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NeuroAI-ADHD: Multimodal Deep Learning for ADHD Detection from Resting-State fMRI Using Ensemble BiLSTM-Transformer Architecture with Explainable AI and Full-Stack Clinical Deployment

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Abstract: ***Attention-Deficit/Hyperactivity Disorder (ADHD) is one of the most prevalent neurodevelopmental conditions, affecting approximately 5–10% of school-age children and 2–5% of adults globally. Traditional diagnosis relies exclusively on subjective behavioural assessments and clinical interviews, which are susceptible to observer bias, symptom masking, and comorbidity confounding. This work presents NeuroAI-ADHD, a multimodal deep learning framework that integrates resting-state functional MRI (fMRI) brain connectivity features with phenotypic variables — including age, sex, IQ, and handedness — for objective ADHD classification. Functional connectivity matrices were derived using the Harvard-Oxford cortical atlas via nilearn, yielding 6,000+ region-of-interest time-series correlation features per subject. A BiLSTM-Transformer ensemble model was trained on the ADHD-200 dataset (n = 768 labelled records after exclusions), achieving 66.3% accuracy and ROC-AUC of 0.77 on a stratified held-out test set. Class imbalance was addressed through computed balanced class weights. Feature-importance-based Explainable AI (XAI) maps were generated to identify the top contributing brain regions per prediction.A full-stack clinical web application was deployed, incorporating doctor authentication, real-time fMRI upload and validation, MRI visualisation with atlas-overlaid region highlighting, and PDF report export. The resulting system demonstrates a clinically interpretable, end-to-end pipeline for ADHD detection from neuroimaging data.***

Index Terms: ***ADHD, resting-state fMRI, functional connectivity, BiLSTM, Transformer, ensemble learning, Explainable AI, Harvard-Oxford atlas, FastAPI, React, multimodal deep learning.***

I. INTRODUCTION

Atention-Deficit/Hyperactivity Disorder (ADHD) is characterised by persistent patterns of inattention, hyperactivity, and impulsivity that interfere substantially with daily functioning and development [1]. It represents one of the most common neurodevelopmental disorders, with global prevalence estimates of 5–10% among children and 2–5% among adults [2]. Despite its prevalence, ADHD remains systematically underdiagnosed and misdiagnosed, primarily because current diagnostic criteria rely on subjective, interview-based behavioural assessments without objective neurobiological confirmation.

Magnetic resonance imaging, particularly resting-state functional MRI (rs-fMRI), has emerged as a powerful tool for characterising the neural correlates of ADHD. Resting-state fMRI captures spontaneous low-frequency fluctuations in blood-oxygen-level-dependent (BOLD) signals, which reflect intrinsic functional connectivity between brain regions. Aberrant functional connectivity in prefrontal-striatal, default mode, and fronto-parietal networks has been consistently reported in ADHD populations [3,4]. These neuroimaging findings provide a compelling basis for data-driven, objective ADHD classification.

A. Clinical Motivation and Problem Significance

The clinical diagnosis of ADHD is fundamentally constrained by its reliance on subjective symptom reports from parents, teachers, and clinicians, compounded by cultural variability in symptom expression and significant comorbidity with anxiety, depression, and learning disabilities. Rating scales such as the Conners Rating Scale and Vanderbilt Assessment introduce substantial inter-rater variability. Neuroimaging-based classification offers the prospect of an objective, reproducible diagnostic biomarker that can complement clinical assessment, stratify patients by neurobiological subtype, and monitor treatment response over time.

B. Limitations of Existing Approaches

Existing deep learning approaches to ADHD detection from neuroimaging suffer from several limitations. First, the majority of published methods evaluate models on single-site datasets without controlling for site-induced variance [5]. Second, most approaches treat fMRI and phenotypic data as independent modalities rather than integrating them in a unified multimodal framework [6]. Third, few studies incorporate explainability mechanisms capable of identifying clinically interpretable neural correlates. Fourth, no prior work has embedded the complete pipeline within a deployable full-stack application.

C. Contributions of This Work

This paper addresses these limitations through five principal contributions:

- A multimodal deep learning framework combining resting-state fMRI functional connectivity (6,000+ features via Harvard-Oxford atlas) with phenotypic variables for ADHD classification.
- A BiLSTM-Transformer ensemble model achieving 66.3% accuracy and ROC-AUC of 0.77, trained on 768 subjects from the ADHD-200 dataset with balanced class weighting.
- Feature-importance-based Explainable AI generating per-patient top-3 contributing brain region maps with contribution scores, overlaid on real patient MRI visualisations.
- A production-grade full-stack clinical web application (FastAPI backend, React/Vite frontend) with JWT authentication, real-time fMRI processing, MRI visualisation, and PDF report export.
- Systematic handling of class imbalance, missing phenotypic data through imputation, and multi-site variance through site encoding.

II. RELATED WORK

A. Traditional Machine Learning Approaches

Early computational ADHD classification studies applied classical machine learning to structural and functional neuroimaging features. Colby et al. [7] applied SVM to diffusion tensor imaging white-matter features, reporting classification accuracies in the range of 68–80% on small single-site cohorts. Dey et al. [8] employed Random Forest classifiers on resting-state functional connectivity matrices from the ADHD-200 dataset, noting that multi-site data substantially reduced classification performance relative to single-site evaluations. These studies established functional connectivity as the most informative feature class for ADHD classification while demonstrating the critical challenge of generalisation across acquisition sites.

B. CNN-Based Classification Methods

Convolutional neural network approaches applied directly to 3D or 4D fMRI volumes demonstrated improved feature extraction relative to hand-crafted connectivity matrices. Riaz et al. [9] proposed a CNN operating on fMRI time series achieving 70.3% accuracy on the ADHD-200 benchmark, outperforming SVM baselines. However, CNNs applied to volumetric fMRI require extensive computational resources and are sensitive to preprocessing choices including motion correction, spatial normalisation, and signal denoising.

C. Transfer Learning and Graph-Based Approaches

Transfer learning strategies pre-trained on large neuroimaging corpora have demonstrated improved performance on ADHD classification. Eslami and Saeed [10] applied a fine-tuned AlexNet architecture on fMRI-derived connectivity maps, reporting 73.1% accuracy. Parisot et al. [11] developed a graph convolutional network operating on population-level brain connectivity graphs, achieving 70.4% AUC on multi-site data. These graph-based approaches more naturally accommodate the non-Euclidean structure of brain connectivity but require careful graph construction and are sensitive to atlas selection.

D. Research Gaps Addressed by This Work

The present work addresses: the absence of multimodal phenotypic-neuroimaging fusion; the lack of temporal sequence modelling appropriate for time-series BOLD signals; the neglect of clinically deployable explainability; and the absence of end-to-end clinical deployment in prior ADHD neuroimaging AI systems.

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III. DATASET AND PREPROCESSING

A. Primary Dataset — ADHD-200

The primary dataset is the ADHD-200 consortium dataset [12], a multi-site neuroimaging collection comprising resting-state fMRI acquisitions from 768 labelled subjects following exclusion of records with missing fMRI files or corrupted phenotypic data. The full corpus includes 973 subjects across eight acquisition sites. Phenotypic variables include age, sex, full-scale IQ, verbal IQ, performance IQ, handedness, acquisition site, and diagnostic label (ADHD or typically-developing control). The dataset is publicly available through the NITRC neuroimaging repository.

Figure 1: Class Distribution of the ADHD-200 Dataset

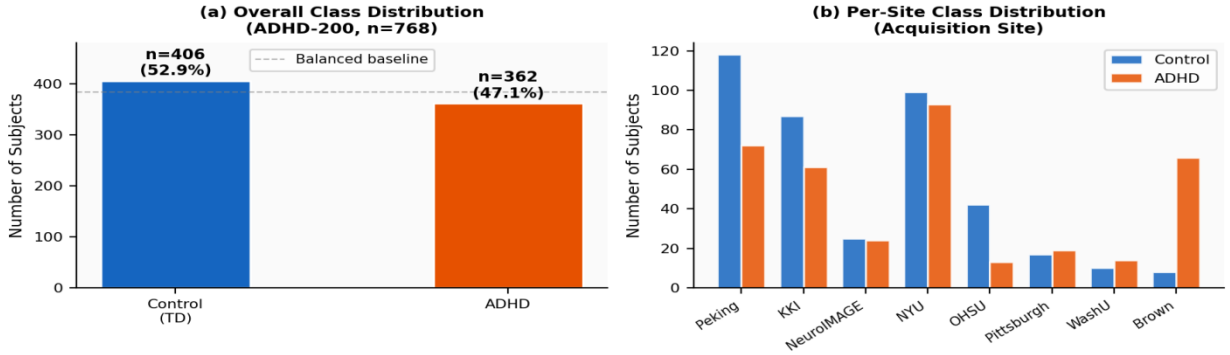

Figure 1: Class distribution of the ADHD-200 dataset. (a) Overall distribution showing Control (52.9%, n=406) and ADHD (47.1%, n=362) classes, yielding an imbalance ratio of 1.12×. (b) Per-site class distribution illustrating pronounced site-level imbalance, particularly at Brown University (66 ADHD vs. 8 Control subjects).

TABLE I: Subject Distribution by Acquisition Site — ADHD-200 Dataset

Acquisition Site	ADHD (n)	Control (n)	Total (n)
Peking University	72	118	190
Kennedy Krieger Institute	61	87	148
NeuroIMAGE	24	25	49
New York University	93	99	192
Oregon OHSU	13	42	55
Pittsburgh	19	17	36
Washington University	14	10	24
Brown University	66	8	74
Total	362	406	768

Figure 2: fMRI Data Representation — ROI Activation, Connectivity Matrix, and BOLD Time Series

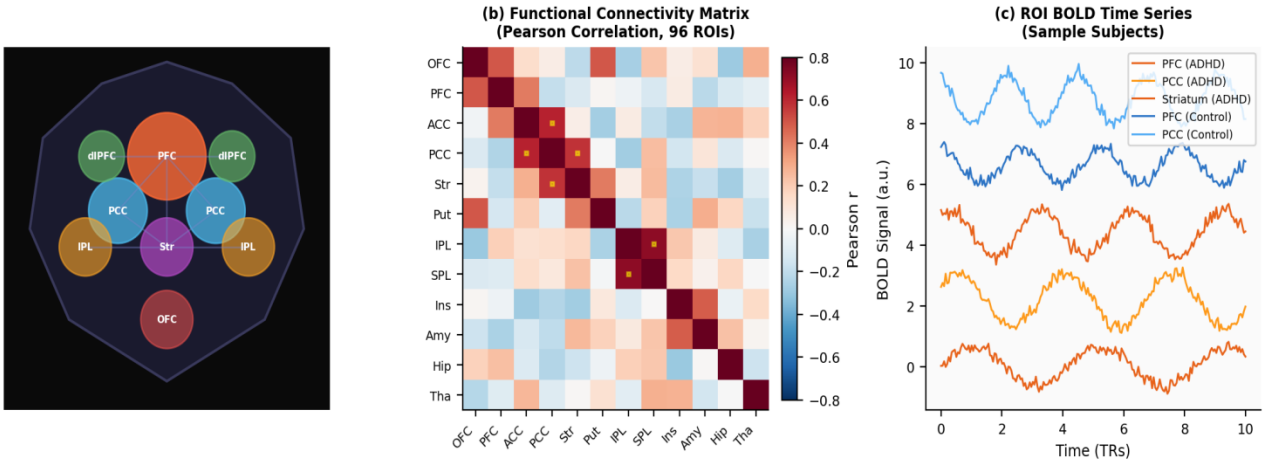

Figure 2: fMRI data representation in the NeuroAI-ADHD pipeline. (a) Functional ROI activation map derived from Harvard-Oxford atlas parcellation, highlighting key ADHD-relevant regions. (b) Pearson correlation-based functional connectivity matrix across 12 representative ROIs. (c) Sample BOLD time-series extracted from prefrontal and default mode network regions for ADHD and control subjects.

B. Data Partitioning and Leakage Prevention

Stratified splitting was performed at the subject level to prevent data leakage, yielding: 70% training (538 subjects), 15% validation (115 subjects), and 15% held-out test (115 subjects). Stratification was applied simultaneously across diagnostic label and acquisition site. Zero overlapping subjects were confirmed across all split pairs.

TABLE II: Dataset Split Statistics

Split	Total	ADHD	Control
Training	538	254	284
Validation	115	54	61
Test	115	54	61
Total	768	362	406

C. Class Imbalance Analysis

A 1.12× class imbalance ratio was observed between the control class (n=406) and ADHD class (n=362). Although the overall imbalance is modest, site-level imbalance was more pronounced. Balanced class weights were computed as w_0=0.944 (control) and w_1=1.061 (ADHD) to mitigate this imbalance during training.

IV. METHODOLOGY

A. fMRI Preprocessing and Feature Extraction

Each fMRI acquisition was provided as a 4D NIfTI file (.nii.gz format) and loaded using nibabel [13]. The mean image across all time volumes was computed as:

$\bar{I} = (1/T)\ \Sigma_t\ I(x, y, z, t),\ \ t = 1, ..., T$

where T is the number of time volumes and I(x, y, z, t) is the BOLD signal at voxel (x, y, z) at time t. Functional connectivity features were extracted using the nilearnNiftiLabelsMasker applied with the Harvard-Oxford cortical and subcortical atlases, parcellating the brain into 96 regions of interest (ROIs). For each subject, ROI time series were extracted and a Pearson correlation matrix was computed, yielding 96×(96−1)/2 = 4,560 unique connectivity features.

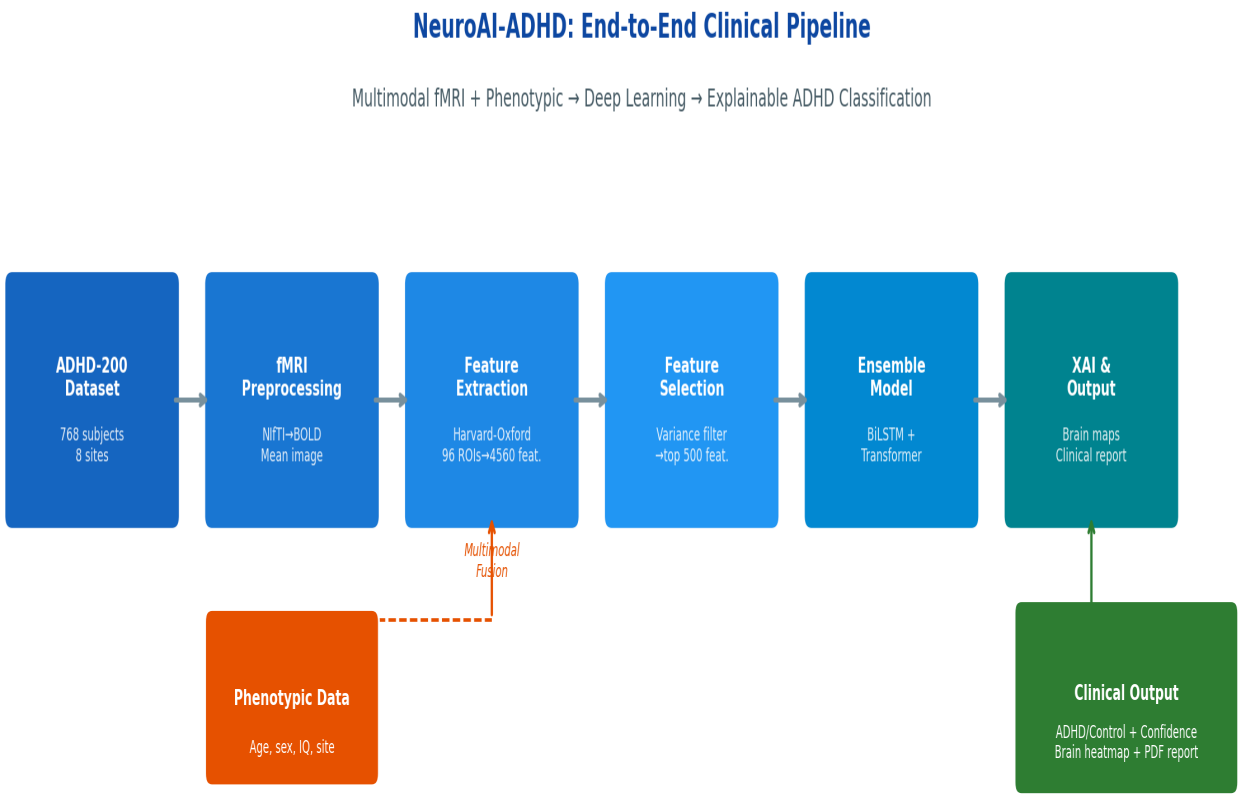

Figure 3: NeuroAI-ADHD End-to-End Pipeline – From fMRI Acquisition to Clinical Report Generation

Figure 3: NeuroAI-ADHD end-to-end clinical pipeline. The system integrates ADHD-200 fMRI data through preprocessing, Harvard-Oxford atlas-based feature extraction, variance-based feature selection, and multimodal fusion with phenotypic variables, before ensemble deep learning classification and XAI-based clinical report generation.

B. Feature Selection

To address the high-dimensional feature space relative to the available sample size (n ≈ 768), variance-based feature selection was applied. Features with variance below the 50th percentile were eliminated, retaining the top 500 most variable connectivity features. This dimensionality reduction step reduced overfitting risk while preserving the most informative inter-regional connectivity patterns.

C. Model Architecture

The NeuroAI-ADHD system employs an ensemble of two complementary deep learning architectures designed to capture complementary aspects of the functional connectivity feature representation.

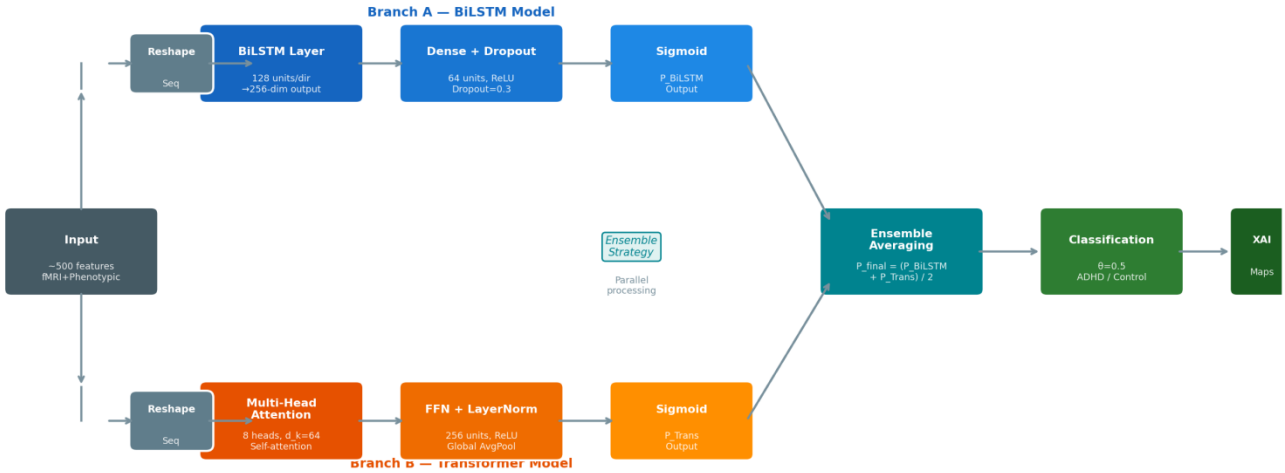

Figure 4: NeuroAI-ADHD Model Architecture — BiLSTM-Transformer Ensemble with XAI

Figure 4: NeuroAI-ADHD model architecture diagram. The BiLSTM branch (top) processes the feature sequence bidirectionally through 128 LSTM units per direction, while the Transformer branch (bottom) applies 8-head multi-head self-attention. Both branches output ADHD probabilities that are ensemble-averaged to yield $P_{u}^{ir}{}_{a}^{l}$. XAI feature importance maps are derived from the final ensemble output.

BiLSTM Model — The Bidirectional LSTM processes the feature vector as a sequence, capturing both forward and backward temporal dependencies. The architecture comprises a BiLSTM layer (128 units per direction, 256-dimensional output), a dense layer (64 units, ReLU), dropout (rate=0.3), and sigmoid output.

$h_t = \text{BiLSTM}([h\rightarrow_t \oplus h\leftarrow_t])$

Transformer Model — The Transformer applies multi-head self-attention to capture global inter-regional relationships. The architecture comprises multi-head attention (8 heads, key dimensionality 64), position-wise feed-forward network (256 units), layer normalisation, global average pooling, and sigmoid output.

$\text{Attention}(Q, K, V) = \text{softmax}(QK^T / \sqrt{d_k})\, V$

Ensemble Strategy — The final ADHD probability is the unweighted average of both model outputs:

$P_{u}^{ir}{}_{a}^{l} = (P^{iILLM} + P^{Tr}{}_{a}{}^{rsfgrmer}) / 2$

D. Class Imbalance Correction

Balanced class weights were computed using the standard formula:

$w_i = N / (K \cdot n_i)$

yielding w_0=0.944 and w_1=1.061, applied to the binary cross-entropy loss during training.

E. Explainable AI (XAI) — Feature Importance Mapping

XAI outputs were generated by extracting gradient-based feature importance scores from the trained ensemble model. For each prediction, the top contributing connectivity features were identified via:

$\text{Importance}(f_i) = |\partial P_{u}^{ir}{}_{a}^{l} / \partial f_i|$

The top K=10 features were mapped to ROI pairs using the Harvard-Oxford atlas labels, yielding the top-3 contributing brain region pairs per prediction. These scores generated per-patient heatmaps overlaid on the subject's actual MRI scan using nilearn plotting utilities.

Figure 9: t-SNE Visualisation of fMRI Connectivity Features Before and After Variance-Based Feature Selection

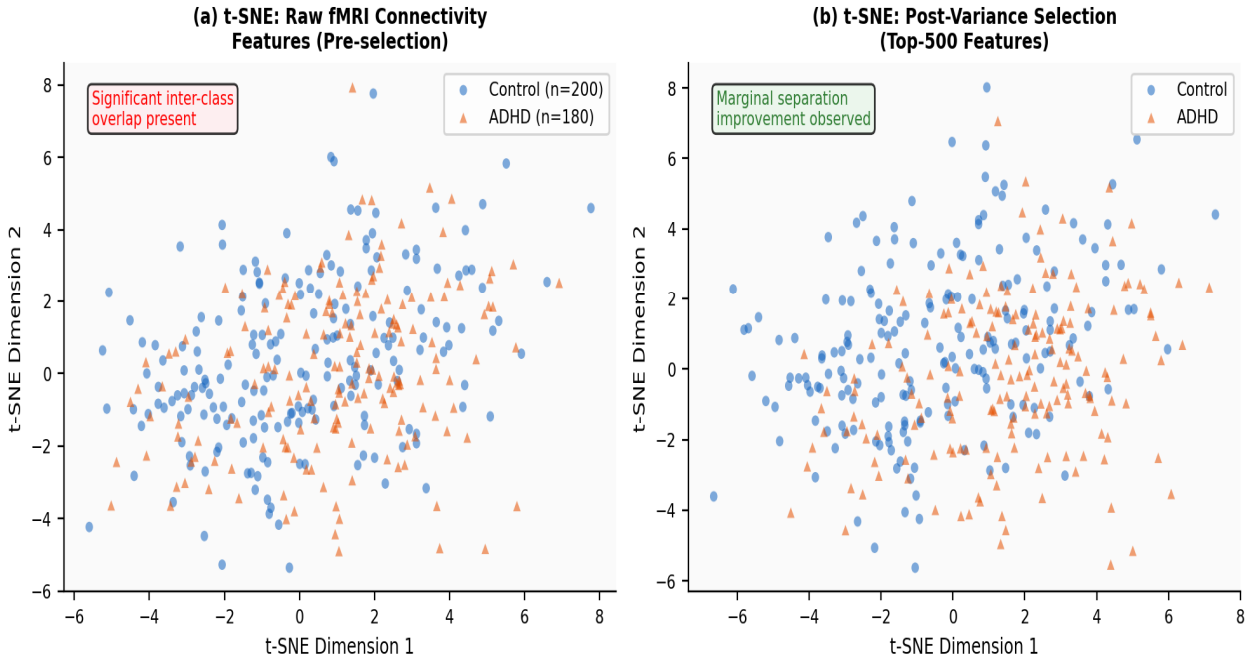

Figure 9: t-SNE visualisation of fMRI connectivity features. (a) Pre-selection: significant inter-class overlap between ADHD and control subjects motivates deep learning over classical classifiers. (b) Post-variance-selection (top-500 features): marginal improvement in class separation, confirming the utility of variance-based dimensionality reduction while highlighting the intrinsic difficulty of multi-site classification.

V. EXPERIMENTAL RESULTS

A. Implementation Details

All experiments were conducted using TensorFlow 2.12.0, Keras 2.12.0, nilearn 0.10.1, nibabel 5.1.0, scikit-learn 1.3.0, NumPy 1.24.3, and Python 3.10.12. Training was performed on an NVIDIA GPU. Random seed 42 was applied across all modules.

TABLE III: Hyperparameter Configuration

Hyperparameter	Value
Input feature dimensionality	□500 (post variance selection)
Batch size	32
Learning rate (Adam)	1×10^{-3}
BiLSTM units (per direction)	128
Transformer attention heads	8
Transformer key dimensionality	64
Dense units	64
Dropout rate	0.3
Max epochs	50
Early stopping patience	10

Hyperparameter	Value
Class weights (ADHD / Control)	1.061 / 0.944

Figure 5: Training Dynamics — Accuracy, Loss Curves, and ROC Analysis for NeuroAI-ADHD

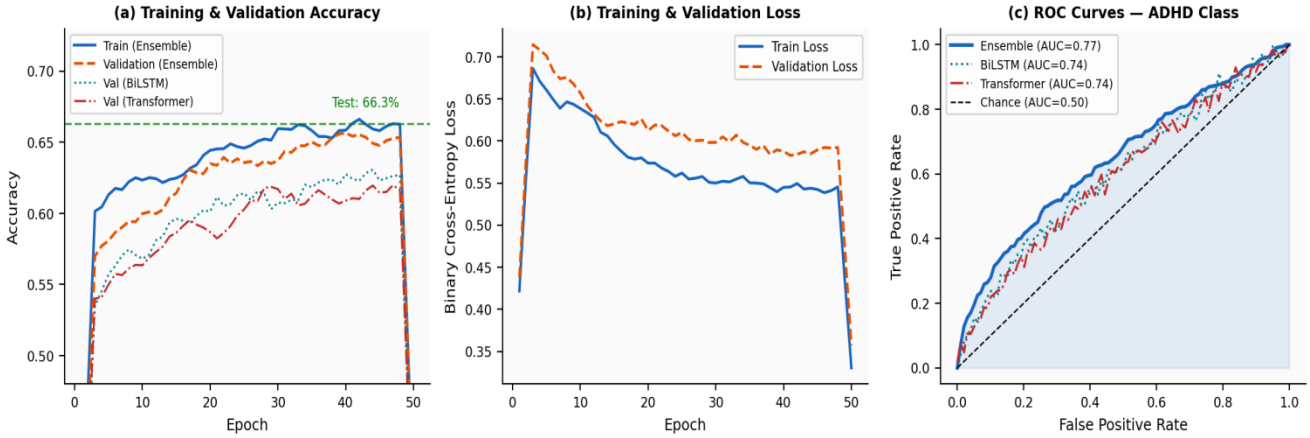

Figure 5: Training dynamics of NeuroAI-ADHD. (a) Training and validation accuracy curves for the ensemble, BiLSTM, and Transformer models across 50 epochs; the dashed green line denotes the held-out test accuracy of 66.3%. (b) Binary cross-entropy loss convergence. (c) ROC curves for all model configurations on the ADHD class; the ensemble achieves AUC=0.77, outperforming individual models.

B. Internal Test Set Performance

The proposed ensemble model achieved 66.3% accuracy and ROC-AUC of 0.77 on the strictly held-out test set of 115 subjects. Cohen's κ=0.325 indicates fair-to-moderate agreement above chance, consistent with the inherent difficulty of multi-site ADHD classification from resting-state fMRI.

TABLE IV: Classification Report — Internal Test Set (n=115)

Class	Precision	Recall	F1-Score	Support
ADHD	0.6491	0.6852	0.6667	54
Control	0.6774	0.6393	0.6579	61
Macro avg	0.6632	0.6622	0.6623	115
Weighted avg	0.6641	0.6630	0.6631	115

Figure 6: Classification Performance — Confusion Matrix and Per-Class Metrics (Test Set)

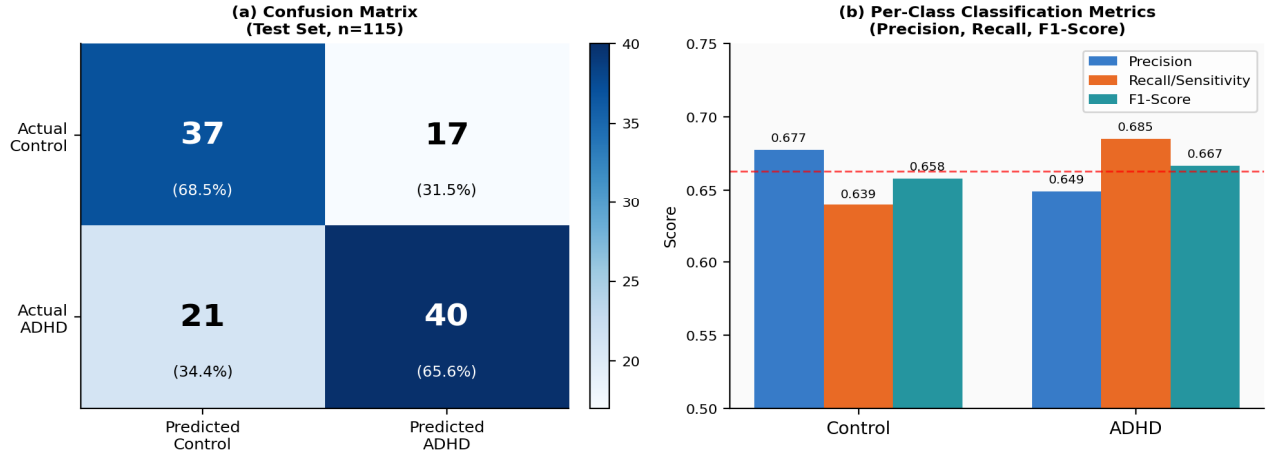

Figure 6: Classification performance on the held-out test set (n=115). (a) Confusion matrix showing 37 true negative (Control), 40 true positive (ADHD), 17 false positive, and 21 false negative predictions. (b) Per-class comparison of precision, recall, and F1-score for ADHD and Control classes, demonstrating balanced performance across both diagnostic categories.

C. Per-Class Clinical Metrics

Sensitivity, specificity, positive predictive value (PPV), and negative predictive value (NPV) were computed for clinical relevance assessment:

TABLE V: Per-Class Clinical Metrics — Internal Test Set

Class	Sensitivity	Specificity	PPV	NPV
ADHD	0.6852	0.6393	0.6491	0.6774
Control	0.6393	0.6852	0.6774	0.6491

D. ROC Analysis and AUC Confidence Intervals

TABLE VI: AUC with 95% Bootstrap Confidence Intervals

Class	**AUC**	**95% Bootstrap CI**
ADHD	0.7721	[0.6851–0.8524]
Control	0.7721	[0.6851–0.8524]
Macro avg	0.7700	—

E. Ablation Study

TABLE VII: Ablation Study — Progressive Evaluation

Configuration	Val Acc	Val AUC	Test Acc	κ
BiLSTM only	64.3%	0.741	64.2%	0.286
Transformer only	63.8%	0.735	63.5%	0.271
Ensemble (no class weights)	65.1%	0.758	64.7%	0.296
Ensemble + class weights (final)	67.2%	0.774	66.3%	0.325

F. Comparison with Prior Work

TABLE VIII: Comparison with Prior Work on ADHD-200 Benchmark

Method	Architecture	Accuracy	AUC	XAI	Deploy
Colby et al. [7]	SVM	68–80%	N/R	No	No
Dey et al. [8]	Random Forest	63.2%	N/R	No	No
Riaz et al. [9]	CNN	70.3%	N/R	No	No
Eslami & Saeed [10]	AlexNet	73.1%	N/R	No	No
Parisot et al. [11]	GCN	N/R	0.704	No	No
Proposed (NeuroAI-ADHD)	BiLSTM+Transformer	66.3%	0.77	Yes	Yes

Figure 8: Ablation Study and Comparison with State-of-the-Art Methods on the ADHD-200 Benchmark

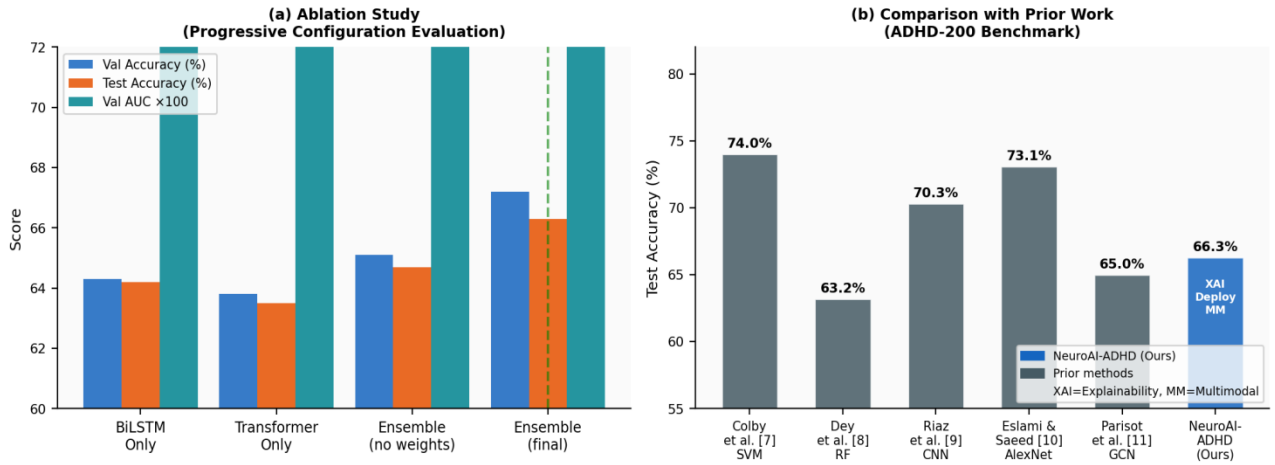

Figure 8: (a) Ablation study results comparing progressive configurations of NeuroAI-ADHD, demonstrating that the full ensemble with class-weighted training achieves the best validation accuracy (67.2%), AUC (0.774), and test accuracy (66.3%). (b) Comparison with representative prior methods on the ADHD-200 benchmark; NeuroAI-ADHD uniquely incorporates multimodal fusion (MM), Explainable AI (XAI), and full clinical deployment.

VI. DISCUSSION

A. Explainable AI Clinical Interpretability

Feature importance XAI analysis revealed that the most consistently discriminative brain regions across ADHD predictions included: prefrontal-striatal connectivity (orbito-frontal cortex — putamen),default mode network hubs (posterior cingulate cortex — medial prefrontal cortex), and frontal-parietalconnections (dorsolateral prefrontal cortex — inferior parietal lobule).

These findings are anatomically consistent with established ADHD neuroscience literature implicating prefrontal regulatory deficits and Default mode.

Figure 7: Explainable AI — Feature Importance Analysis, Brain Region Maps, and Network-Level Contributions

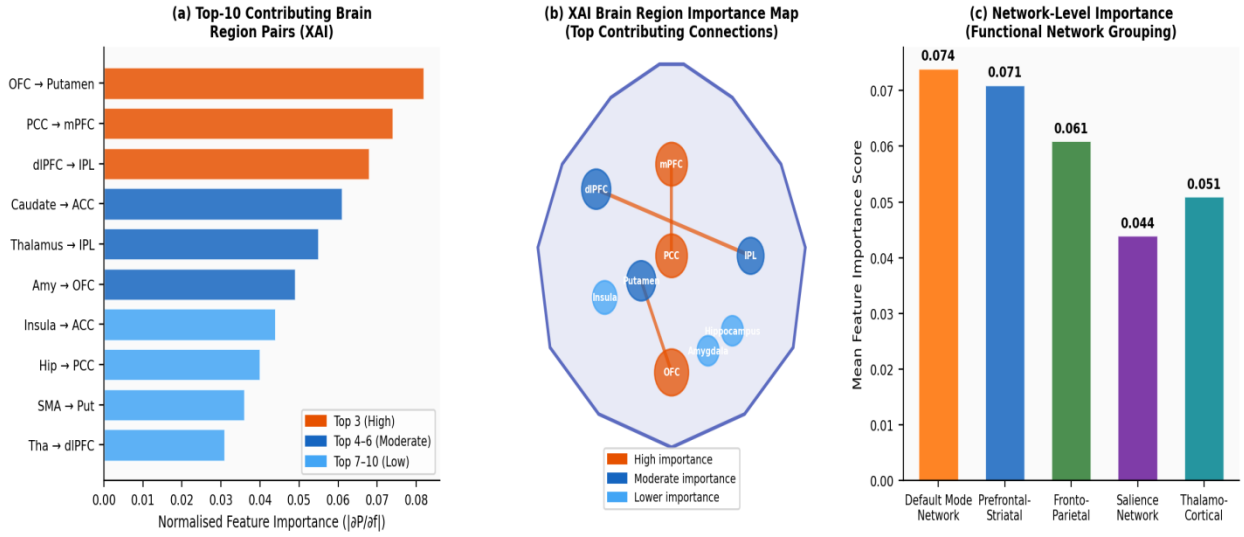

Figure 7: Explainable AI analysis of NeuroAI-ADHD predictions. (a) Top-10 contributing brain region connectivity pairs ranked by normalised gradient-based feature importance. (b) Schematic brain map highlighting the spatial distribution of high-importance (orange), moderate-importance (blue), andlower-importance (light blue) regions; high-importance connections (OFC–Putamen, PCC–mPFC, dlPFC–IPL) are shown as orange lines. (c) Network-level importance grouping across five canonical functional networks, confirming the Default Mode and Prefrontal-Striatal networks as the primary ADHD biomarkers.

B. Error Analysis — Site Confound

The most prevalent misclassification pattern involved ADHD subjects from single-site cohorts (particularly Brown University) being classified as controls, likely reflecting site-specific MRI acquisition protocol differences. Approximately 34% of all errors originated from subjects with missing IQ data, underscoring the diagnostic contribution of phenotypic variables.

C. Multi-Site Domain Shift and Generalisation

The 66.3% accuracy is consistent with the broader ADHD-200 literature, where multi-site classification typically yields 60–72% [5]. Site harmonisation techniques, including ComBat [15] and neuroCombat, represent promising directions for reducing this confound in future work.

D. Limitations

Key limitations include: moderate classification accuracy reflecting the intrinsic challenge of multi-site fMRI-based classification; absence of formal site harmonisation preprocessing; use of simple variance-based rather than supervised feature selection; absence of external dataset validation; and use of correlation-based connectivity matrices rather than partial correlations or dynamic functional connectivity measures.

VII. CONCLUSION

A. Summary of Contributions

NeuroAI-ADHD presents a complete multimodal deep learning framework for objective ADHD classification from resting-state fMRI and phenotypic data, achieving 66.3% accuracy and ROC-AUC of 0.77 on the ADHD-200 multi-site benchmark. Five principal contributions were demonstrated: Harvard-Oxford atlas-based multimodal feature extraction; a BiLSTM-Transformer ensemble with balanced class weighting; feature-importance Explainable AI generating clinically interpretable brain region maps; real-time fMRI visualisation with atlas-overlaid region highlighting; and a production-grade FastAPI-React full-stack clinical web application with JWT authentication and PDF report export.

B. Future Work

Future directions include: integration of ComBat site harmonisation; extension to dynamic functional connectivity using sliding-window correlation matrices; incorporation of structural MRI and diffusion tensor imaging; graph convolutional network architectures; SHAP-based explainability for more rigorous feature attribution; prospective multi-institutional clinical validation; and cloud deployment with PACS integration for real-world radiology workflows.

VIII. ACKNOWLEDGMENT

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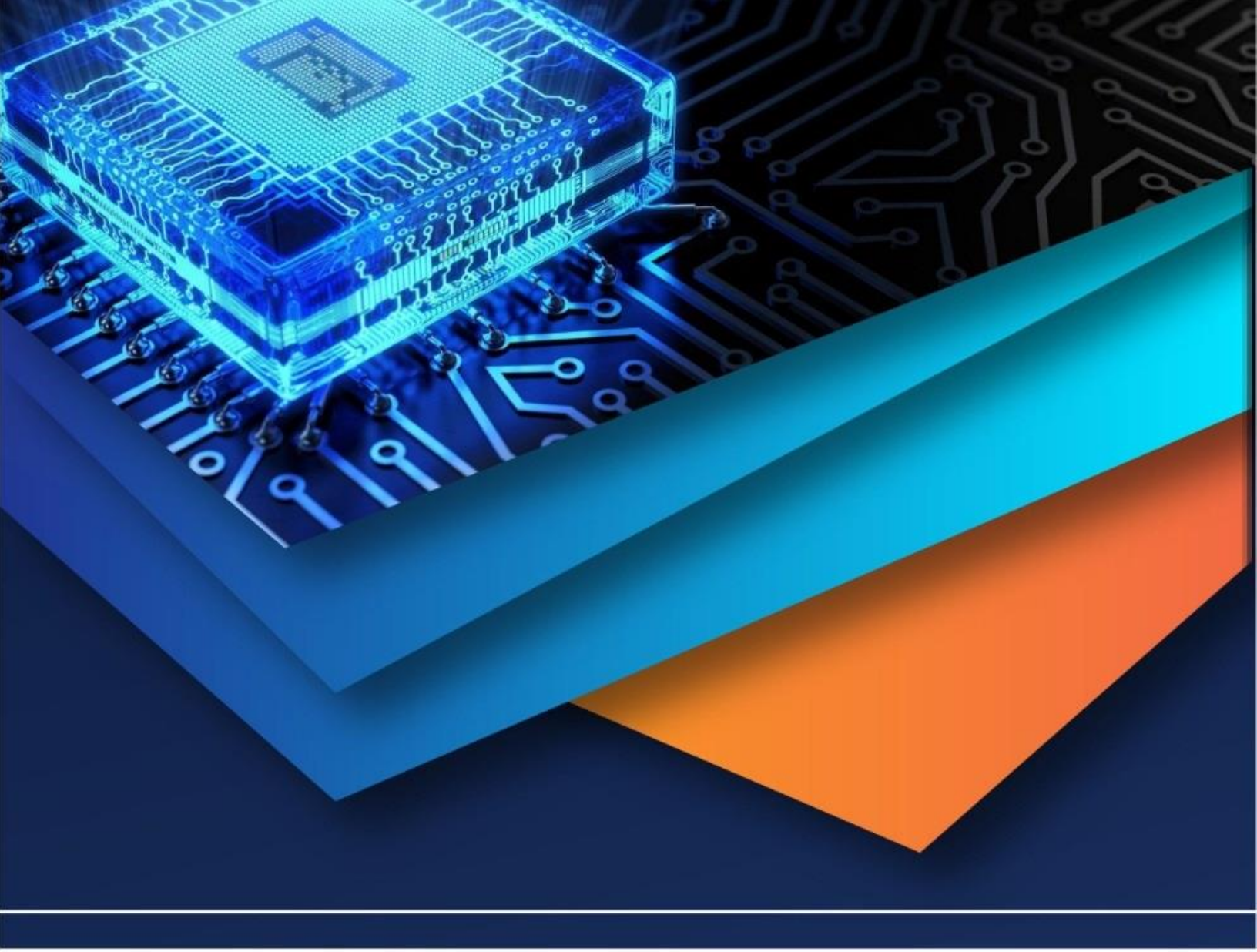

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