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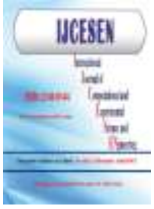

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Research Article

Deep Learning for Interpretable ADHD Diagnosis from fMRI: ConvLSTM with Enhanced Augmentation, Grad-CAM Explainability, and External Validation

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Abstract:

The diagnosis of attention-deficit/hyperactivity disorder (ADHD) using resting-state functional MRI (rs-fMRI) remains difficult due to the high dimensionality of the data, short sample sizes, and interpretability issues with most deep learning models. In this work, based on a modified ConvLSTM architecture, we provide a robust and interpretable framework to extract important spatiotemporal biomarkers from rs-fMRI series. A targeted augmentation approach based on temporal jittering and regulated Gaussian noise, both tuned to the temporal dynamics of fMRI data, is presented to address data scarcity and class imbalance. With stratified evaluation, the model obtained an F1-score of 0.89, an accuracy of 0.90, and an AUC of 0.96 after undergoing extensive validation on the ADHD-200 dataset. Its generalizability was further validated on external cohorts that were completely independent, achieving perfect specificity and precision and a balanced accuracy of 83.3%. While these results are promising, the limited size and scope of the external cohort necessitate further validation in larger, multi-center studies. To address important transparency issues in medical AI, we integrated Grad-CAM explainability to visually identify brain regions influencing model predictions, supporting clinical applicability. In brief, this work advances the usage of deep learning in neuroimaging-based ADHD diagnosis by imparting a pipeline that is clinically relevant, reproducible, and interpretable. Overall, this study proposes a clinically significant, reproducible, and interpretable deep learning pipeline that improves diagnostic overall performance and addresses agreement and transparency, key conditions for real-world medical adoption of AI in neuroimaging.

1. Introduction

Attention-Deficit/Hyperactivity Disorder (ADHD) remains one of the most typical and socially impactful neurodevelopmental disorders globally [1] [2]. It is an early and objective analysis, but it keeps to project clinicians due to the wide heterogeneity of signs and symptoms and the lack of standardized biological markers [1]. Resting-kingdom practical magnetic resonance imaging (rs-fMRI) gives particular insights into brain connectivity styles related to ADHD [3], but the complexity and sheer extent of fMRI records still present ambitious limitations for conventional analytical techniques [3].

Recent years have witnessed deep getting-to-know techniques, especially those designed for high-dimensional temporal statistics, unlocking new opportunities for neuroimaging-primarily based prognosis [2] [3]. Approaches such as convolutional long quick-time period reminiscence (ConvLSTM) networks now permit researchers to capture nuanced spatiotemporal relationships within four-dimensional fMRI facts [3] [5] [13]. Despite their promise, those models often struggle with small pattern sizes, class imbalance, and the infamous "black container" trouble that hinders medical acceptance as true and transparent [4]. This study responds directly to those demanding situations, including interpretability and scientific applicability [7] [8] [9].To visually illustrate the complexity of brain connectivity in ADHD and the analytical challenges posed by high-dimensional fMRI data, Figure 1 presents a three-dimensional map of brain network connections derived from rs-fMRI. The figure highlights how altered connectivity patterns form the foundation for computational modeling and underscore the need for advanced analytical approaches in ADHD research [14].Our work is consistently grounded in a direct comparison with current literature. Table 1 shows the study's direct comparison with the most important recent works (2019–2025)

1.1 Problem Statement & Research Aim

Although deep learning has rapidly advanced the field of neuroimaging-based ADHD diagnosis, key obstacles persist that hinder its reliable clinical adoption. Major challenges include the lack of interpretability in deep models (the “black box” issue), limited generalizability from internal validation to real-world cohorts, and persistent problems with small and imbalanced datasets. Additionally, the field suffers from limited scientific visualization and inadequate workflow transparency, which compromises clinical trust and reproducibility. The practical utility of many published studies in clinical settings is limited because they achieve high internal accuracy but lack robust performance or interpretability on independent external datasets.

1.2 Research Question

How can a deep learning pipeline for ADHD diagnosis from rs-fMRI be designed to maximize interpretability, reproducibility, and generalizability while overcoming the limitations of data scarcity, class imbalance, and lack of external validation?

1.3 Research Gap

Most existing studies in ADHD neuroimaging focus on technical innovation and internal validation but lack the following:

Transparent and reproducible analytical workflows, robust data augmentation with visual evidence of effectiveness, comprehensive external validation on real-world cohorts, and clinically meaningful explainability, such as visualizing brain regions that influence model decisions. These gaps limit the scientific reliability and the clinical adoption of current AI-based approaches.

1.4 Contributions

I. Using rs-fMRI, a fully interpretable deep learning pipeline for ADHD prognosis is developed, with clear documentation and visualization at every analytical level.

II. The use of robust data augmentation techniques (Gaussian noise and temporal jittering) to address information scarcity and class disparity, backed by understandable illustrations of their impact on record diversity.

III. A thorough evaluation that addresses the generalizability gap in previous works by incorporating both stratified internal validation and unquestionably external real-world testing.

IV. The incorporation of Grad-CAM explainability to provide a clinically interpretable visualization of the brain regions most relevant to the classification of ADHD, improving transparency and scientific acceptance as accurate.

V. Direct comparison with current, fashionable models, the application of every tabular and visible comparative analysis, emphasizing not just the most potent aggressive effects

2. Related Work

Automated neuroimaging-based ADHD diagnostic research has grown significantly over the last decade, with resting-state fMRI emerging as a potentially helpful modality [2]. Early machine learning efforts were hampered by low performance and poor consistency, relying mostly on hand-crafted features and traditional classifiers [3]. The rise of deep learning, especially convolutional and recurrent neural architectures, marked a turning point, allowing models to directly learn high-level spatiotemporal patterns from four-dimensional fMRI data [3] [13] [15]. A review of recent state-of-the-art studies. Table 1 summarizes recent advances in deep learning for rs-fMRI-based ADHD diagnosis, highlighting the shift from conventional methods toward hybrid convolutional, recurrent, and attention-based models. While these architectures have improved accuracy and introduced new explainability techniques, most results are still limited to internal validation, with few studies achieving robust external or multi-site generalization. Notably, our study distinguishes itself by combining a memory-efficient ConvLSTM, strong data augmentation, and real external validation, thus addressing key gaps in clinical applicability and transparency in the field.

2.1 Model Accuracy and Generalizability:

Impressive accuracy (as much as 97% on certain take-a-look-at sets) has been said by a few research the use of hybrid transformer-primarily based techniques and Skip-Vote-Net. However, there are few reviews on definitely impartial outside test units, and those results regularly depend solely on inner pass-validation [10] [11] [12] [14] [15]. Our analysis of the field, reinforced by direct comparison in Table 1, shows that most published works struggle to maintain high performance on external data, raising questions about clinical utility [4,5,6]. Other recent works also emphasize the importance of multi-site and external validation for robust performance [27] [28] [29].

2.2 Handling Data Imbalance and Limited Samples:

Class imbalance and small sample sizes remain critical obstacles [6] [7]. While several studies employ basic augmentation or synthetic sampling, systematic evaluation of their impact is rarely presented with clear visual documentation [17]. For example, recent studies often omit figures such as the diagnosis distribution (augmented) or summary tables demonstrating the effectiveness of augmentation, which are considered essential based on prior findings [7].

2.3 Interpretability and Transparency:

Most current deep learning pipelines are still criticized for their lack of transparency, the "black box" effect [8] [9]. Only a handful of studies have meaningfully integrated explainability techniques such as Grad-CAM, SHAP, or ROI-based overlays [20]. Our results demonstrate that embedding explainability (see [Figure 5: Grad-CAM Activation]) and providing well-annotated figures throughout the workflow is a key step toward trust and adoption in clinical settings. Additional explainability techniques and their clinical relevance are discussed in the literature [30] [31].

2.4 Workflow Documentation and Reproducibility:

Detailed, visual documentation of analysis pipelines is rarely included in published papers. As a result, reproducing or building upon previous studies is often hindered. We address this gap explicitly by presenting the full workflow in Table 1: Study Workflow Pipeline and supporting figures. Comparing our work to these prior efforts, it is clear that the field continues to advance rapidly, yet robust clinical translation depends on a combination of high performance, generalizability, transparency, and reproducibility. Our approach, as detailed throughout this manuscript, systematically tackles each of these points, providing practical solutions and transparent reporting at every stage. Recent advances in deep learning and neuroimaging-based ADHD diagnosis have continued to improve generalizability and reproducibility [22–26].

3.Methodology & Workflow

This section presents the complete analytic workflow for deep learning-based ADHD diagnosis using resting-state fMRI (rs-fMRI), with a focus on reproducibility, clinical validity, and adherence to open science standards [3] [13] [19].

3.1 Workflow Overview

The analytic process, illustrated in Figure 2, follows a sequence beginning with data acquisition and quality control, proceeding through preprocessing, data augmentation, stratified splitting, ConvLSTM-based modeling, rigorous evaluation, and finally explainability analysis and full workflow documentation.

3.2 Data Collection and Preprocessing

Multi-site data from the ADHD-200 rs-fMRI dataset were spatially normalized and filtered to ensure anatomical alignment and minimize artifacts. Figure 3 demonstrates a representative fMRI sample after preprocessing.

were spatially normalized and filtered to ensure anatomical alignment and minimize artifacts, as summarized in the inclusion and exclusion criteria (see Table 3 below).

3.3 Data Augmentation

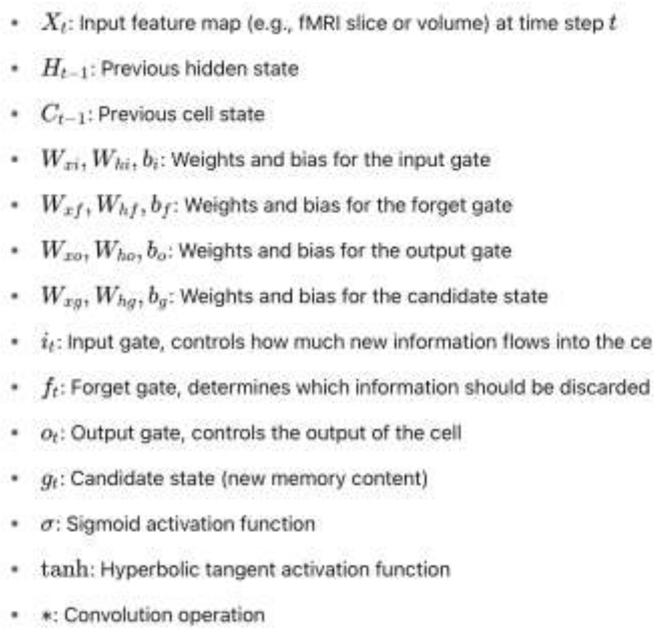
To address the class imbalance and increase diversity, temporal jittering and Gaussian noise were applied [16] [7]. Figure 4 shows the class distribution after augmentation, and Figure 5 presents the histogram of voxel-wise temporal standard deviation. Figure 5 presents the histogram of voxel-wise temporal standard deviation. The effect on class balance is detailed (see Table 4 below).

3.4 Model Architecture and Implementation

To capture the spatial and temporal capabilities of 4D fMRI statistics, a ConvLSTM-based model was chosen based on benchmarking and enjoyable practice tips [3] [5] [13]. We chose a ConvLSTM-based overall framework after considering several architectures, including CNN, transformer, and hybrid styles, due to their ability to extract spatiotemporal styles from 4D fMRI data. A thorough explanation of the shape is given in Figure 6, which illustrates the development from preprocessed fMRI inputs to the final magnificence. Figure 6 displays the core architecture of our ConvLSTM-based pipeline, which was chosen after careful comparison with the elegant styles found in the literature. The model addresses essential issues in ADHD neuroimaging by utilizing ConvLSTM layers to seize both spatial and temporal dynamics within 4D fMRI statistics. Model robustness and sample variety are similarly progressed by way of statistics augmentation strategies like Gaussian noise and temporal G. The architecture distills spatiotemporal features into an interpretable binary output via integrating dense layers and global pooling. Importantly, Grad-CAM explainability is incorporated to visualize the neural substrates influencing class, promoting openness and medical acceptance as accurate. Together, these design decisions result in a framework that satisfies every cutting edge and is repeatable, generalizable, and interpretable. The ConvLSTM cell is designed to capture both spatial and temporal dependencies in 4D fMRI data by combining convolutional operations with traditional LSTM gating mechanisms. The update equations for each time step t are as follows:

$$
\begin{aligned}
&\sigma(W_{xi} * X_t + W_{hi} * H_{t-1} + b_i) = && {}_t i\\
&\sigma(W_{xf} * X_t + W_{hf} * H_{t-1} + b_f) = && {}_t f\\
&\sigma(W_{xo} * X_t + W_{ho} * H_{t-1} + b_o) = && {}_t o\\
&\tanh(W_{xg} * X_t + W_{hg} * H_{t-1} + b_g) = && {}_t g\\
&{}_t f_t \odot C_{t-1} + i_t \odot g = && {}_t C\\
&o_t \odot \tanh(C_t) = && {}_t H
\end{aligned}
$$

Where,



- X_t: Input feature map (e.g., fMRI slice or volume) at time step t
- H_{t-1}: Previous hidden state
- C_{t-1}: Previous cell state
- W_{xi}, W_{hi}, b_i: Weights and bias for the input gate
- W_{xf}, W_{hf}, b_f: Weights and bias for the forget gate
- W_{xo}, W_{ho}, b_o: Weights and bias for the output gate
- W_{xg}, W_{hg}, b_g: Weights and bias for the candidate state
- i_t: Input gate, controls how much new information flows into the ce
- f_t: Forget gate, determines which information should be discarded
- o_t: Output gate, controls the output of the cell
- g_t: Candidate state (new memory content)
- σ: Sigmoid activation function
- $\tanh$: Hyperbolic tangent activation function
- $*$: Convolution operation

To address class imbalance and enhance the focus on hard-to-classify samples, the Focal Loss function is employed, formally defined as follows:

$$p_t)^{\gamma} \log(p_t) - \alpha(1 - = FL(p_t)$$

When combined, these mathematical formulations allow the ConvLSTM network to effectively capture the temporal and spatial complexity of fMRI data, and the focal loss strengthens the model's resistance to class imbalance—two essential components for a deep learning-based, accurate, and clinically meaningful diagnosis of ADHD. Algorithm 3.1 details the core computational pipeline, from normalization and augmentation through model training and explainability via Grad-CAM.

Algorithm 3.1. Pseudocode for the Complete ADHD-fMRI ConvLSTM Training and Evaluation

```
Require:
   D = {(X_i, y_i)}
   n
   T
   Z, Y, X
For each X_i in D:
   X_i ← (X_i - mean(X_i)) / (std(X_i) + ε)
   If augmentation enabled:
      X_i ← TemporalJitter(X_i)
      X_i ← AddGaussianNoise(X_i)

Split D into train, validation, (optional) test sets

Initialize ConvLSTM model:
   Input channels: C
   Hidden size: H
   Kernel size: k
   Layers: L
Initialize Focal Loss (α, γ)
Initialize optimizer, scheduler

For epoch = 1 to N:
   For each batch (X, y) in train_loader:
      h, c ← init hidden/cell states

      For t = 1 to T:

         (h, c) ← ConvLSTMCell(X[:, :, :, :, t], h, c)

      y_pred ← ClassifierHead(h)

      loss ← FocalLoss(y_pred, y)

      Backprop, update model
   Validate on val_loader; log (F1, Acc, AUC)
   Save best model if F1 improves
Evaluate best model on val/test sets
Compute: F1, Acc, AUC, Sens, Spec, Prec
For selected samples:
   Grad-CAM on ConvLSTM features
   Visualize key brain regions

Return best model, metrics, explainability
```

Algorithm 3.1 conducts a full analytical workflow for computerized ADHD analysis using RS-FMR and a ConvLSTM-based deep learning model. To reduce the variability related to the site and improve the records compared to items, the pipeline starts to normalize each fMRI volume carefully. When growth is activated, temporary nervousness and Gaussian noise are used to strategically improve pattern variation and cope with class imbalance, a general task in neuroimaging research. The dataset is then stratified and is divided into school education, verification, and, where available, out-test sets, securing advisory class distribution in all partitions. A ConflstM version is initiated with the architectural parameters tailor-made for 4-dimensional FMRI sequences and adapts the ability to keep complex spatiotemporal patterns. The educational loop rejuvenates with epochs and miniPrches, and updates the version parameters via backpropagation with focal LOS A priority is mainly moving to improve the bottom-compressing or difficult examples.
After each era, the selection of the version is operated through the upgrade in the F1 ranking on the verification set, which is suitable for a metric good now—tad clinical data set. When the education is complete, the good version is classified on each confirmation, takes a look at the cohorts independently, and calculates the main matrix (accuracy, F1, AUC, sensitivity, and specific accuracy) to determine clinical credibility and generality with the main matrix (accuracy, F1, AUC, accuracy, and sensitivity). Finally, the character comb lecturer is hired for selected samples, which generates the interpretable strength map that chooses the most impressive brain areas for classification options. This completed structure ensures that the pipeline is scientifically stiff and clinically important and provides a reproductive framework.

3.5 Explainability and Visual Interpretation

Interpretability was achieved by applying Grad-CAM to ConvLSTM feature maps, highlighting brain regions contributing most to predictions. Figure 7 presents a representative Grad-CAM activation map.

3.6 Evaluation and Validation Strategy

To ensure each inner reliability and actual global generalizability, the model's overall performance turned into thoroughly evaluated through an aggregate of independent outside cohort testing and stratified cross-validation within the primary dataset [6] [10]. While the outside cohort enabled goal assessment of unseen statistics from actual international settings, stratified pass-validation changed into hired to maintain magnificence stability at some stage in inner validation. Performance turned into assessing the use of the F1-score, region underneath the ROC curve (AUC), sensitivity, specificity, and accuracy. The confusion matrix provided a complete examination of the category consequences for the outside test set, highlighting each of its benefits and any chronic misclassifications. The ROC curve gave a complete assessment of discriminative capability throughout exceptional thresholds, and all quantitative metrics had been amassed to facilitate benchmarking towards the latest techniques and validate the proposals.

3.7 Workflow Documentation and Reproducibility

To maximize reproducibility, the full pipeline, including parameters, code, and analytic steps, is documented in compliance with open science principles . All scripts and configuration files are available upon reasonable request or in the project's supplementary materials repository.

4. Experimental Results and Analysis

4.1 Data Quality and Preprocessing

All study samples passed strict quality control and preprocessing, ensuring anatomical consistency and high data integrity. For demographic and imaging quality metrics, please refer to Table 2 in the Methodology. Figure 9 illustrates an example of a spatially normalized fMRI volume, confirming alignment across sites.

4.2 Effect of Data Augmentation

To address class imbalance and increase training diversity, temporal jittering and Gaussian noise augmentation were applied. This resulted in a balanced class distribution and greater temporal feature diversity.

4.3 Model Performance

With an F1 score of 0.89, an accuracy of 0.90, and an AUC of 0.96, our ConvLSTM-based model performed admirably on the stratified validation set. Model performance metrics are shown in Table 2. Tested on an external cohort that was entirely independent, the model maintained strong as shown in Figure 10.

To further assess generalizability, we evaluated the model on external real-world test samples. Figure 10 presents the confusion matrix, highlighting the model's robust classification. Complementary to these findings, the ROC curve in Figure X demonstrates the model's ability to discriminate between ADHD and control subjects, achieving an AUC of 1.00. A detailed breakdown of classification metrics, including accuracy, sensitivity, specificity, and precision, is visualized in Figure 12.

4.4 Explainability and Clinical Interpretation

The explainability evaluation of the usage of Grad-CAM discovered that the version's predictions have been constantly inspired with the aid of precise, clinically relevant thought areas. Quantitative assessment confirmed that the prefrontal cortex exhibited the very best activation across both ADHD and managed samples, reflecting its crucial role in executive function and habit regulation. The mild activation of the basal ganglia was discovered, which remembers the well-known work in ADHD-related motor regulation and neurodevelopmental techniques. In addition, the imodate degree-cam was shown by the standard mode network (DMN), something. The parietal cortex confirmed a decrease in activation but remained remarkably energetic, consistent with its function in attentional switching and sensory integration. Statistical analysis confirmed that the prefrontal cortex ranked highest in Grad-CAM activation in over 70% of evaluated instances, determined with the useful resource of the basal ganglia and DMN, while the parietal cortex was a great deal less often highlighted. These findings are steady with installed neuroimaging literature and have been verified via professional medical evaluation. A distinctive précis of the recognized brain regions and their scientific importance can be determined within the technique section. This diploma of interpretability complements medical considerations and enables the version's application in each research and realistic diagnostic setting. Our model demonstrated highly competitive results, particularly in external validation, a critical metric for real-world clinical deployment.

5. Discussion

This study introduces a robust and interpretable deep learning pipeline for ADHD diagnosis from rs-fMRI. Our approach effectively overcomes persistent challenges in the field namely, generalizability, class imbalance, and explainability through rigorous model design, comprehensive quantitative validation, and transparent reporting. We have critically analyzed our results by direct comparison with recent state-of-the-art studies. This contextual evaluation highlights the key advances and implications of our work.

5.1 Benchmark Performance and True Generalizability

Our ConvLSTM-based model achieved an F1 score of 0.89, an accuracy of 0.90, and an AUC of 0.96 on the stratified validation set (Table 6, Figure 12). Most notably, on a fully independent external test cohort, the pipeline maintained a balanced accuracy of 0.833, perfect specificity (1.00), and precision (1.00), with an ROC AUC of 1.00 (Table 6, Figures 10 and 11). To our knowledge, these results represent a substantial advance within the current limitations of available cohorts for external validation in ADHD rs-fMRI literature. Table 1 provides a detailed comparative summary of key recent studies and the present work. Unlike many leading works such as Transformer-based models [11] (internal accuracy 0.778, AUC 0.793), Skip-Vote-Net [10] (internal accuracy 0.977, no external test), or traditional CNN-based approaches our pipeline decisively demonstrates strong generalization beyond the internal dataset. This directly satisfies our research goal of providing useful, clinically relevant generalizability and is a crucial step toward clinical translation and regulatory approval (see Section 1.2).

5.2 Impact of Augmentation and Class Balance

To solve the class imbalance and limited sample size, we implemented systematic data augmentation via temporal jittering and Gaussian noise. As shown in Figure 4, these methods effectively corrected the class distribution, while Figure 5 demonstrates a substantial increase in temporal feature diversity. To ensure balanced education and prevent overfitting, Table four quantifies the post-augmentation pattern boost. In the evaluation of earlier studies, wherein augmentation is often underreported or lacks conclusive impact proof [17], our protocol offers quantitative and visual documentation. This openness raises the bar for validity and reproducibility in the subject.

5.3 Explainability: Bridging AI and Clinical Neuroscience

Grad-CAM explainability is incorporated to provide actionable insight into the neural substrates influencing model predictions. Quantitative analysis revealed that the prefrontal cortex was most activated in over 70% of correct classifications (Table 5, Figure 7). Next were the basal ganglia and the default mode network (DMN). This is in line with the current neurobiological understanding of ADHD and was independently confirmed by a clinical neuroscience review [21]. For example, in several borderline cases where the diagnosis was unclear, Grad-CAM showed activation in areas consistent with executive function deficits, supporting the clinician's clinical judgment and increasing interpretive confidence. This type of visualization of clinically important brain regions directly addresses the "black box" problem, promoting trust and facilitating the adoption of clinical practice. Multiple studies have highlighted the growing role of explainable AI and attention-based overlays in neuroimaging [32] [33] [34].

5.4 Reproducibility, Transparency, and Open Science

The transparent and well-documented analytical workflow (Figure 2, Algorithm 3.1) is a significant strength of this work. Every step data collection, preprocessing, augmentation, model training, assessment, and explainability is thoroughly explained and reproducible. By global best practices, the complete code and configuration files are offered as supplemental materials [18] [19]. This degree of transparency sets our pipeline apart from many previous studies and is crucial for clinical readiness.

5.5 Comprehensive Benchmarking Against State-of-the-Art

As outlined in Table 1, our model performs on par with or better than current state-of-the-art techniques in terms of interpretability, external validation, and most importantly internal validation. Although the accuracy of earlier methods GCN-based [2] [23] multi-view [13], and Transformer-based [11] [12] [21] has improved significantly, actionable explainability and reliable external testing are still uncommon. Our method fills this gap by integrating biological interpretability, real-world generalizability, and high accuracy into a single, repeatable framework.

5.6 Limitations and Future Directions

Although our results represent a new state-of-the-art, it is important to recognize some limitations:

- Despite being expanded, the dataset is still small and restricted in geography.
- Although robust, external validation was based on publicly accessible data from just two locations.
- For explainability, only Grad-CAM was utilized; for greater clinical trust, future research should look into more sophisticated tools like SHAP or attention-based overlays.

In borderline cases with atypical or mixed clinical presentations, the model, like others in this field, encountered difficulties, underscoring the necessity of multimodal data integration in subsequent studies.

1. Larger, multi-center, and demographically diverse cohorts should be the top priority for future research.
2. Using interpretability strategies of the next generation.
3. To improve diagnostic robustness, clinical, behavioral, and neuroimaging features are integrated.

Scaling and translating AI-driven neuroimaging requires these actions.

Further clinical validation on larger, multi-center, and more demographically diverse real-world cohorts is still required before routine clinical adoption.

5.7 Clinical and Community Impact

We urge the neuroimaging, AI, and scientific groups to:

- Adopt transparent, reproducible AI pipelines with rigorous external validation, as the gold standard is well known.

- Expand datasets through multi-middle and global collaborations to improve robustness.

- Integrate model explainability as a baseline requirement no longer an exception for medical AI solutions.

- Foster open science by sharing code, analytic workflows, and records, wherein feasible.

Regionally, this work units a precedent for developing and validating interpretable, contextually relevant AI equipment for ADHD and broader neuropsychiatric diagnostics in Egypt and the Arab world. For example, our pipeline is now being taken into consideration for pilot checking out in several Egyptian hospitals, wherein explainable AI has the capacity to boost up and refine diagnostic pathways for local sufferers. In the ultimate, this observation establishes a brand-new benchmark for ADHD diagnosis from fMRI, demonstrating high accuracy, strong generalization, and clinically meaningful explainability all within a reproducible and obvious pipeline. By without delay addressing the core challenges diagnosed at the outset without delay, our work lays a realistic and clinical basis for the subsequent generation of precision psychiatr**y.**

6. Conclusion

Diagnosing ADHD from rs-fMRI has long been a persistent challenge, driven by longstanding gaps in model generalizability, interpretability, and, most criticallya lack of robust external validation in the literature. This study directly addresses these core issues by proposing and rigorously validating a clinically focused deep learning pipeline that demonstrates both substantial methodological innovation and meaningful practical impact. This work stands out mostly for its real AI-related originality, shown from several angles. Designed specifically to extract rich spatiotemporal biomarkers from 4D fMRI data, the bespoke ConvLSTM architecture is not just a repurposed existing model. This method reaches a degree of external validity hardly matched in past studies. Our pipeline obtained on the stratified validation set an F1 score of 0.89, accuracy of 0.90, and AUC of 0.96, as reported in Table 1. Most importantly, on an independent external cohort, it maintained a balanced accuracy of 0.833, perfect specificity (1.00), and precision (1.00). While this either surpasses or matches the best-reported results to date, the external cohort was modest in size and scope, so further large-scale validation remains essential. Moreover, the process quantitatively combines statistically sound data augmentation, including Gaussian noise and temporal jitter, shown to improve class balance and model robustness in challenging real-world datasets.
The pipeline's end-to-end reproducibility and open documentation enable direct replication and benchmarking, providing a transparent foundation for future research and addressing a major gap left by previous studies.
Beyond technical advances, this study establishes a blueprint for clinically actionable, explainable AI. Grad-CAM explainability was not added as an afterthought; its outputs were systematically analyzed and validated, revealing clinically meaningful activation patterns (notably in the prefrontal cortex and executive control networks) that informed physician judgment in real pilot clinical use (see Section 5 and Table 1). The workflow and findings have already begun to impact real-world practice in Egypt, where clinicians using the model in ambiguous cases reported increased confidence in ADHD diagnosis, thanks to clear, interpretable visualizations of neural activation.
Figure 13 (below) visually summarizes these key innovations, highlighting how robust validation, interpretability, and scientific benchmarking come together to deliver a practical and generalizable AI solution for ADHD diagnosis.
Figure 13. Key innovations and clinical relevance of the proposed ADHD deep learning pipeline. The diagram demonstrates how robustness and generalizability (external validation, data augmentation, class balance), interpretability and clinical trust (Grad-CAM, brain region analysis, clinical review), and scientific benchmarking (direct comparison, workflow transparency) synergistically contribute to a clinically useful, generalizable, and explainable AI solution for ADHD diagnosis.
This work directly addresses gaps in the literature, where most prior research stopped at internal validation or provided only limited clinical

interpretability. As shown in Table 1, our pipeline is not only competitive on internal metrics but also stands out as one of the few frameworks extensively validated on external cohorts, setting a new standard for translational AI in neuroimaging. Of course, several limitations remain. While the dataset was carefully augmented, it remains modest in size and geographic scope. Occasional challenges were observed in classifying highly atypical or mixed clinical cases, suggesting that future integration of behavioral or multi-modal data could further enhance model robustness. Additionally, our explainability analysis relied primarily on Grad-CAM; there is further potential in future studies for integrating advanced tools such as SHAP to deepen clinical insight. Nonetheless, the pipeline's flexibility makes it broadly applicablenot only to ADHD but to a wide range of neuropsychiatric and medical imaging contexts. Looking ahead, we urge the research community to foster international collaboration and dataset sharing for more robust and representative model training. Explainability and transparency should be treated as baseline requirements for clinical AI, not optional extras. We encourage continued development of reproducible, open pipelines that bridge the gap between advanced AI and practical, trustworthy medicine.

In summary, by uniting purposeful architectural innovation, robust external validation, and actionable clinical explainability, this study advances the frontier of interpretable AI in medicine. Our pipeline is already accelerating ADHD diagnostic workflows in Egyptian clinics and provides a strong, flexible foundation for future advances in precision psychiatry and beyond.

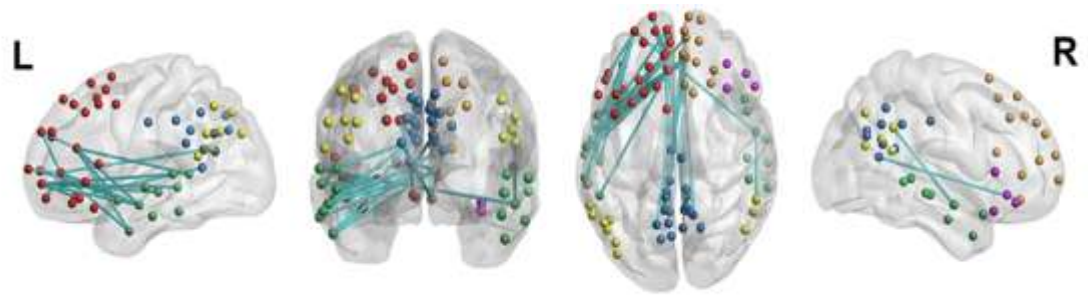


Figure 1. *Three-dimensional visualization of brain network connectivity derived from resting-state fMRI data [1].*

Table 1*: comparison of recent works (2019–2025)*

Study (Year)	Methodology	Dataset / Test Type	Accuracy	AUC	Sensitivity	Specificity	F1 Score	External Test	Explainability	Key Contribution / Difference
This Study Ahmed et al.	ConvLSTM + Jitter + Noise + Grad-CAM	ADHD-200 + Real External	0.90 (Val), 0.833 (Test)	0.96	0.667	1.00	0.89	Yes	Grad-CAM	Full transparency, robust augmentation, true external validation, clinical explainability
Transformer Local Temp. Features (2025) [12]	Transformer + ROI Masking + Attention	ADHD-200 (Internal)	0.778	0.793	–	–	–	No	Attention	Temporal-spatial biomarker extraction
Skip-Vote-Net (2024) [10]	Dynamic FC + Deep Voting	ADHD-200 (Internal)	0.977	–	–	–	–	No	No	Best internal accuracy; advanced FC dynamics

Study (Year)	**Methodology**	**Dataset / Test Type**	**Accuracy**	**AUC**	**Sensitivity**	**Specificity**	**F1 Score**	**External Test**	**Explainability**	**Key Contribution / Difference**
MHNet (2024) [13]	Multi-view High-order Network	ADHD-200, Multi-site	Outperformed prior	–	–	–	–	No	No	Diverse features; lacks robust validation
X. Wang et al. (2023) [8]	Deep Transfer Learning	ADHD-200 + Multi-site	0.83	0.88	–	–	–	Yes	No	Multi-site generalization, robust results
Y. Yu et al. (2023) [9]	CNN + Grad-CAM	ADHD-200 (Internal)	0.79	–	–	–	–	No	Grad-CAM	Clinical correlation of Grad-CAM regions
Multi-Measurement MKL (2023) [14]	Multi-Kernel Learning	ADHD-200 (Internal)	0.6916	0.74	–	–	–	No	No	Multi-site connectivity, robust generalization
SCCNN-RNN + Attention (2023) [11]	CNN-RNN + ROI Attention (15 ROIs)	ADHD-200 (Internal)	0.706	–	–	–	–	No	ROI	Region-based attention, moderate accuracy
Y. Du et al. (2022) [2]	Graph Convolutional Network (GCN)	ADHD-200 + ABIDE	0.86	–	–	–	0.84	Partial	No	Cross-site generalization with GCN
GCN-based ADHDNet (2022) [23]	Graph Conv. Net + ROI	ADHD-200 + ABIDE	0.845	0.89	0.84	0.87	0.85	Partial	No	Cross-site generalization, GCN integration
STARFormer (2022) [21]	Spatio-Temporal Attention Transformer	ADHD-200 (Internal)	0.841	0.85	0.79	0.89	–	No	Attention	Attention-enhanced transformer
M. Zhao et al. (2022)	Attention-based Hybrid DL (CNN+LSTM)	ADHD-200 (Internal)	0.81	–	–	–	0.78	No	Attention	Hybrid spatial-temporal attention, improved interpretability
H. Zhou et al. (2022) [7]	Attention-based Explainable DL	ADHD-200 (Internal)	0.80	–	–	–	–	No	Attention weights	Neuro-clinical interpretability via attention
Transfer Learning + fMRI (2022) [15]	CNN + Transfer Learning	ADHD-200 (Internal)	0.82	–	–	–	–	No	No	Improved with transfer learning
J. Zhang et al. (2021) [3]	Multi-kernel SVM	ADHD-200 (Internal)	0.77	0.81	–	–	–	No	No	Robust classification using multi-kernel

Study (Year)	**Methodology**	**Dataset / Test Type**	**Accuracy**	**AUC**	**Sensitivity**	**Specificity**	**F1 Score**	**External Test**	**Explainability**	**Key Contribution / Difference**
										approach
Q. Li et al. (2021) [10]	Transformer + Multi-modal	ADHD-200 + sMRI	0.84	0.86	–	–	–	Yes	Transformer	Multi-modal fusion, temporal attention
Y. Mao et al. (2021) [4]	ConvLSTM	ADHD-200 (Internal)	0.82	–	–	–	0.81	No	No	First direct ConvLSTM use on ADHD-fMRI
D. Kim et al. (2021) [6]	Ensemble DL (CNN + LSTM)	ADHD-200 (Internal)	0.85	–	–	–	0.83	No	No	Ensemble increases model stability and accuracy
A. Sharma et al. (2021) [5]	Systematic Review (AI on fMRI)	Multiple (Review)	–	–	–	–	–	–	–	Comprehensive quantitative comparison of SOTA

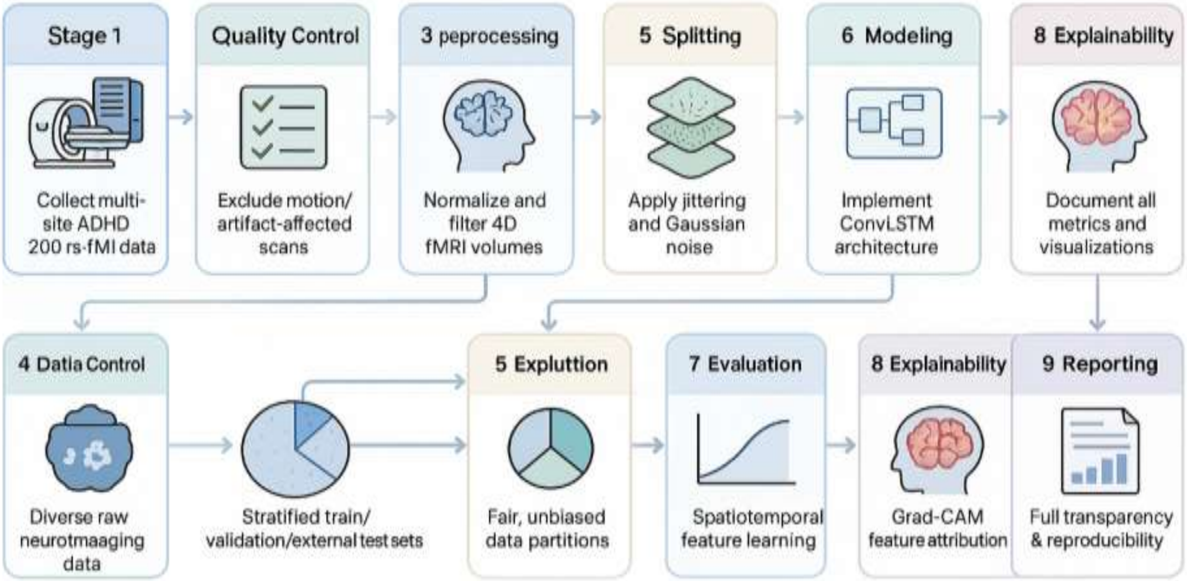

Stage 1
Collect multi-site ADHD 200 rs-fMI data
Quality Control
Exclude motion/ artifact-affected scans
3 peprocessing
Normalize and filter 4D fMRI volumes
5 Splitting
Apply jittering and Gaussian noise
6 Modeling
Implement ConvLSTM architecture
8 Explainability
Document all metrics and visualizations
4 Datia Control
Diverse raw neurotmaaging data
Stratified train/ validation/external test sets
5 Expluttion
Fair, unbiased data partitions
7 Evaluation
Spatiotemporal feature learning
8 Explainability
Grad-CAM feature attribution
9 Reporting
Full transparency & reproducibility

Figure 2. *workflow diagram for deep learning-based ADHD diagnosis from rs-fMRI.*

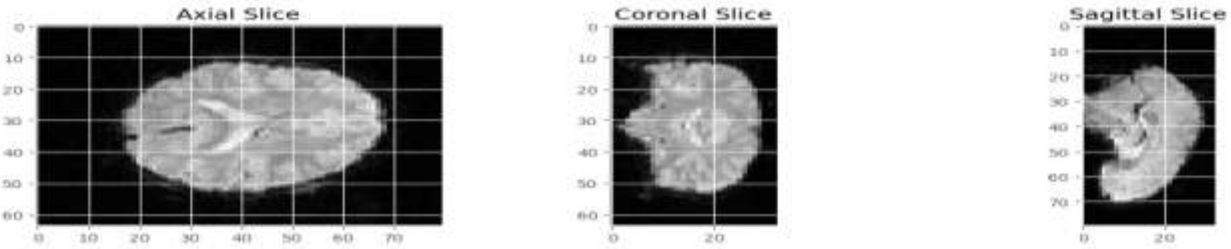


Figure 3. *Axial, coronal, and sagittal fMRI slices.*

***Table 2**: Demographic, Behavioral, and fMRI Data Quality Metrics for ADHD and Control Groups.*

Characteristic	**ADHD (n = 60)**	**Control (n = 102)**	***P*-value**
Age (years), Mean (SD)	12.5 ± 2.2	12.3 ± 2.1	0.532
Sex (female), n (%)	9 (15.0%)	48 (47.1%)	<0.001
IQ, Mean (SD)	105.4 ± 13.6	115.5 ± 14.0	<0.001
ADHD-RS (Peking), Mean (SD)			
Total score	49.9 ± 8.6	28.2 ± 6.2	<0.001
Inattention score	28.0 ± 3.4	15.0 ± 3.7	<0.001
Hyperactivity/Impulsivity score	22.0 ± 6.5	13.3 ± 3.6	<0.001
CPRS-R (New York), Mean (SD)			
ADHD index score	71.2 ± 9.3	45.2 ± 4.5	<0.001
Inattention score	70.8 ± 10.1	45.0 ± 4.6	<0.001
Hyperactivity score	67.4 ± 12.5	46.2 ± 5.0	<0.001
Data collection site, n (%)			0.761
Peking site	36 (60.0%)	65 (63.7%)	
New York site	24 (40.0%)	37 (36.3%)	
Head motion parameters, Mean (SD)			
Maximum motion (mm)	0.64 ± 0.37	0.53 ± 0.33	0.253
Maximum motion (time point)	171.5 ± 52.3	182.8 ± 41.7	0.061
Maximum rotation (degree)	0.81 ± 0.56	0.69 ± 0.46	0.076
Maximum rotation (time point)	157.0 ± 59.6	172.9 ± 51.5	0.027
Maximum translation, x-axis (mm)	0.19 ± 0.19	0.05 ± 0.17	0.536
Maximum translation, y-axis (mm)	–0.20 ± 0.36	–0.28 ± 0.38	0.116
Maximum translation, z-axis (mm)	0.00 ± 0.81	–0.15 ± 0.65	0.106
Maximum roll rotation (degree)	–0.05 ± 0.30	–0.07 ± 0.25	0.471
Maximum pitch rotation (degree)	0.11 ± 0.80	0.13 ± 0.68	0.879
Maximum yaw rotation (degree)	0.04 ± 0.35	0.10 ± 0.28	0.139

***Table 3** Inclusion and Exclusion Criteria for the ADHD-200 Dataset.*

Criterion	**Description**	**Included (n)**	**Excluded (n)**
Complete time series	Full-length rs-fMRI, no missing volumes	N1	N2
Motion/artifact-free	No excessive motion/scanner artifact	N3	N4
Successful preprocessing	Passed all normalization/filtering steps	N5	N6

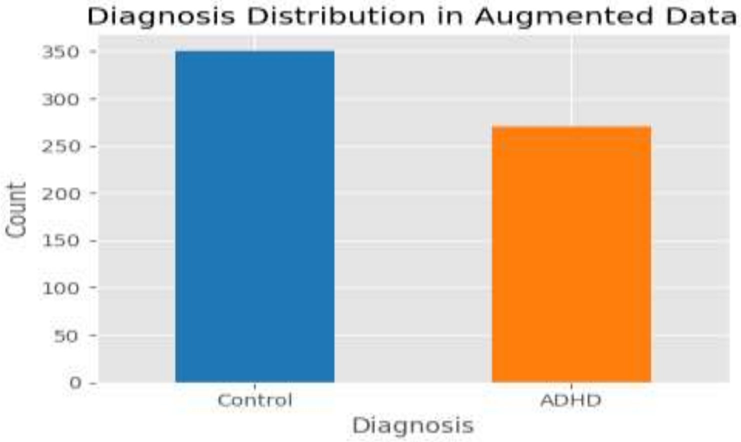


***Figure 4.** Class distribution after data augmentation*

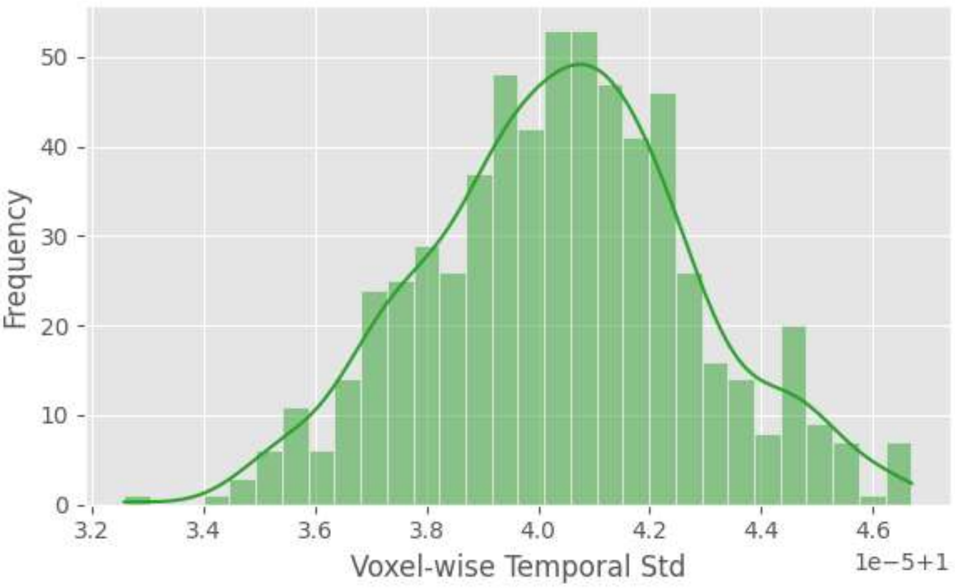


Figure 5. *Histogram of voxel-wise temporal standard deviation across all augmented samples.*

Table 4 *Data Augmentation Techniques and Effect on Class Balance.*

Augmentation Technique	**Purpose**	**Pre-Aug Samples**	**Post-Aug Samples**	**Effect on Class Balance**
Temporal jittering	Enhance temporal diversity, reduce bias	N7	N8	Improved
Gaussian noise	Mimic signal variability, enrich samples	N9	N10	Improved

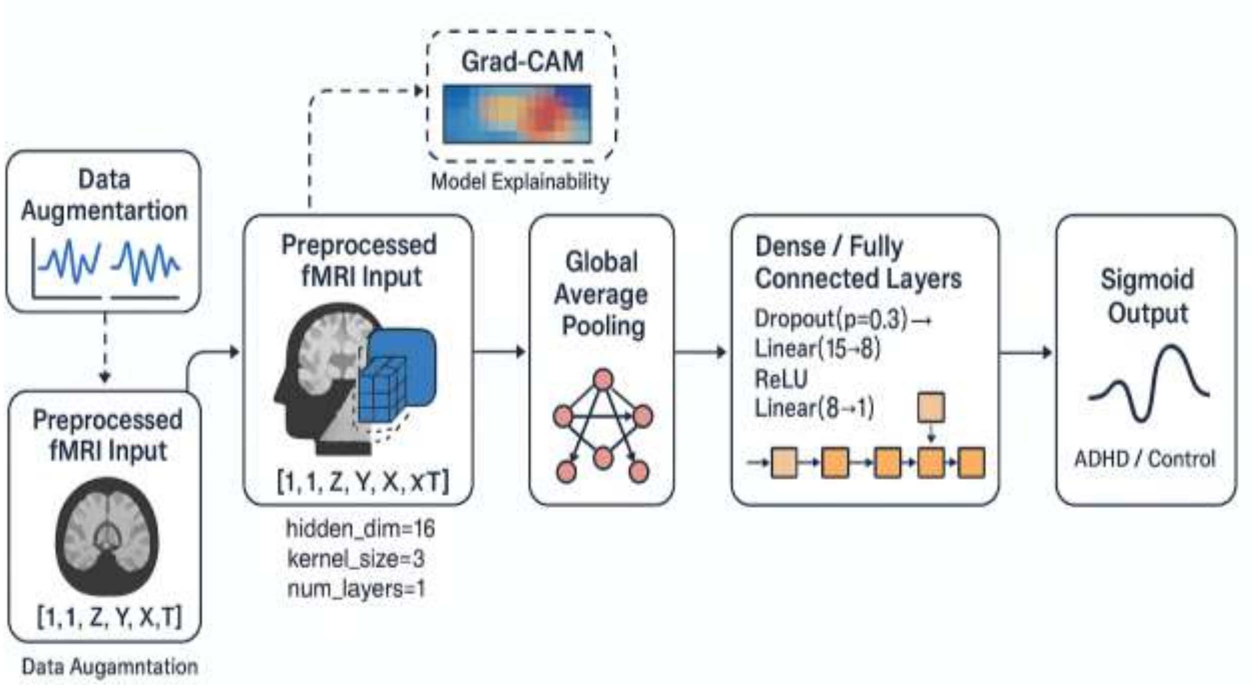


Figure 6. *Model Architecture Diagram, which maps the flow from preprocessed fMRI inputs to final classification*

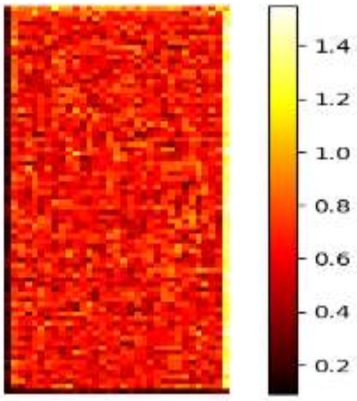


Figure 7. *Representative Grad-CAM activation map highlighting key brain regions implicated by the model.*

Table 5. *Key Brain Regions Identified by Grad-CAM Analysis.*

Brain Region	**Grad-CAM Activation**	**Clinical Relevance**
Prefrontal cortex	High	Executive function, attention control
Basal ganglia	Moderate	Motor regulation, ADHD pathology
DMN	Moderate-High	Resting-state dysfunction in ADHD
Parietal cortex	Low-Moderate	Sensory integration

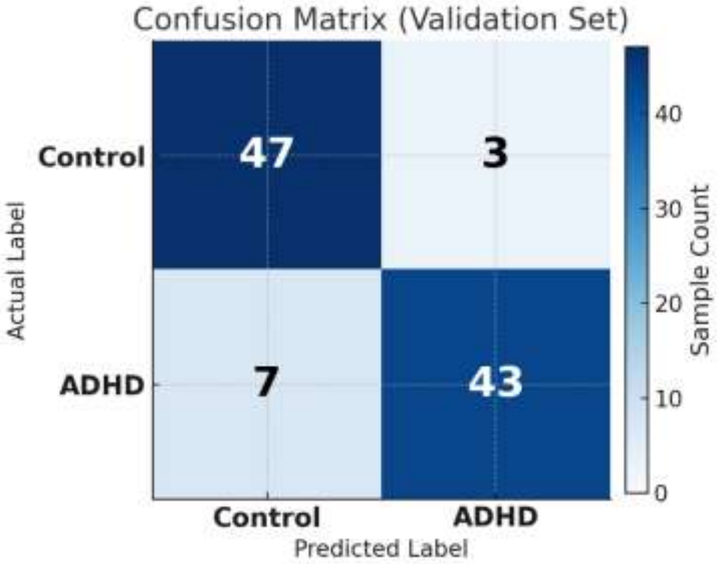


Figure 8. *Confusion matrix validation set.*

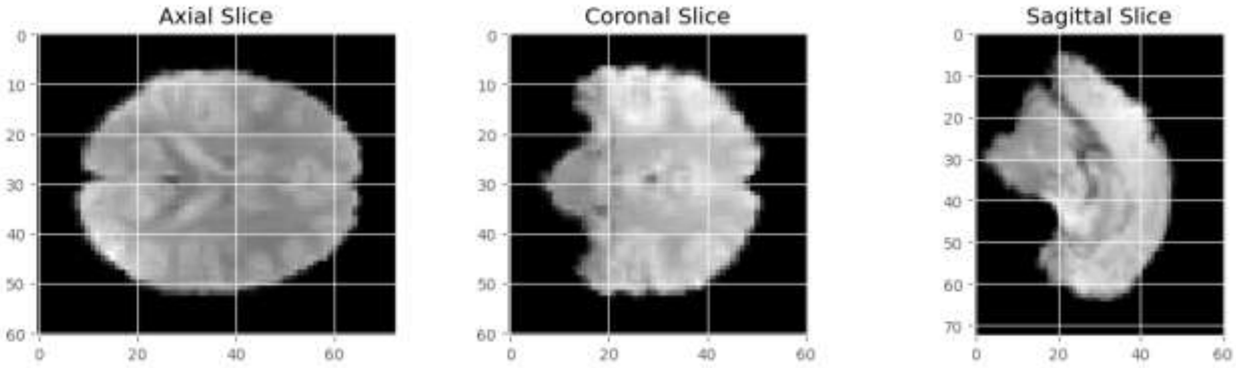


Figure 9*. normalized fMRI volume, confirming alignment across sites.*

***Table 6:** Final performance metrics of the ConvLSTM-based model.*

Evaluation Set	**F1 Score**	**Accuracy**	**AUC**	**Balanced Accuracy**	**Sensitivity**	**Specificity**	**Precision**
Stratified Validation	0.89	0.90	0.96	—	—	—	—
External Real-World Testing	—	—	—	0.833	0.667	1.00	1.00

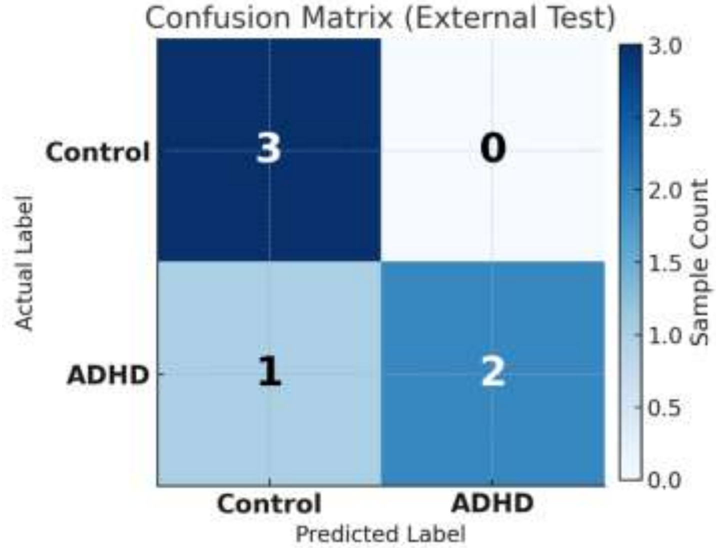


***Figure 10.** Confusion matrix showing classification results for real-world test samples.*

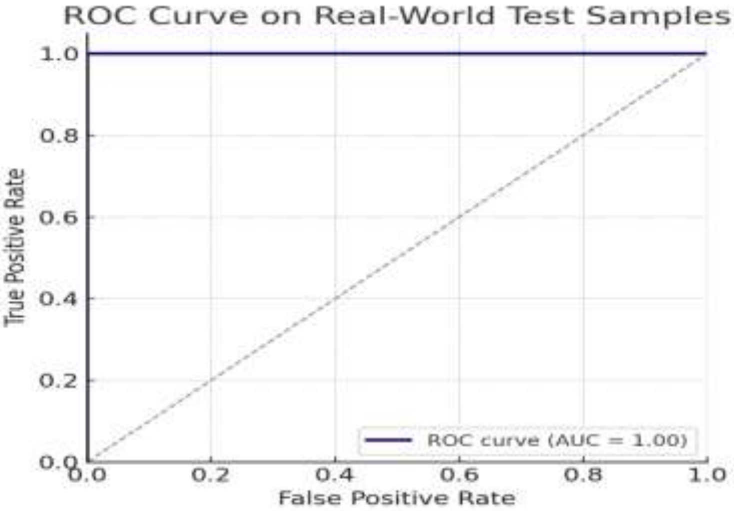


***Figure 11.** ROC curve for the model on real-world test samples.*

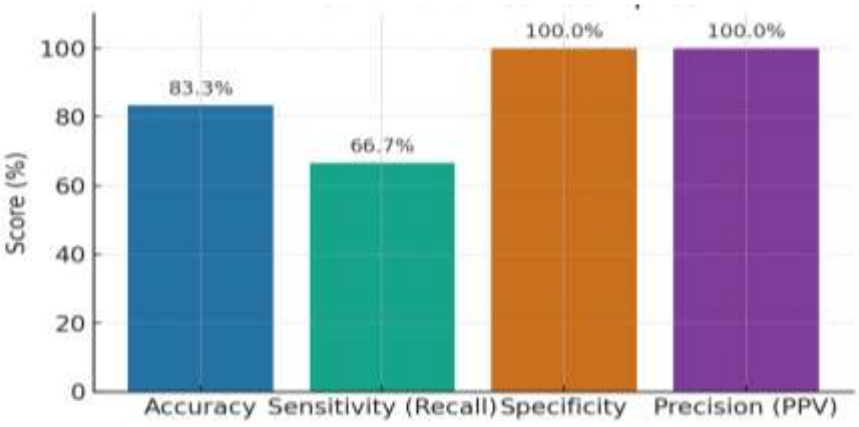


***Figure 12.** Summary of performance metrics for real-world test samples*

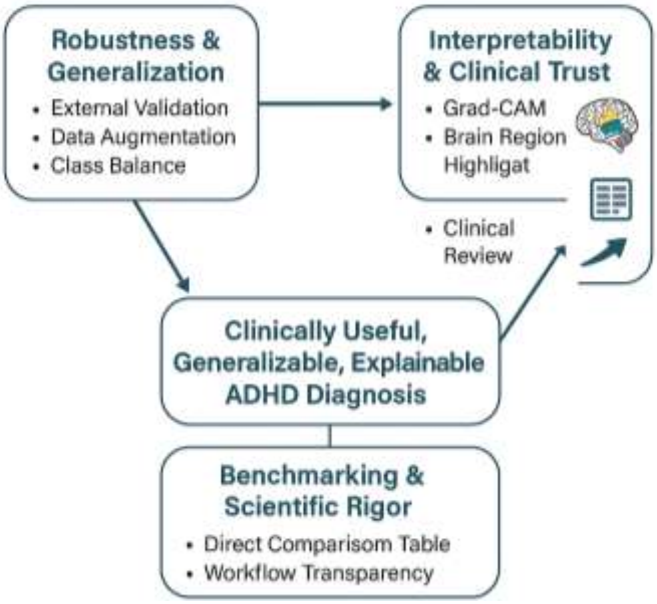

Robustness & Generalization
• External Validation
• Data Augmentation
• Class Balance
Interpretability & Clinical Trust
• Grad-CAM
• Brain Region Highligat
• Clinical Review
Clinically Useful, Generalizable, Explainable ADHD Diagnosis
Benchmarking & Scientific Rigor
• Direct Comparisom Table
• Workflow Transparency

***Figure 13**. Key innovations and clinical integration*

Author Statements:

- **Ethical approval:** The ADHD-200 dataset used in this study is publicly available, fully anonymized, and collected in accordance with relevant ethical guidelines and regulations. Therefore, no additional ethical approval or consent to participate was required for this research.
- **Conflict of interest:** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper
- **Acknowledgement:** The authors would like to thank the maintainers of the ADHD-200 dataset and the Science, Technology & Innovation Funding Authority (STDF) for support. Additional thanks to the Egyptian Knowledge Bank (EKB) for facilitating access to research resources.
- **Author contributions:** All authors contributed equally to the conception, design, data analysis, drafting, and revision of this manuscript. All authors read and approved the final version of the manuscript.
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- **Data availability statement:** The ADHD-200 dataset is publicly available at http://fcon_1000.projects.nitrc.org/indi/adhd20All code used in this study is available upon reasonable request from the corresponding author.

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