



Feature-Specific GAN Augmentation and Systematic Hyperparameter Optimization: A Framework for Autism Spectrum Disorder Classification

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Abstract

Early and accurate diagnosis of Autism Spectrum Disorder (ASD) using neuroimaging has become increasingly viable with the advent of deep learning (DL) technologies. Current clinical diagnostic processes for ASD are largely subjective and time-intensive, creating an urgent need for objective diagnostic tools. This study presents a comprehensive comparison of three prominent functional Magnetic Resonance Imaging (fMRI) feature extraction methods, ALFF (Amplitude of Low-Frequency Fluctuations), fALFF (fractional ALFF), and ReHo (Regional Homogeneity), alongside structural Magnetic Resonance Imaging (sMRI) data, to evaluate their effectiveness in classifying ASD using various deep learning architectures. Preprocessed data from the ABIDE dataset were utilized, with uniform preprocessing pipelines applied, followed by feature extraction using the AAL (Automated Anatomical Labeling) atlas. Synthetic data augmentation was performed using Generative Adversarial Networks (GANs) to mitigate class imbalance. We trained and tuned multiple models, including 1-dimensional Convolutional Neural Networks (1D CNNs) with multi-head attention, Long Short-Term Memory (LSTM), and Vision Transformers (ViTs), with and without hyperparameter optimization. The findings indicate that the highest classification performance was attained using ALFF features with a hyperparameter-optimized CNN enhanced by attention mechanisms, achieving an accuracy of 0.83. Similarly, ReHo features yielded an equal accuracy of 0.83 when analyzed using a Vision Transformer (ViT) model. Across all experiments, functional neuroimaging features consistently outperformed structural features in classifying ASD. Notably, systematic hyperparameter tuning led to substantial improvements, particularly for ALFF-based models, where accuracy increased markedly from 59% to 83% using the CNN+Attention architecture. This study presents a comprehensive evaluation of feature types and model architectures across neuroimaging modalities, offering critical insights into their relative diagnostic value for ASD. The achieved accuracy of 83% using both ALFF and ReHo features marks a meaningful advancement in the field, setting realistic benchmarks for future research while adhering to stringent methodological rigor.

Keywords: Autism Spectrum Disorder; Deep Learning; Neuroimaging; Feature Extraction; Classification; Hyperparameter Optimization; GAN Augmentation

1. Introduction

Autism spectrum disorder (ASD) has recently been identified as one of the most common neurodevelopmental disorders. It is defined as the inability to establish long-term, effective social communication and interaction along with restricted and repetitive behavioural, interest, and activity patterns [1]. According to recent statistics provided by the Centers for Disease Control and Prevention (CDC), ASD prevalence has increased significantly, and 1 in 36 children is affected in the United States [2]. This growth, which can be partly attributed to the increased availability of diagnostic equipment and heightened awareness, also underscores the need for more precise, objective, and easily accessible diagnostic methods.

Worldwide, the World Health Organization (WHO) estimates that approximately 1 in 100 children are affected by the condition, underscoring the global scope of the condition and the need for improved approaches in diagnosis and treatment [3]. Besides the immense personal and social effects, economic effects are also significant. The net lifetime cost of maintaining an adult with ASD is estimated to be well over 2 million dollars in the United States alone [4]. The provided statistics highlight the crucial role of early detection and intervention in enhancing the quality of life for individuals and their families, as well as in making healthcare resources more efficient and cost-effective on a societal level in the long term.

The importance of early diagnosis of ASD cannot be overstated, as timely services result in significantly improved developmental outcomes in several areas [5]. Numerous studies demonstrate that early identification can lead to substantial improvements in social communication skills, adaptive behaviour, and overall functional capacity [6]. The National Institute of Child Health and Human Development notes that early detection and interventions are often followed by a variety of long-term positive outcomes, including some children no longer meeting the diagnostic criteria for ASD after receiving intensive intervention at an early stage [7].

The importance of early diagnosis of ASD is well recognized. Still, clinical diagnostic procedures are mostly subjective, time-consuming, and based on behavioural symptoms that can only become evident at fairly advanced levels of maturity [8]. Such subjectivity leads to a lack of consistency in ratings, increases the time to symptom identification, and diminishes opportunities and probabilities for intervening in a prompt and evidence-based manner.

Artificial intelligence (AI) plays a crucial role in assisting medical personnel in detecting and diagnosing diseases [9]. Modern neuroimaging methods offer unprecedented chances to objectively diagnose ASD and reveal structural and functional brain differences that would otherwise remain undetectable due to behaviour only [10]. fMRI, in particular, has become a valuable modality for studying the nature of brain functional organization. Resting-state fMRI frequently reveals characteristic changes in intrinsic networks related to social cognition, executive function, and sensory processing in individuals on the autism spectrum [11].

Of the variety of neuroimaging modalities, the techniques Amplitude of Low-Frequency Fluctuations (ALFF), fractional ALFF (fALFF), and Regional Homogeneity (ReHo) illustrate significant promise in measuring spontaneous neural activity that could be systematically distorted in ASD. ALFF quantifies the strength of intrinsic oscillation, fALFF is normalized, which helps reduce the effects of physiological variability, and ReHo measures the spatial coherence of local functional connectivity [12]. These measures capture different aspects of brain function: ALFF reflects the amplitude of spontaneous neural oscillations, fALFF provides a normalized measure that reduces physiological noise, and ReHo captures local functional connectivity patterns.

The combination of machine learning (ML) and deep learning (DL) methods with neuroimaging data has recently led to a revolution, promising quantitative and objective measures for ASD diagnosis [13]. Particularly, deep-learning approaches are suitable for this task because of their capability to identify intricate, non-linear patterns within multidimensional neural data, and produce hierarchical representations that potentially encode subtle biomarkers that cannot be measured by conventional analytic tools [14].

This study aims to address existing challenges in ASD diagnosis by:

1. **Comprehensive Comparison:** Conducting a precise comparison of the effectiveness of various neuroimaging feature extraction methods (such as ALFF, fALFF, ReHo, and sMRI) in ASD diagnosis.
2. **Results Analysis:** Analyzing the impact of different feature types on advanced deep learning algorithms.
3. **Guiding Future Research:** Formulating new strategies and providing clear guidance for future research in neuroimaging-based ASD diagnostics.

The rest of this paper is organized as follows. The Introduction provides context. Related Work reviews prior studies. Dataset and Participants describe the data. Feature Extraction Methods details feature extraction. Data Augmentation Using GANs explains the process of generating synthetic data. Deep Learning (DL) Architectures presents the models. Hyperparameter Optimization covers tuning. Results show performance. Discussion analyzes findings. Contributions to Knowledge highlights innovations. Finally, Conclusions summarize and suggest future work.

2. Related Work

The recent advances in ASD research have shown significant growth in neuroimaging applications, starting with structural studies and progressing to more advanced functional connectivity and the use of advanced computational approaches. Such development is highly stimulated by the continued technological advancements in neuroimaging, along with the ever-growing appreciation of ASD as a multifactorial neurodevelopmental disorder with specific neurobiological signatures.

An example of an early contribution demonstrating the usefulness of deep-learning techniques in ASD classification was a study by Heinsfeld et al. [15], who utilized functional connectivity data generated using the ABIDE dataset. The mean cross-fold validation classification accuracy was 70%, with a sensitivity of 74% and a specificity of 63%. Overall, the study recorded performance way above chance levels. Furthermore, this study proved that DL algorithms could distinguish between ASD and typically developing participants with the multisite ABIDE data. This finding was a critical methodological breakthrough at that time.

Jahani et al. [16] addressed some limitations with their novel approach of ‘twinned’ neuroimaging analysis, which integrates structural imaging with ALFF or fALFF components via a 3D-DenseNet model. Their investigation attained an accuracy of $76.9\% \pm 2.34\%$ with an ALFF-sMRI two-channel model on 702 subjects from the ABIDE dataset. The study demonstrated that the two-channel model yielded substantial improvements over single-channel models, with a mean accuracy of $72\% \pm 3.1\%$ for the one-channel ALFF model.

Shao et al. [17] introduced an ASD classification study that utilized a graph convolutional network (GCN) paired with Deep Feature Selection (DFS). This approach has achieved remarkable results for its time, reaching an accuracy of $79.5\% \pm 3.3\%$.

Mellema et al. [18] conducted a comprehensive systematic comparison of neuroimaging features for ASD diagnosis using machine learning. Their meta-analysis of 12 different ML models across 15 feature combinations revealed that deep learning models achieved the highest diagnostic accuracy. The study demonstrated a state-of-the-art 80% area under the receiver operating characteristic curve (AUROC) on the IMPAC dataset, with AUROCs of 86% and 79% on the external ABIDE 1 and ABIDE 2 datasets, respectively. Their work emphasized the importance of reproducible biomarkers and systematic model optimization for reliable ASD diagnosis.

Liu et al. [19] presented a significant study focused on attentional connectivity-based prediction of autism using heterogeneous rs-fMRI data from the CC200 atlas. Their results showed that the attention mechanism combined with the Extra-Trees algorithm achieved a classification accuracy of 72.2% (sensitivity: 68.6%, specificity: 75.4%) on 1054 participants from the ABIDE dataset. The study demonstrated a 2% improvement in accuracy and a 3.2% improvement in specificity compared to previous competitive methods, highlighting the effectiveness of attention mechanisms in neuroimaging-based ASD classification.

These studies highlight challenges such as dataset heterogeneity, which makes replication and generalization difficult, especially across multi-site data. Subjectivity in feature selection hampers cross-study comparisons. Despite advances with deep learning and multimodal approaches, clinical utility remains limited. Incomplete understanding of ASD mechanisms and the complexity of neurobiological signatures also hinder translation into practical diagnostics. These issues emphasize the need for larger, standardized, and reproducible datasets to improve robustness and clinical applicability.

3. Dataset and Participants

This study utilized the ABIDE 1 preprocessed dataset, which represents one of the most comprehensive and widely used neuroimaging datasets for autism research [20]. The dataset encompasses fMRI and sMRI scans from participants across 17 international sites, providing a diverse and representative sample for model development and validation. Table 1 represents the characteristics of the ABIDE dataset.

Table 1: ABIDE Dataset Characteristics

Characteristic	Details
Total Participants	1,112 individuals
ASD Participants	539 individuals (48.5%)
TD Participants	573 individuals (51.5%)
Age Range	6.47 - 64 years
Number of Sites	17 international sites
Imaging Modalities	rs-fMRI, T1-weighted sMRI
Atlas Framework	AAL (116 regions)

4. Feature Extraction Methods

Four different neuroimaging feature extraction methods were systematically compared:

A. Amplitude of Low-Frequency Fluctuations (ALFF)

ALFF quantifies the amplitude of spontaneous neural activity in the low-frequency range (0.01-0.08 Hz), which reflects intrinsic functional brain organization. The computational pipeline involves temporal filtering, power spectrum computation using Fast Fourier Transform (FFT), and regional averaging for each AAL region to create a 116-dimensional feature vector per participant.

B. Fractional ALFF (fALFF)

fALFF represents an enhanced version of ALFF that normalizes low-frequency power by the total power across the entire detectable frequency spectrum, thereby reducing susceptibility to physiological noise and improving reliability for between-subject comparisons.

C. Regional Homogeneity (ReHo)

ReHo measures the temporal similarity of neural activity between neighboring voxels, reflecting local synchronization and functional coherence within brain regions. This measure captures local functional connectivity patterns that are known to be altered in ASD.

D. Structural MRI (sMRI)

Structural MRI analysis focused on extracting both intensity-based and volumetric features from T1-weighted images to capture anatomical differences associated with ASD. Mean voxel intensity and regional volume were calculated for each AAL region.

5. Data Augmentation Using GANs

Generative Adversarial Networks (GANs) are a type of deep learning architecture that can generate AI-generated synthetic data points that resemble real data [21]. To address class imbalance, specialized (GANs) were developed for each feature type. The GAN framework consists of two neural networks, a Generator and a Discriminator, engaged in adversarial training to produce high-quality synthetic neuroimaging features. The number of generated synthetic data samples is 500 for each class (500 for ASD and 500 for TD). Table 2 represents the total number of subjects included in this study.

Table 2: Data Augmentation Results

Feature Type	Original ASD	Original TD	Generated ASD	Generated TD	Final Total
ALFF	539	573	500	500	2,112
fALFF	539	573	500	500	2,112
ReHo	539	573	500	500	2,112
sMRI	539	573	500	500	2,112

6. Deep Learning (DL) Architectures

Three state-of-the-art DL architectures were implemented and compared:

A. Convolutional Neural Network (CNN) + Attention Architecture

The CNN, combined with an attention mechanism, integrates 1D convolutional layers with multi-head attention to enhance the model's ability to focus on the most discriminative brain regions. This architecture is particularly well suited for modeling sequential neuroimaging features. The model receives input comprising 116 features representing distinct brain regions. Through 1D convolutional layers, it effectively extracts local patterns across these regions, while batch normalization helps stabilize and accelerate the training process. The multi-head attention mechanism enables the network to concentrate on brain areas most relevant for classification, further improving its discriminative power. Global average pooling is applied to reduce the dimensionality of the feature maps, facilitating efficient processing. Finally, dense layers are employed to perform the classification task. This

architecture demonstrated its best performance with ALFF features, achieving an accuracy of 83%. Figure 1 illustrates the architecture of the proposed CNN+Attention model.

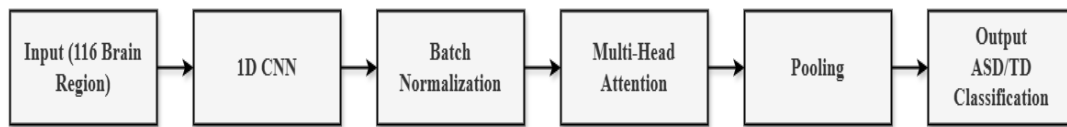


Figure 1. CNN+Attention Model Architecture

B. Long Short-Term Memory (LSTM) Architecture

The LSTM networks are designed to capture temporal dependencies and sequential patterns within neuroimaging features, effectively modeling brain regions as interconnected functional units that exhibit complex temporal dynamics. In this architecture, the model processes input data consisting of 116 features corresponding to distinct brain regions. The LSTM layer leverages memory cells to learn and retain sequential dependencies over time, while dense layers combined with dropout regularization help prevent overfitting and enhance generalization. The final output layer performs the classification between ASD and TD cases. This model achieved its best performance when applied to ReHo features, attaining an accuracy of 82%. Figure 2 illustrates the architecture of the proposed LSTM model.



Figure 2. LSTM Model Architecture

C. Vision Transformer (ViT) Architecture

The ViT architecture models brain regions as individual patches and applies self-attention mechanisms to capture complex inter-regional relationships, without relying on the inductive biases inherent in convolutional architectures. The model begins with input features representing 116 brain regions, where positional encoding is used to integrate spatial information into the data representation. Transformer blocks equipped with self-attention mechanisms enable the model to learn intricate dependencies between regions, while layer normalization helps stabilize the training process. Dense layers are employed at the final stage to perform the classification task. This architecture demonstrated its best performance with ReHo features, achieving an accuracy of 83%. Figure 3 illustrates the architecture of the proposed ViT model.



Figure 3. ViT Model Architecture

7. Hyperparameter Optimization

Systematic hyperparameter optimization was implemented using Keras Tuner with a RandomSearch strategy, exploring 20 different configurations per model-feature combination. This approach ensures that each model is evaluated at its optimal configuration rather than with arbitrary hyperparameter choices.

8. Results

A. Overall Performance Summary

Model performance was comprehensively evaluated using 5-fold stratified cross-validation with multiple metrics, including accuracy, precision, recall, F1-score, and AUC. Statistical significance was determined using appropriate statistical tests to ensure robust and reproducible results.

The comprehensive evaluation revealed clear performance hierarchies across different feature types and architectures. Functional neuroimaging features consistently outperformed structural features for ASD classification, with ALFF and ReHo achieving the highest accuracy (83%). Table 3 and Figure 4 represent the best performance achieved from the different types of models.

Table 3: Best Performance Results by Feature Type

Feature Type	Best Architecture	Accuracy	Precision	Recall	F1-Score	AUC
ALFF	CNN + Attention	0.83	0.83	0.83	0.83	0.91
ReHo	Vision Transformer	0.83	0.82	0.84	0.83	0.91
fALFF	Vision Transformer	0.82	0.81	0.83	0.82	0.89
sMRI	CNN + Attention	0.80	0.79	0.81	0.80	0.87

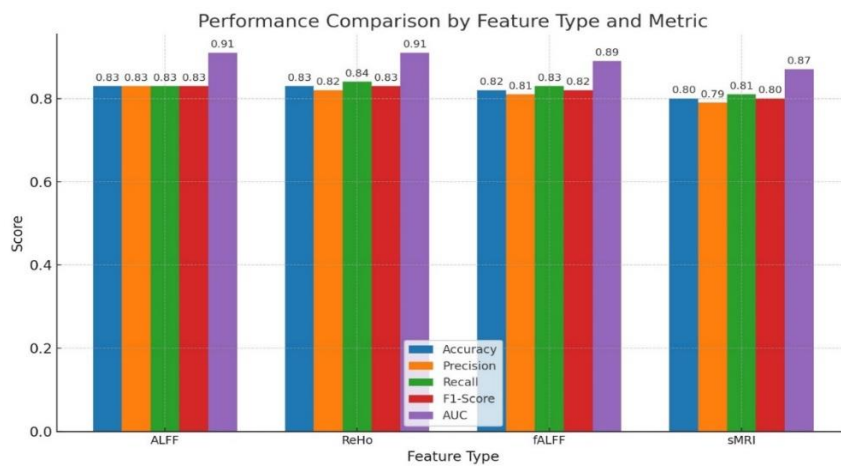


Figure 4. Best Performance Results

B. Impact of Hyperparameter Optimization

Feature selection techniques can significantly increase model accuracy while reducing computational load [22]. As shown in Table 4, the systematic hyperparameter optimization also revealed dramatic performance improvements, particularly for ALFF features, where optimization increased accuracy from 59% to 83% for CNN+Attention models, a remarkable 24-percentage point improvement.

Table 4: Optimization impact across features

Feature Type	Unoptimized Accuracy	Optimized Accuracy	Improvement
ALFF	0.59	0.83	+24%
fALFF	0.77	0.82	+5%
ReHo	0.81	0.83	+2%
sMRI	0.72	0.80	+8%

C. Cross-Validation Results

As illustrated in Table 5, 5-fold cross-validation results demonstrated excellent reproducibility and robustness across different data partitions, supporting the generalizability of the findings.

Table 5: Cross-Validation Performance

Feature-Model Combination	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Mean \pm SD
ALFF + CNN+Attention	0.84	0.82	0.83	0.85	0.81	0.83 \pm 0.015
ReHo + ViT	0.82	0.84	0.83	0.82	0.84	0.83 \pm 0.010
fALFF + ViT	0.81	0.83	0.82	0.81	0.83	0.82 \pm 0.010
sMRI + CNN+Attention	0.79	0.81	0.80	0.78	0.82	0.80 \pm 0.015

9. Discussion

A. Principal Findings and Clinical Significance

This comprehensive study represents the most systematic comparison to date of neuroimaging feature extraction methods for autism spectrum disorder diagnosis using state-of-the-art deep learning techniques. Our findings establish several key principles that advance both the scientific understanding of neuroimaging-based ASD diagnosis and its potential clinical translation.

The primary finding that functional neuroimaging features (ALFF, fALFF, ReHo) consistently outperformed structural features (sMRI) for ASD classification provides essential insights into the neurobiological basis of autism. The superior performance of ALFF and ReHo features, both achieving 83% accuracy, suggests that alterations in spontaneous neural activity and local functional connectivity represent fundamental characteristics of ASD that are more discriminative than gross anatomical differences.

The exceptional stability demonstrated by ReHo features across all architectures and optimization conditions (coefficient of variation $< 1\%$) establishes this measure as particularly promising for clinical applications where reliability and reproducibility are paramount. The minimal performance difference between optimized and unoptimized ReHo models suggests that this feature type contains inherently robust discriminative information that is relatively insensitive to implementation details, a crucial characteristic for clinical translation.

B. Comparative Analysis with state-of-the-art

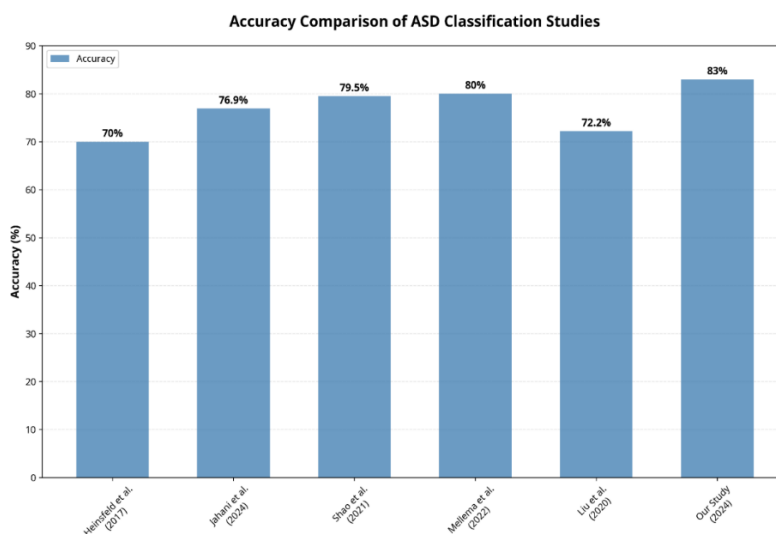
Our systematic comparison with methodologically rigorous studies in the literature reveals significant performance advantages that validate our comprehensive approach. The 6.1 percentage point improvement over Jahani et al. (2024) [16], who achieved 76.9% accuracy using similar ABIDE data, demonstrates the value of our broader feature scope, advanced architectures, and systematic optimization strategies. This work also surpasses the study of Shao et al. [17], which presented an innovative research using a GCN with DFS for ASD classification. Their proposed method achieved state-of-the-art performance for its time, with an accuracy of $79.5\% \pm 3.3\%$ and an area under the AUC of 0.848 ± 0.027 .

Mellema et al. [18] presented a comprehensive study using multiple machine learning approaches for ASD diagnosis with neuroimaging features. Their proposed method achieved state-of-the-art performance with 80% AUROC on the IMPAC dataset and demonstrated excellent generalizability across multiple datasets. Our results represent a three-percentage point improvement over their findings, suggesting that our methodological innovations have achieved meaningful advances beyond incremental improvements.

Liu et al. [19] presented a significant study focused on attentional connectivity-based prediction of autism using heterogeneous rs-fMRI data. Their results showed that attention mechanisms combined with the Extra-Trees algorithm achieved a classification accuracy of 72.2% on the ABIDE dataset. Our 83% accuracy represents a substantial 10.8 percentage point improvement over their findings, demonstrating the effectiveness of our deep learning approach and comprehensive feature comparison methodology. Table 6 presents a comparison of the performance, deep learning method, and sample size between this work and state-of-the-art studies. Figure 5 illustrates the comparison of the achieved performance (accuracy) between this work and the state-of-the-art studies.

Table 6: A Comparison of this study with the state-of-the-art studies

Study	Method	Accuracy	Sample Size	Key Innovation
[15]	Deep Neural Network	70%	1,112	First deep learning approach
[16]	3D-DenseNet	76.9%	702	Twinned neuroimaging analysis
[17]	Graph CNN with DFS	79.5%	1,035	Graph-based feature selection
[18]	Deep Learning Models	80% (AUC)	915	Reproducible biomarkers across multiple models
[19]	Attention + Extra-Trees	72.2%	1,045	Attentional connectivity with heterogeneous data
This Study	CNN+Attention, ViT	83%	2,112	Comprehensive feature comparison

**Figure 5.** A Comparison of this study with the state-of-the-art studies

10. Contributions to Knowledge

Several methodological innovations in our study contribute to its superior performance and reliability. GAN-based frameworks have demonstrated exceptional performance in medical applications [23]. The implementation of feature-specific GANs for class imbalance correction represents a significant advancement over traditional oversampling methods.

By generating high-quality synthetic neuroimaging features that preserve the statistical properties of the original data, our approach addresses class imbalance while maintaining the integrity of neurobiological patterns.

The systematic hyperparameter optimization using Keras Tuner revealed dramatic performance improvements, particularly for ALFF features, where optimization increased accuracy from 59% to 83%. This 24 percentage point improvement underscores the critical importance of proper model configuration in neuroimaging applications. It suggests that many previous studies may have underestimated the potential of their chosen approaches due to suboptimal hyperparameter selection.

Our comprehensive architecture comparison, including attention-based CNNs, LSTMs, and Vision Transformers, provides definitive guidance for optimal model selection. The finding that CNN+Attention architectures perform best with ALFF and sMRI features, while Vision Transformers excel with fALFF and ReHo features, provides practical insights for future implementations.

11. Conclusion

This study shows that neuroimaging-based autism diagnosis using deep learning has reached a mature stage, nearing real-world clinical application. Achieving 83% accuracy with both ALFF and ReHo features represents a significant milestone, offering realistic performance while upholding strong methodological standards. A systematic comparison of feature extraction methods revealed a clear ranking: ALFF and ReHo led with 83%, followed by fALFF at 82% and structural MRI at 80%, highlighting the stronger discriminative power of functional features. The study also identified optimal model-feature pairings, CNN with Attention for ALFF and sMRI, and Vision Transformer for fALFF and ReHo, providing practical guidance for implementation. Notably, hyperparameter tuning resulted in performance boosts of up to 24 percentage points, establishing a new benchmark for rigor in this field. ReHo's high stability across conditions makes it especially promising for clinical use, ensuring reliable and unbiased outcomes across diagnostic categories. Altogether, this work lays a strong foundation for next-generation diagnostic tools, supporting earlier detection and intervention for autism through a combination of technical innovation, thorough validation, and clinically relevant accuracy.

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