Additionally, the presence of restricted and repetitive patterns of behavior, such as adherence to routines, intense focus on specific interests, and repetitive movements or actions, further contributes to the complexity of managing daily activities and adapting to changing environments.

For parents and caregivers, supporting individuals with ASD involves navigating these unique challenges while ensuring access to appropriate educational, therapeutic, and community resources. The variability in symptoms and strengths among individuals with ASD underscores the importance of personalized approaches to intervention and support. Despite these challenges, many individuals with ASD demonstrate remarkable strengths in areas such as attention to detail, problem-solving abilities, and creativity, highlighting the need for a holistic understanding that embraces neurodiversity.

The gold standard for diagnosing ASD is through extensive clinical evaluation conducted by the neurologist, developmental pediatrician and other clinical experts [1] by the use of Autism Diagnostic Observation Schedule (ADOS) [2] and can be with conjunction with Diagnostic and Statistical Manual of Mental Disorders (DSM IV and DSM-5)[3]. On-going researches aim to uncover the underlying biological and genetic factors contributing to ASD, particularly through the identification of reliable biomarkers that can predict autism. These biomarkers are essential for improving early diagnosis and intervention strategies, thereby enhancing outcomes for individuals across the spectrum. Research navigated through brain anatomy of patients [4] with autism has been examined noninvasively by several magnetic resonance imaging (MRI) in vivo for the last 25 years [5]. Several MRI techniques have been used to identify structural abnormalities in autistic subjects [6]. Because of its high contrast sensitivity and spatial resolution, MRI has become the method of choice for brain morphology investigation. Structural Magnetic Resonance Imaging (sMRI) has emerged as a promising tool in this regard, allowing for detailed anatomical images that facilitate exploration of brain abnormalities associated with ASD [7].

Structural MRI (sMRI) has afforded researchers various methods to investigate structural alterations in the brains of individuals with ASD. One of it is the morphological features such as surface area, cortical thickness, cortical curvature, folding index, and volume have been used to describe the structural changes in autism [8]. Research has identified that certain areas of the brain, including the frontal lobes, amygdala, cerebellum, corpus callosum, and basal ganglia, have been associated with autism[9]. Despite identifying these brain regions there is still no consensus in the scientific community about the specific structural changes in the brain associated with autism.

The growing emphasis on both fMRI and sMRI in ASD research necessitates the availability of large datasets for analysis. In this regard, the Autism Brain Imaging Data Exchange II (ABIDE II) which is a successor of the ABIDE I dataset, was established by the International Neuroimaging Laboratory, Psychiatric and Neurodevelopmental Disorders (INLP-PND) consortium to aide in various research techniques and strategies. ABIDE II is a publicly

available archive of MRI data from individuals with ASD and typically developing controls[10]. Various studies have explored brain abnormalities in the cerebellum [11], gray matter (GM) volumes [12] and brain functional connectivity (FC) [13] and others using statistical methods [14]. Machine learning (ML) models and deep learning (DL) techniques have recently become attractive to be applied in the diagnosis of diseases like Parkinson's [15] and epilepsy[16]. Conventional ML methods facilitate the exploration of complex abnormal imaging patterns and consider the relationships between different brain regions [17]. In ASD detection, however, some of the researches[18][19][20][21] extensively used both ML and DL on both fMRI and sMRI data to capture the effects of ASD on the brain. sMRI is commonly used to examine brain morphology because of its high contrast sensitivity, spatial resolution, and the fact that it does not need exposure to ionizing radiation; this is especially significant for children and adolescents [22]. sMRI delivers various sequences of brain tissue (e.g., T1, T2, and FLAIR) created by altering excitation and repetition durations to view multiple brain regions [23].

However, the primary challenge in applying machine learning to neuroimaging data for autism research is the curse of dimensionality [22],[24], [25]. This phenomenon arises when the number of features (p) exceeds the number of samples (n). To mitigate this issue, researchers typically explore two main strategies: increasing sample size or reducing feature space through methods such as feature selection or feature extraction. Given the constraints of limited computational resources in this study, expanding the sample size is impractical. Therefore, the study focused on feature extraction, a method that transforms original features obtained from segmentation processes into a reduced, yet informative, set of features in a lower-dimensional space. This approach aims to capture the essential underlying structures of the neuroimaging data more effectively [26].

The application of machine learning in ASD diagnosis using ABIDE II data is an opportunity to explore novel detection methods with promising potential. This study focuses on leveraging morphological brain attributes as inputs to a classifier. It employs a robust preprocessing pipeline to enhance raw data for classification purposes. Methodologically, the study integrates both traditional linear machine learning techniques such as SVM and LR, and advanced deep learning models like DeepMLP and CNN featuring DenseNet, a cutting-edge convolutional neural network. These approaches are designed to assess their effectiveness in identifying patterns within structural MRI datasets. By investigating the structural brain signatures associated with ASD, this research aims to deepen our understanding of the disorder and support the development of targeted interventions

2. Materials and Methods

In this study, fig. 1 shows a comprehensive account of the procedures and tools employed to investigate ASD using neuroimaging data from the ABIDE II dataset. The study design encompassed a preprocessing pipeline, segmentation, feature extraction, and detection.

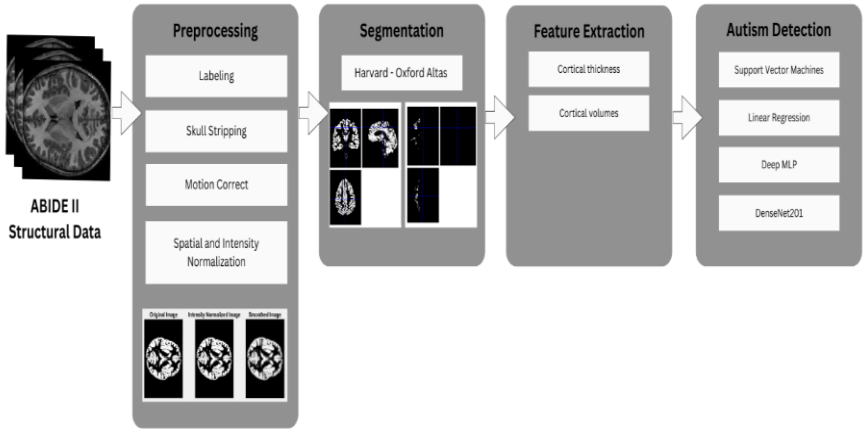

Figure 1.Block diagram of the proposed methodology

A. Dataset Acquisition

The ABIDE (Autism Brain Imaging Data Exchange) Dataset II contains MRI data used in this research, comprising a total of 1,054 subjects. The dataset includes two classes: the ASD group with 497 subjects and the typical control (TC) group with 555 individuals. For this study, only the baseline data was used for the sites that have longitudinal data. Alongside the MRI data, phenotypic and other pertinent information about the datasets, such as diagnosis, age, handedness, IQ, and more, were also downloaded for reference and labelling purposes. These datasets were obtained from the ABIDE II website. The Autism Brain Imaging Data Exchange II (ABIDE II) is a large-scale initiative that aggregates and shares brain imaging data from individuals with autism spectrum disorder (ASD) and typically developing controls. The ABIDE II datasets are contributed by numerous international sites, including the Barrow Neurological Institute (BN), Erasmus University Medical Center (EMC), ETH Zurich (ETH), Indiana University (IU), Institut Pasteur (IP), Katholieke Universiteit Leuven (KUL), Kennedy Krieger Institute (KKI), University of Miami (MIA), New York University 1 and 2 (NYU1, NYU2), Olin Neuropsychiatry Research Centre (ONRC), Oregon Health & Science University (OHSU), San Diego State University (SDSU), Stanford University (Stanford), Trinity Centre for Health Sciences, University of California, Los Angeles (UCLA), University of California Davis (USD), University of Utah School of Medicine(USM), University of Pittsburgh School of Medicine (UPSM). These sites contributed a variety of data, including structural and functional MRI scans, along with detailed phenotypic information. For this study, specifically, the structural MRI dataset was utilized.

B. Preprocessing pipeline

To prepare the structural MRI (sMRI) data for machine learning classification, a comprehensive preprocessing pipeline was employed to optimize data quality for feature extraction and model training. This process commenced with categorization or labeling and skull stripping, meticulously removing non-brain tissues such as the skull, scalp, and meninges to ensure the analysis focused exclusively on brain tissues. Subsequently, motion realignment corrected any head movements during data acquisition, thereby ensuring the model learns from an accurate representation of the brain's anatomy. Spatial normalization was performed to

standardize the anatomical space across different images, facilitating enhanced data comparability and consistency in analysis. Intensity normalization adjusted the intensity values of the NIfTI images to a range of [0, 1], addressing variations in voxel intensity caused by scanner settings or head position. This normalization process, which used the minimum and maximum intensity values within each image, was crucial for mitigating technical artifacts and allowing the model to concentrate on underlying anatomical features. By integrating these preprocessing steps, high-quality, standardized representations of brain anatomy were achieved within the MRI data. This meticulous preprocessing ultimately enhances the robustness and generalizability of machine learning models applied to brain image classification tasks.

C. Cortical Segmentation

In this study, cortical parcellation was conducted using the Harvard-Oxford (HO) Atlas, which segments the cortical surface of the brain into distinct regions based on anatomical landmarks, aligning each subject's brain anatomy to a standardized map. The HO atlas used in this study was downloaded from https://identifiers.org/neurovault.image:1698. During the parcellation process, the preprocessed structural MRI (sMRI) data was segmented into predefined regions. Each voxel in the MRI image was assigned a label corresponding to a specific cortical region as defined by the atlas.

Following the parcellation, cortical thickness and cortical volume were extracted from the segmented regions. These morphological features were then utilized as input for various machine learning classifiers, facilitating the analysis and classification of the data. Output of this step are numerical feature matrices of cortical thickness and cortical volume.

D. Machine Learning

Various classifiers, both linear and non-linear, were employed to classify Autism Spectrum Disorder (ASD) using features extracted in earlier stages of the study. Prior to classification, cortical thickness and cortical volume matrices were concatenated for each subject. This concatenation ensured that each subject's features were represented as a unified input vector, facilitating the classification process across different machine learning models.

A linear kernel SVM model was employed in this study. X_train and y_train represent the training data used to train the Support Vector Machine (SVM) classifier. X_train is a matrix where each row corresponds to a subject's feature vector (concatenated cortical volumes and thickness), and y_train is a vector of labels indicating whether each subject has ASD (1) or is a Typical Control (0). These data are learned by the model and finds a linear hyperplane that optimally separates the feature vectors of ASD and TC subjects based on their cortical volume and thickness features. The dataset is divided into 10 subsets (folds). During each iteration, 9 folds are used for training, and 1 fold is used for validation. This approach ensures that every data point is used for both training and validation exactly once, providing a robust estimate of the model’s performance.

Linear regression was implemented Logistic Regression employed to classify between ASD and TC based on cortical volume and cortical thickness features extracted from MRI data. Stratified K-Fold cross-validation is used to split the data into training and validation sets across 10-fold cross validation. This ensures that each fold preserves the percentage of

samples for each class. Within each fold, a logistic regression model is trained on the training set on both classes. The model predicts labels (y_pred) and probabilities (y_proba) on the validation set (X_test). y_pred indicates whether each MRI sample is predicted to belong to the ASD group (1) or the TC group (0).

Moreover, DenseNet-201 is a convolutional neural network architecture that belongs to the DenseNet family. It is a variant with 201 layers. It has been designed to be deep while maintaining efficiency in terms of computational resources and memory usage. Initially, this model requires different dimensions of feature data so, data is first reshaped to fit the classifier's requirements. The output layer is then set to a binary output layer ready for classification. Stochastic Gradient Descent with Momentum (SDG) is used as an optimizer that incorporates momentum to accelerate convergence in the gradient descent process. DenseNet-201 effectively leverages its deep learning capabilities to learn discriminative features from cortical MRI data, distinguishing between ASD and TC subjects based on their cortical structure. Cross-validation approach ensures that the model's performance is robustly evaluated, providing insights into its generalization ability and reliability across different data splits.

Finally, a Deep MLP (Multilayer Perceptron) is utilized as a classification model where it is a type of artificial neural network that consists of multiple layers of neurons, each layer fully connected to the next one. Beginning with the integration of cortical volume and thickness features extracted from MRI scans, the process unfolds through a series of meticulously orchestrated steps. These include the standardization of input data to ensure uniformity in feature contributions, followed by a cross-validation strategy that divides the dataset into folds for robust model evaluation. The heart of the operation lies in a Deep MLP configuration, comprising multiple densely connected layers enriched with ReLU activations and dropout regularization to foster complex pattern recognition while guarding against overfitting.

Through iterative training epochs facilitated by Adam optimization and monitored by binary cross-entropy loss, the model learns to predict probabilities of ASD classification with sigmoid output activation. Sigmoid are in the range [0,1]. This property makes it suitable for binary classification tasks where the output can be interpreted as a probability of belonging to one class (e.g., ASD or TC). This approach not only aims for high accuracy but also strives to uncover meaningful insights into cortical structural differences associated with ASD, fostering advancements in neuroscientific understanding and diagnostic precision.

3. Results and Discussion

Table 1. Average performance for each model in a 10-fold cross validation

Model	Accuracy	Precision	Recall	AUC	Validation Accuracy
SVM	0.5633	NaN	0.000145	0.5256	0.5633
LR	0.5631	0.4609	0.0018	0.5279	0.5631
Deep MLP	0.5742	0.6892	0.1363	0.5949	0.5829
DenseNet201	0.5321	0.60596	0.39139	-	50.4763

Table 1 shows the mean accuracy, precision, recall, AUC, and validation accuracy of each classifier in classifying cortical features from the preprocessed sMRI data. SVM achieved an accuracy of 56.33% with consistent performance in validation accuracy. However, precision

could not be calculated, because of potential issues factor calculating theaffecting precision. Similarly, LR achieved an accuracy of 56.31% and a validation accuracy of 56.31%. Its precision (46.09%) and recall (0.18%) were relatively low, indicating challenges in correctly identifying positive cases.

Moreover, DenseNet201 had the lowest accuracy at 53.21% and a validation accuracy of 50.48%. While it demonstrated moderate precision (60.60%) and recall (39.14%), its overall performance in discriminating between classes was suboptimal. Deep MLP, on the otherhand demonstrated the highest accuracy among the models at 57.42%, with good validation accuracy (58.29%). It also showed the highest average precision (68.92%) and moderate recall (13.63%), suggesting it could effectively capture complex patterns in the data.

Based on the results, linear classifiers such as SVM and LR exhibited comparable but modest accuracy around 56.3%, indicating their limited capability to distinguish between ASD and typical controls. However, they struggled to achieve high precision and recall, highlighting potential limitations in capturing the complex patterns inherent in the data. In contrast, the non-linear Deep MLP model outperformed the linear classifiers with an accuracy of 57.4%, demonstrating superior performance in learning intricate data relationships. Its higher average precision (68.9%) and moderate recall (13.6%) suggest that the Deep MLP may be more suitable for tasks requiring nuanced classification of ASD based on structural indices.

4. Conclusions

The conclusion of this study underscores the potential of machine learning models, particularly deep learning approaches like Deep MLP, in classifying autism spectrum disorder (ASD) based on cortical structural features. While linear classifiers such as SVM and LR provide a baseline, they exhibit limitations in capturing complex relationships within the data. The superior performance of Deep MLP in accuracy and ability to discern patterns suggests its suitability for more nuanced ASD classification tasks. However, the models currently fall short of medical standards due to challenges in interpretability and integration into clinical diagnostic frameworks. Future research should focus on enhancing model interpretability, potentially through multimodal dataset integration, to improve clinical utility and reliability in diagnosing ASD.

5. Implications

Based from the results of the experiments, the Deep MLP model outperformed SVM, LR, and DenseNet201 in terms of accuracy and precision, suggesting that its ability to learn complex representations from your data might be more suitable for this kind of classification task. Regarding the robustness of the models, the variability observed across different metrics (accuracy, precision, recall) underscores the importance of evaluating model robustness and generalizability across diverse datasets and potential biases.

In terms of clinical relevance, the study's results suggest that while the models hold potential for applications like diagnosis or risk assessment, they currently do not meet medical standards. This is primarily due to the necessity for improved explanation of model decisions

and their integration into established diagnostic frameworks. Therefore, relying solely on cortical features such as thickness and volume may not reliably detect the presence or absence of the disorder. To enhance classification performance, it is advisable to consider multimodal datasets that integrate other types of data, such as resting-state data from the ABIDE dataset, which could provide complementary insights into autism spectrum disorders.

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