Neuropsychiatric Disease and Treatment

Dovepress
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ORIGINAL RESEARCH

# Electroencephalogram (EEG) Based Prediction of Attention Deficit Hyperactivity Disorder (ADHD) Using Machine Learning

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**Objective:** Attention Deficit Hyperactivity Disorder (ADHD) is a neurodevelopmental condition with challenges in timely and accurate diagnosis. This study evaluates the effectiveness of combining electroencephalogram (EEG) data with machine learning techniques to enhance ADHD diagnostic accuracy.

**Methods:** A total of 168 participants, comprising 107 ADHD and 61 neurotypical (NT) individuals, were assessed using the Kiddie Schedule for Affective Disorders and Schizophrenia Present and Lifetime Version Korean Version (K-SADS-PL-K). EEG data from 19 channels were analyzed across five frequency bands: delta (1–4 hz), theta (4–8 hz), alpha (8–12 hz), beta (12–30 hz), and gamma (30–51 hz). The Extreme Gradient Boosting (XGBoost) classifier was employed for classification, and Leave-One-Subject-Out (LOSO) cross-validation was used to ensure model robustness.

**Results:** Data augmentation through 30-second segmentations generated 2434 EEG segments for ADHD and 1060 for NT. The XGBoost model achieved a test accuracy of 90.81% and an F1-score of 0.9347. Feature importance analysis using SHAP (SHapley Additive exPlanations) values identified middle beta frequency features, particularly from the O1 electrode site, as significant contributors to classification.

**Conclusion:** EEG-based machine learning models, such as the XGBoost classifier, show potential as non-invasive tools for ADHD diagnosis, offering high accuracy and interpretability. The novelty of this approach lies in combining SHAP analysis with data augmentation techniques and LOSO cross-validation, ensuring both explainability and robust generalizability. Future research with larger datasets and diverse populations is recommended to validate findings and explore clinical applications.

**Keywords:** attention deficit hyperactivity disorder, ADHD, machine learning, quantitative electroencephalography, diagnosis

## Introduction

Attention Deficit Hyperactivity Disorder (ADHD) is a common neurodevelopmental disorder characterized by inattention, hyperactivity, and impulsivity, affecting both children and adults globally.[1] The prevalence of ADHD in children is estimated to be approximately 5%, while around 4.4% of adults are reported to exhibit persistent ADHD symptoms.[2] As of 2020, when adjusted for global population characteristics, the prevalence of ADHD starting in childhood and persisting into adulthood was estimated at 2.58%, translating to approximately 139.84 million individuals. Additionally, the prevalence of adult ADHD symptoms unrelated to childhood onset was reported at 6.76%, corresponding to about 366.33 million individuals worldwide. These figures highlight the significant public health burden posed by ADHD on a global scale.[3]

In addition to core symptoms such as inattention, hyperactivity, and impulsivity, children with ADHD are known to experience deficits in executive functions, including working memory, inhibitory control, and planning, when compared



Received: 28 November 2024
Accepted: 7 February 2025
Published: 13 February 2025

to their neurotypical peers.[4] These deficits often lead to long-term challenges, such as poor academic achievement, difficulties in interpersonal relationships, and an increased likelihood of delinquent behavior.[5] These symptoms frequently persist into adulthood, causing lifelong impairments and imposing significant academic, social, financial, and employment-related burdens on both individuals and their families. Early diagnosis and intervention are therefore essential to ensure the well-being and future prospects of individuals with ADHD. However, the underlying pathophysiology of ADHD remains unclear, making early diagnosis particularly challenging. Currently, ADHD diagnosis relies on an extensive process that includes comprehensive interviews, behavioral assessments, third-party observations, and detailed personal histories. Diagnostic decisions are typically made based on the criteria outlined in the *Diagnostic and Statistical Manual of Mental Disorders, Fifth Edition (DSM-5)*, published by the American Psychiatric Association.[6] However, these subjective behavioral assessment approaches can lead to inconsistencies and biases. Accurate diagnosis is crucial for timely intervention but is often complicated by the reliance on subjective assessment tools and the symptom overlap with other conditions. As a result, there is increasing interest in objective, data-driven diagnostic methods.

Electroencephalography (EEG) has emerged as a promising non-invasive tool for evaluating brain activity patterns associated with ADHD. Advances in quantitative EEG (qEEG) have enabled detailed analysis of frequency-specific brain activity, highlighting its potential for clinical applications. Studies have reported distinct differences in the brain wave patterns of individuals with ADHD compared to controls, such as increased delta and theta waves and decreased alpha and beta waves.[7] Efforts to differentiate typically developing children from those with ADHD using qEEG have continued over time. The theta-to-beta ratio (TBR) has gained attention as a strong candidate for a biological marker in children with ADHD.[8] However, subsequent research has revealed limitations, including a high rate of false positives and increased TBR levels even in control groups, suggesting that TBR may not be a reliable diagnostic marker.[9]

To overcome these limitations, it is necessary to move beyond traditional statistical analyses of EEG signal data and adopt machine learning methods. Machine learning techniques have emerged as powerful tools for processing complex datasets and detecting subtle patterns in neurophysiological signals. A previous study analyzed morphological and power spectral density (PSD) features associated with ADHD using resting-state EEG signals from 61 children with ADHD and 60 healthy controls. Classification algorithms such as AdaBoost, k-nearest neighbor (KNN) classifier, Naive Bayes, and random forest were applied, with the Bernoulli Naive Bayes classifier achieving the highest accuracy of 96%.[10] Another study reported a diagnostic accuracy of 94.67% on test data using a deep learning algorithm, specifically a convolutional neural network (CNN), to diagnose ADHD.[11] In addition, a study employing four machine learning-based algorithms—support vector machine (SVM), k-nearest neighbors (KNN), multilayer perceptron (MLP), and logistic regression—demonstrated an accuracy of 94.2%, a sensitivity of 93.3%, an F1-score of 91.9%, and an AUC of 0.964 in classifying children with ADHD.[12] Recent studies have explored advanced methods for ADHD classification, such as the use of empirical mode decomposition (EMD) and discrete wavelet transform (DWT) for feature extraction, combined with machine learning algorithms. ADHD dataset classified using the AdaBoost algorithm achieved an accuracy of 1.00, with F1-score values of 0.71, respectively. In comparison, the Random Forest (RF) algorithm achieved slightly lower metrics, with an accuracy of 0.98 and an F1-score of 0.71. These results highlight the potential of machine learning models in achieving high accuracy for ADHD classification.[13]

In 2024, significant progress was observed in leveraging wearable EEG devices and multimodal strategies to enhance ADHD detection. Notably, recent studies highlighted that combining EEG-derived features with behavioral assessments led to improved diagnostic performance, particularly by emphasizing the role of high-frequency gamma activity in the occipital region.[14] However, challenges persist in achieving a balance between diagnostic accuracy, model interpretability, and generalizability across diverse cohorts.

A critical research gap exists in developing models that not only deliver high classification accuracy but also offer meaningful insights into the neurophysiological mechanisms of ADHD. Addressing this gap, our study integrates quantitative EEG (qEEG) data with SHAP (SHapley Additive exPlanations) analysis and utilizes the Extreme Gradient Boosting (XGBoost) algorithm. This method enhances diagnostic accuracy while ensuring interpretability by identifying key features such as middle beta activity. Additionally, the robustness of the model is validated through Leave-One-Subject-Out (LOSO) cross-validation.

# Methods

## Participants

Children aged 8 to 15 years were recruited between 2019 and 2021 from the Department of Psychiatry at Daegu Catholic University Medical Center, Seoul National University Hospital, and Hanyang University Seoul Hospital. Written informed consent was obtained from both the children and their parents after they were provided with detailed information about the study and its procedures.

ADHD diagnoses were determined using the Diagnostic and Statistical Manual of Mental Disorders, Fifth Edition (DSM-5) criteria, assessed through the Kiddie Schedule for Affective Disorders and Schizophrenia-Present and Lifetime Version, Korean Version (K-SADS-PL-K), a semi-structured clinical interview. Children with a history of congenital genetic conditions, brain injury, neurological disorders, or psychiatric conditions such as schizophrenia spectrum disorder, autism spectrum disorder, obsessive-compulsive disorder, major depressive disorder, or bipolar disorder were excluded. Additionally, participants with an IQ below 70, as determined by the Korean-Wechsler Intelligence Scale for Children-Fourth Edition (K-WISC-IV), were also excluded. The ADHD group comprised children who met the diagnostic criteria for ADHD based on the K-SADS-PL-K. The Neurotypical group included children who did not exhibit any abnormalities according to DSM-5 criteria and had no prior history of psychological or related disorders. A total of 168 participants were included in the study, divided into an ADHD group (n = 107) and a Neurotypical group (n = 61).

The study protocol was approved by the Institutional Review Boards of Daegu Catholic University Medical Center (CR-19-064), Seoul National University Hospital (H-1905-145-1035), and Hanyang University Seoul Hospital (HYUH 2020–02-025-005). The study adhered to the ethical principles outlined in the Declaration of Helsinki (World Medical Association: Ethical Principles for Medical Research Involving Human Subjects, 1964). Additionally, the study was registered at ClinicalTrials.gov (registration number: NCT04469335; registered on July 14, 2020).

## EEG Recording and Pre-Processing

A flowchart illustrating the workflow of the EEG-based ADHD classification technique is presented in Figure S1. This diagram outlines the key steps, including data acquisition, preprocessing, feature extraction, and classification, providing a visual overview of the methodology used in this study. EEG data were recorded using four different systems: the Compumedics Grael-4K System (Compumedics, Australia), the Nihon Kohden Corporation Neurofax EEG-1200K System (Nihon Kohden, Japan), the Grass Technologies Comet-Plus System (Grass Technologies, USA), and the Ybrain MINDD-SCAN system (Ybrain, Republic of Korea). EEG signals were collected from 19 electrodes positioned according to the international 10–20 system, including Fp1, Fp2, F3, F4, F7, F8, Fz, C3, C4, Cz, T3, T4, T5, T6, P3, P4, Pz, O1, and O2. Depending on the hospital and the specific device used, sampling rates varied between 400 hz, 500 hz, and 512 hz. During the EEG recordings, participants were seated comfortably in a chair with their eyes closed.

The preprocessing of EEG data was conducted using Python, with the SciPy and MNE-Python libraries. Initially, detrending was applied to remove the DC component, followed by normalization to facilitate data comparability. The data were then resampled to a standardized sampling rate of 250 hz across all datasets. For consistency, the EEG signals were re-referenced to an average reference. A bandpass filter (1–100 hz) and a 60 hz notch filter were applied to remove high-frequency noise and power line interference.

Independent component analysis (ICA) was employed to identify and remove artifacts, including eye blinks, muscle activity, and cardiac noise. The ICLabel algorithm was used to label the decomposed signals, and non-brain components, such as those associated with muscle, eye, heart, line, and channel noise, were excluded. Finally, the artifact-free EEG data were segmented into equal 30-second epochs for further analysis.

## Feature Extraction

For spectral analysis, five frequency bands were defined: delta (1–4Hz), theta (4–8Hz), alpha (8–12Hz), beta (12–30Hz), and gamma (30–51Hz). Power spectral analysis was conducted using Welch's method, with a 1000ms time window,


https://doi.org/10.2147/NDT.S509094

500ms overlap, and a Hamming window, implemented in MNE-Python software. The absolute power for each frequency band was averaged across all time windows and frequencies.

Cross-frequency phase-amplitude coupling (CFPAC) between theta and gamma oscillations was evaluated to examine cross-frequency interactions.[15] The theta signal (4–8Hz) phase and the gamma signals' amplitude (in the ranges of 30–33Hz, 33–36Hz, 36–39Hz, 39–42Hz, 42–45Hz, 45–48Hz, 48–51Hz) were extracted from the EEG data using the Hilbert transform. The phase-amplitude coupling between the theta phase and each gamma amplitude was measured using the Phase-Locking Value (PLV) method. All computations were performed using the Tensorpac toolbox. Relative powers, power ratios, and phase-amplitude coupling values were calculated and used as features for classification.

## Classifier

To investigate the problem of classifying the ADHD group versus the neurotypical group, the Extreme Gradient Boosting (XGBoost) classifier was employed.[16] The XGBoost classifier is an extension of the Gradient Boosting classifier, designed with a particular emphasis on enhancing both speed and performance. The goal of the model was to maximize the F1-score, which balances precision and recall, a grid search algorithm was employed to tune the model's hyperparameters. To evaluate the model's performance, Leave-One-Subject-Out (LOSO) cross-validation was utilized.[17] The data from each subject is iteratively left out as a test set, while the model is trained on the remaining data from all other subjects. This process is repeated for each subject, providing a comprehensive evaluation across all individuals in the dataset. The performance metrics were computed for each iteration, and the final model performance is reported as the average of these metrics across all subjects.

# Results

## Dataset Characteristics

The dataset comprised EEG signals from a total of 168 participants, including 107 individuals in the ADHD group and 61 in the neurotypical (NT) group. The mean age of the ADHD group was 10.23 years (SD = 1.93), while the mean age of the NT group was 11.24 years (SD = 1.84). To address the issue of limited data, the dataset was augmented by segmenting each participant's EEG signals into 30-second intervals. This preprocessing step generated 2434 EEG segments for the ADHD group and 1060 segments for the NT group, which were then utilized to train the artificial intelligence model.

Statistical analysis of frequency band power revealed significant differences between the ADHD and NT groups, particularly in the beta and gamma bands. Additionally, Fisher Ratio calculations were performed for each feature to evaluate their discriminative power for machine learning applications. This analysis assesses the degree of separability between the two classes, with higher values indicating greater class separability. Gamma and beta signals from the occipital region were identified as key factors contributing to the differentiation between groups (Figure 1).

## Model Performance

The XGBoost classifier demonstrated strong performance, achieving a test accuracy of 90.81% and an F1 Score of 0.9347, precision of 0.9258, recall (sensitivity) of 0.9437, and specificity of 0.8264 (Table S1). These results indicate the model's reliability and precision in differentiating between ADHD and Neurotypical subjects (Figure 2). Leave-One-Subject-Out (LOSO) cross-validation was employed to ensure the generalizability of the model across individuals. This approach provided a comprehensive evaluation by iteratively leaving one participant's data as the test set while training the model on the remaining dataset. The results confirmed the model's ability to generalize effectively without overfitting to specific subjects.

## Feature Importance Analysis

Feature importance analysis using SHAP (SHapley Additive exPlanations) values identified middle beta frequency features, particularly those derived from the O1 electrode site, as the most significant contributors to classification. Another notable finding was the substantial group-level difference observed in the gamma band within the occipital

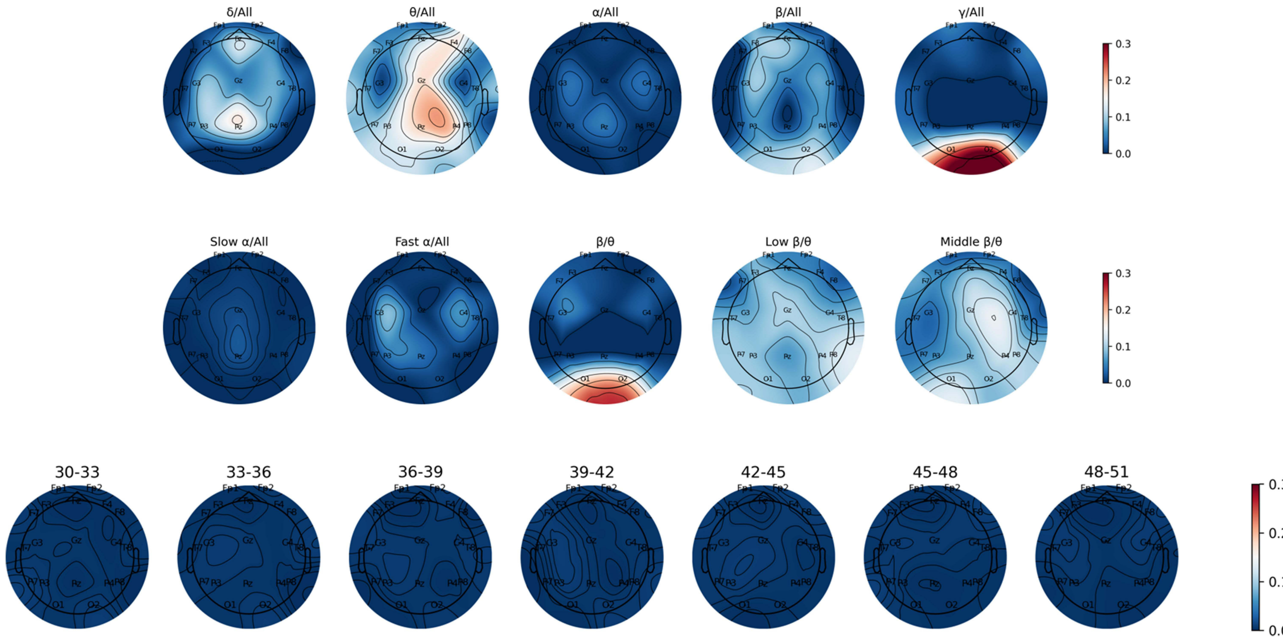


**Figure 1** Fisher Ratio values calculated for each feature to evaluate their discriminative power in the context of machine learning applications. Higher Fisher Ratio values indicate greater separability between classes.

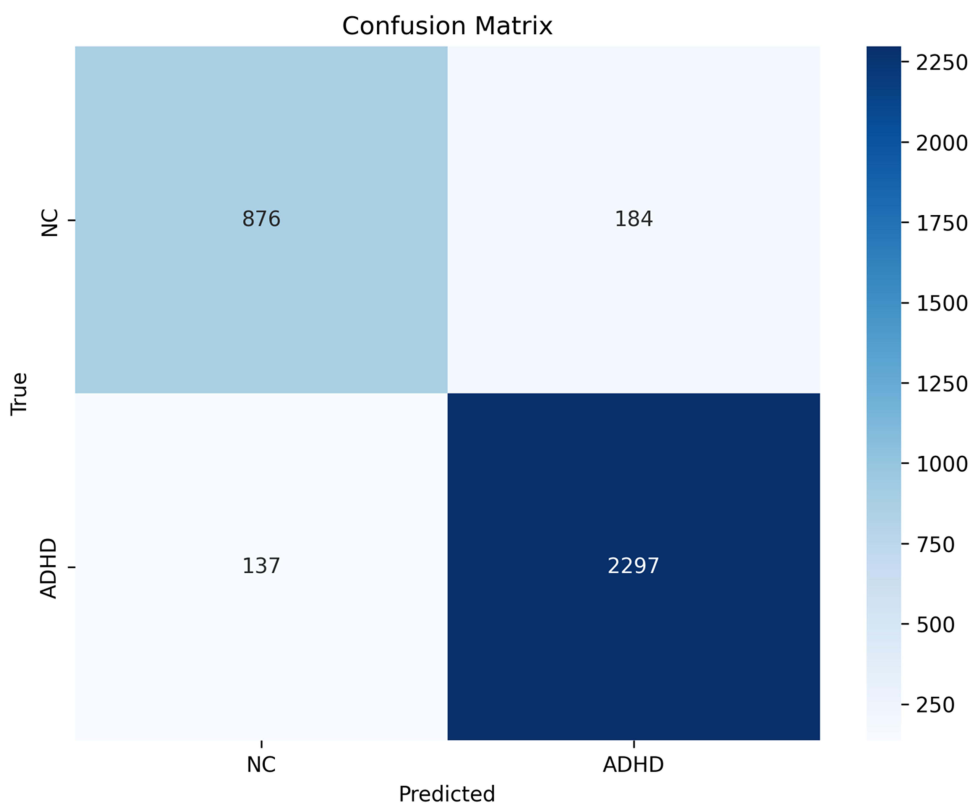


**Figure 2** Performance of the XGBoost classifier in distinguishing ADHD and Neurotypical groups, with a test accuracy of 90.81% and an F1-score of 0.9347.

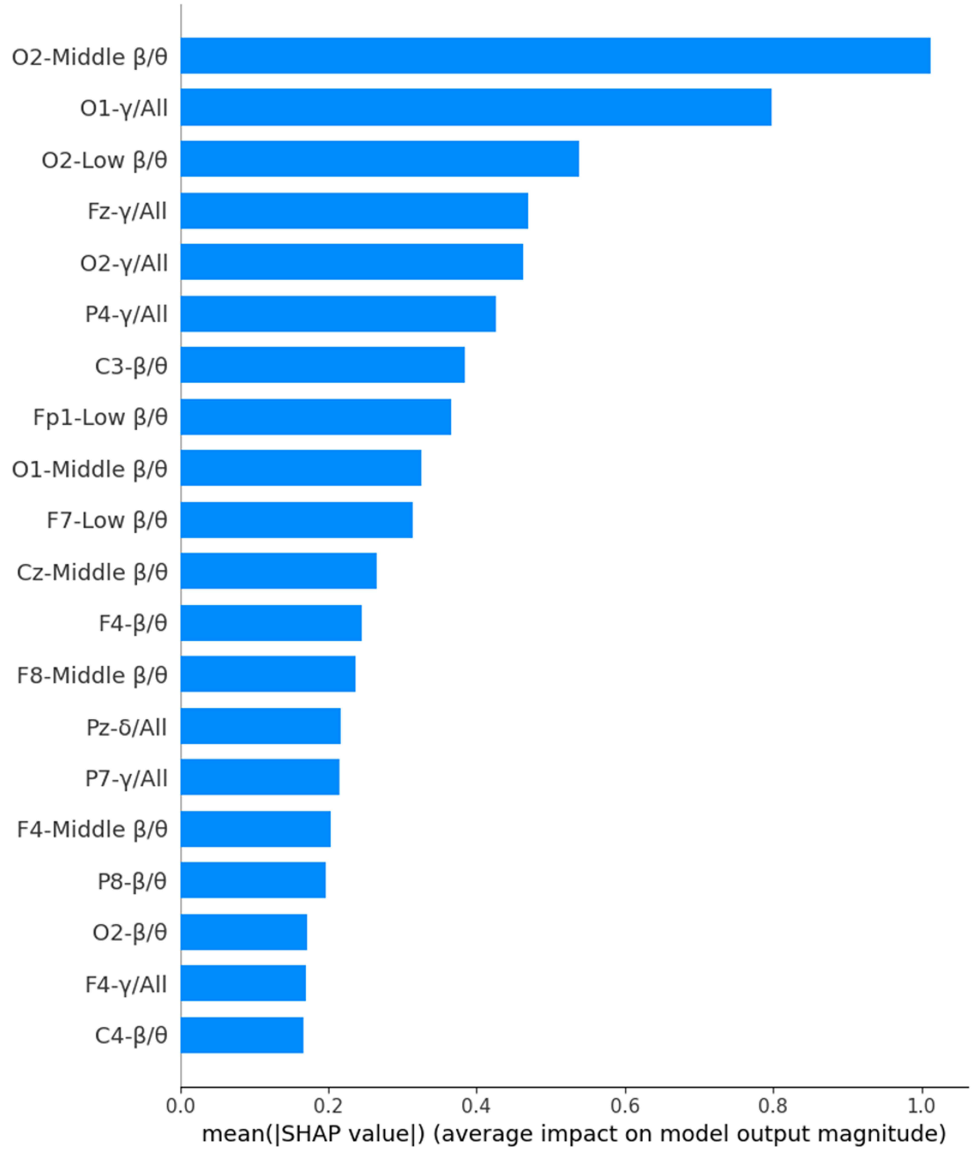


**Figure 3** SHAP value-based feature importance analysis highlights middle beta frequency features from the O1 and O2 electrode sites as the most significant contributors to classification.

region, which further enhanced the distinction between ADHD and NT participants (Figure 3). To further elucidate the spatial and spectral contributions to ADHD classification, we summarized the mean SHAP values for Beta/Theta frequency variations across all electrode sites (Table S2).

Fisher Ratio analysis of feature separability demonstrated high discriminative power for these frequency bands, supporting their critical role in classification. This analysis quantified the features' ability to distinguish between the ADHD and NT groups, with higher Fisher Ratio values indicating greater class separability. These findings are consistent with previous research highlighting altered beta activity as a key neural marker in ADHD populations.

# Discussion

## Comparison with Existing Methods

Traditional ADHD diagnostic approaches rely heavily on subjective measures such as clinical interviews and behavioral assessments, which are vulnerable to bias and variability.[18] In contrast, EEG-based machine learning offers an objective, data-driven alternative with greater reproducibility. While prior studies using EEG have achieved moderate success, challenges such as small sample sizes and suboptimal validation approaches have hindered generalizability. This study addressed these limitations through data augmentation and the application of a robust Leave-One-Subject-Out (LOSO) cross-validation strategy, ensuring that the model's performance reflects its ability to generalize across individuals.

The segmentation of EEG data into 30-second intervals allowed effective data augmentation, significantly increasing the dataset size without introducing noise. This approach not only improved training outcomes but also enabled the model to capture temporal dynamics in EEG signals, a key factor in distinguishing ADHD-related neural patterns.

### Interpretation of Findings

This study demonstrates the significant potential of EEG-based machine learning models for enhancing the diagnostic accuracy of ADHD. The XGBoost classifier achieved a high-test accuracy of 90.81% and an F1-score of 0.9347, indicating strong model performance in distinguishing ADHD participants from neurotypical (NT) controls. The use of SHAP values for feature importance analysis identified middle beta frequency features, particularly from the O1 and O2 electrode sites, as critical contributors to classification accuracy. These findings align with prior research that implicates alterations in beta activity as key markers of ADHD-related neural dysregulation.[19]

The middle beta frequency band is associated with attention, arousal, and cognitive control, processes often impaired in individuals with ADHD.[20] Notably, activity in the occipital region (O1 and O2 electrodes) may reflect visual processing and attentional mechanisms, which are known to be atypical in ADHD populations.[21] Additionally, significant group-level differences observed in gamma activity further support the role of these frequency bands in ADHD diagnosis, reinforcing their utility as biomarkers.[22]

### Clinical Implications and Practical Implementation

The use of EEG-based machine learning models holds several advantages in clinical practice. First, it provides a non-invasive, relatively low-cost diagnostic tool that can complement existing methods. Second, it offers rapid analysis, which could expedite the diagnostic process and facilitate early intervention. Finally, the interpretability of the model through SHAP analysis enhances its clinical utility by providing insights into the neural underpinnings of ADHD, aiding clinicians in understanding individual cases.

The identification of middle beta activity and occipital region signals as key features highlights promising targets for intervention. Neurofeedback training, for example, could be tailored to modulate beta activity, enhancing attentional control. One widely used protocol in clinical practice is the theta-beta protocol,[23] which aims to reduce theta waves while increasing beta activity-a strategy that aligns with the findings of this study. While gamma activity is regarded as an indicator of brain network functionality essential for higher cognitive processes, research on ADHD-related differences in the gamma frequency range remains limited. Studies suggest that gamma activity is strongly associated with cognitive deficits in individuals with ADHD and may be influenced by dopamine polymorphisms linked to the disorder.[24] However, no specific intervention targeting the gamma band has been established to date. Leveraging gamma band features, such as theta-gamma coupling, to enhance diagnostic accuracy could offer significant clinical advantages.[15,25]

However, noise and variability in EEG recordings present significant challenges in real-world settings. To address this, our study incorporated robust preprocessing techniques, including Independent Component Analysis (ICA), bandpass filters, and artifact removal algorithms, to mitigate the impact of noise and enhance signal quality. These preprocessing methods effectively handled common artifacts, such as eye blinks and muscle movements, ensuring reliable data for model training and validation. However, future implementations could integrate adaptive filtering and real-time artifact detection algorithms to further improve the system's robustness under diverse clinical and environmental conditions.

## Limitations

While this study provides promising results, several limitations must be acknowledged. The relatively small sample size (n = 168) may restrict the generalizability of the findings to broader populations. Although data augmentation through segmentation effectively increased the dataset size, the original sample represents a specific demographic, limiting its applicability across diverse cultural or age groups. Additionally, the focus on resting-state EEG data, while common, may overlook ADHD-related neural activity during cognitive or attentional tasks. Incorporating task-based EEG data in future studies could provide a more comprehensive understanding of ADHD. The study also did not fully account for confounding factors, such as comorbid conditions, developmental variations, or medication effects, which could influence EEG patterns. Notably, 81 participants in the ADHD group were on medication, with an average dose of atomoxetine at 38.3 mg or methylphenidate at 31.6 mg. These factors should be considered in future research to improve the robustness of findings. Finally, a limitation of this study is the inherent imbalance in the dataset, with more participants in the ADHD group than in the neurotypical group. To address this issue, EEG recordings were segmented into 30-second intervals, which significantly expanded the dataset and improved the representation of both classes. This approach helped to mitigate potential biases in model training and contributed to more reliable performance metrics. Additionally, the XGBoost classifier was configured to assign higher weights to the minority class, ensuring that the model accounted appropriately for underrepresented neurotypical participants. These adjustments collectively supported the balanced classification performance observed in the study, as evidenced by the model's F1-score of 0.9347.

## Future Directions

To build on these findings, future research should prioritize larger, more diverse datasets to validate the model's generalizability. Expanding the demographic scope to include different age groups, cultural backgrounds, and clinical profiles (eg, ADHD subtypes) would enhance the robustness of the results. Multimodal approaches combining EEG with behavioral, genetic, or neuroimaging data could further improve diagnostic accuracy and provide a more comprehensive understanding of ADHD. In addition, exploring other machine learning algorithms, such as deep learning models, may uncover complex patterns and interactions within EEG data that are not captured by tree-based methods like XGBoost.

## Conclusion

This study demonstrates the potential of EEG-based machine learning models, particularly the XGBoost classifier, as non-invasive tools for ADHD diagnosis. The model achieved high accuracy (90.81%) and provided interpretable insights through SHAP analysis, highlighting middle beta activity and occipital region signals as key biomarkers. To advance this system into clinical practice, further validation is necessary in diverse settings with larger, more heterogeneous populations to ensure robustness across age groups, ADHD subtypes, and cultural contexts. Longitudinal studies are also essential to evaluate the model's utility over time, particularly in monitoring ADHD progression and treatment responses. Finally, integrating automated preprocessing and user-friendly interfaces will facilitate its adoption in routine clinical workflows. These steps will help establish this model as a practical and reliable tool, supporting the broader application of objective diagnostic methods.

## Data Sharing Statement

The datasets generated or analyzed during the study are available from the corresponding author on reasonable request.

## Acknowledgments

This research was supported by a grant of the Korea Health Technology R&D Project through the Korea Health Industry Development Institute (KHIDI), funded by the Ministry of Health & Welfare, Republic of Korea (grant number: HI19C0844).

## Disclosure

The authors report no conflicts of interest in this work.

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