**Predicting Youth OCD Symptoms from Brain Morphology**

*A Machine Learning Approach to Informant Disagreement*

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Acknowledgements

Abstract

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Introduction

Obsessive-Compulsive Disorder

Obsessive-compulsive disorder (OCD) is recognized as a prevalent and persistent neuropsychiatric condition, impacting an estimated 2-3% of individuals worldwide (de Mathis et al., 2013). It is defined in the *Diagnostic and Statistical Manual of Mental Disorders, Fifth Edition*(DSM-5) as the presence of obsessions, compulsions, or both. Obsessions are recurrent, intrusive, and unwanted thoughts, urges, or images that typically cause significant anxiety or distress, and which the individual attempts to ignore or neutralize. Compulsions are repetitive behaviors or mental acts performed in response to obsessions or rigid rules and are aimed at reducing distress or preventing a feared outcome, though they are not realistically connected to the outcome or are clearly excessive (American Psychiatric Association, 2013).

OCD is documented as a clinically and etiologically heterogeneous disorder, with symptom profiles that vary widely across individuals (Bragdon & Coles, 2017). These symptoms are shaped by a convergence of genetic, neurobiological, and environmental influences (Bragdon & Coles, 2017; Shephard et al., 2021). Onset frequently occurs during childhood or adolescence, with reports indicating that up to half of adults with OCD first experienced symptoms during early life, with prevalence rates in these age groups ranging from 1-4% (Nazeer et al., 2020). This developmental period is particularly important to consider, as adolescence is marked by significant brain maturation processes, including synaptic pruning, increased myelination, and cortical remodeling in brain regions implicated in OCD, such as the prefrontal cortex, striatum, and limbic system (Casey et al., 2008). These changes influence emotional regulation and self-control, potentially heightening vulnerability to compulsive and intrusive thought patterns.

Comorbid psychiatric conditions are common in individuals with OCD, further complicating diagnosis and treatment. Studies show that individuals with pediatric-onset OCD often experience higher rates of co-existing disorders, many of which overlap with conditions considered in the differential diagnosis process (Saad et al., 2017). These include mood disorders, anxiety disorders, Tourette’s disorder, eating disorders, and various personality disorders (Anagnostopoulos et al., 2016; Ivarsson et al., 2008; Wu et al., 2019). Suicidality also emerges as a particularly serious risk in this group, underscoring the need for comprehensive and accurate assessment strategies (Storch et al., 2017). In youth populations, internalizing symptoms such as fear, avoidance, and distress may be especially difficult to detect due to their subjective nature, increasing the likelihood of underdiagnosis.

One methodological challenge in the study of developmental psychopathology is the frequent discrepancy between informants, particularly between youth and their caregivers, regarding the severity and nature of symptoms. This divergence is well-documented in developmental psychopathology literature and is especially pronounced for internalizing symptoms, which are less observable than externalizing behaviors (Achenbach et al., 1987; De Los Reyes & Kazdin, 2005). Discrepancies can lead to significant variations in diagnostic conclusions, treatment planning, and interpretations of clinical or research outcomes. OCD presents a particularly informative case for this investigation, as it encompasses both internalizing (e.g., obsessions) and externalizing (e.g., compulsions) symptom dimensions, and clinical diagnosis during adolescence is often based primarily on parent-reported information.

Traditional statistical models may fall short in handling the high dimensionality and variability inherent in neuroimaging data and symptom reports. To overcome these challenges, machine learning approaches grounded in offer a promising alternative. These models prioritize predictive accuracy and generalizability, making them well-suited for identifying patterns in noisy or multi-source data (Luxburg & Schoelkopf, 2008; Shmueli, 2011). In recent years, ML methods have gained traction in clinical neuroscience, with growing applications in psychiatric diagnosis and biomarker discovery. OCD, with its distinct internalizing and externalizing dimensions, presents an ideal context for examining how brain structure correlates with symptoms reported by different informants.

Neurobiology of OCD

From a neurobiological perspective, OCD has been linked to dysfunction within the cortico-striato-thalamo-cortical (CSTC) circuitry, which includes the orbitofrontal cortex, anterior cingulate cortex, thalamus, and basal ganglia (Graybiel & Rauch, 2000). Structural magnetic resonance imaging (sMRI) studies have consistently reported abnormalities in these regions, particularly among pediatric populations (van den Heuvel et al., 2022; Wang et al., 2022). These anomalies are believed to reflect developmental deviations in brain circuits responsible for habit formation, error monitoring, and emotional processing. Furthermore, pharmacological treatment—especially with selective serotonin reuptake inhibitors (SSRIs)—has been shown to modulate these structural features, indicating the importance of accounting for medication effects in neuroimaging research (Wang et al., 2022).

OCD has increasingly been understood as a disorder rooted in atypical brain development, with structural abnormalities emerging across regions critical for emotion regulation, cognitive control, and behavioral flexibility. sMRI studies have played a central role in identifying these neurobiological alterations, particularly in adolescent populations where early interventions may be most effective. Large-scale meta-analytic findings, including those from the ENIGMA-OCD working group, have consistently identified differences in brain morphology between individuals with OCD and healthy controls. In youth, these differences include larger thalamic volumes, reduced cortical thickness in prefrontal and parietal regions, and volumetric anomalies in subcortical structures such as the caudate, putamen, pallidum, and nucleus accumbens (van den Heuvel et al., 2022; Wang et al., 2022).

Importantly, these structural features appear to vary not only by diagnosis but also across developmental stages. Adolescents with OCD have been found to exhibit greater abnormalities in regions associated with reward processing and compulsive behavior, such as the nucleus accumbens and pallidum, while adults often show more pronounced structural changes in the amygdala, a region associated with emotional reactivity (Wang et al., 2022; Wu et al., 2022). These age-related differences suggest that the neuroanatomical underpinnings of OCD may shift over time, reflecting a developmental progression in the disorder’s pathophysiology.

The influence of medication status further complicates interpretation of these findings. Research has shown that unmedicated youth with OCD display larger thalamic volumes compared to controls, whereas medicated youth do not exhibit this difference (van den Heuvel et al., 2022). This suggests that pharmacological treatment, particularly with SSRIs, may alter structural features in ways that should be carefully accounted for in neuroimaging analyses. These structural abnormalities are especially relevant during adolescence, a period marked by rapid neurodevelopmental changes. Deviations from these normative trajectories have been linked to internalizing symptoms, including anxiety, intrusive thoughts, and emotional dysregulation, features central to many cases of adolescent OCD (Milad et al., 2013; Wang et al., 2022).

**Informant Discrepancies in Pediatric OCD Assessment**

Accurately assessing psychological symptoms in youth is inherently complex, and this is especially true for OCD. In both research and clinical settings, evaluations typically depend on multiple informants such as the child, parents, and teachers. However, agreement across these informants is often low to moderate, especially for internalizing symptoms, which are less visible and more subjective (Achenbach et al., 1987; De Los Reyes & Kazdin, 2005). Informant discrepancies are particularly problematic in the case of obsessions, which by definition are internal and may not manifest through observable behavior. In contrast, compulsions are more easily observed and tend to show higher cross-informant agreement. Studies show that discrepancies between youth and parent reports increase with age and are more pronounced in domains like anxiety and intrusive thoughts (Weisz et al., 2005).

Consider the case of Liam, 10-year-old experiencing subthreshold symptoms of OCD. For the past year, Liam had been struggling with persistent, intrusive worries about germs, harm coming to loved ones, and making mistakes. These obsessions caused him significant anxiety, yet he engaged in few observable compulsions. His parent, by contrast, reported minimal concerns, describing Liam as quiet but well-adjusted, with no significant behavioral problems at home. This discrepancy between Liams’s self-reported internal distress and his parent’s perception of functioning reflects a broader challenge in assessing internalizing symptoms in youth. This vignette demonstrates the importance of recognizing that the child's perspective is distinct but equally valid. The insights provided by Liam can differ significantly from those of his mother, highlighting the potential discrepancies in information regardless of whether the goal is clinical assessment or research.

Despite their challenges, discrepancies are not necessarily errors, they reflect meaningful differences in perspectives, settings, and symptom expressions. The foundational work by Achenbach et al. (1987) emphasizes that “no single informant serves as a gold standard.” Rather, multi-informant assessments provide complementary insights and are particularly valuable when interpreted with contextual awareness. In OCD, the diagnostic relevance of internalizing symptoms is especially critical. Parent-reported obsessions have been shown to strongly predict categorical OCD diagnoses, reinforcing the diagnostic weight given to caregiver reports in clinical settings (Ivankovic et al., 2024). However, parallel self- and parent-report measures of broader internalizing symptoms provide an opportunity to examine informant-specific brain–behavior relationships, a core goal of the present study. Ultimately, understanding how symptom reports diverge, and which brain features correspond to these divergences, may help refine diagnostic tools and promote individualized, informant-sensitive assessment strategies in adolescent OCD.

Statistical Learning

Statistical Learning Theory underpins many modern machine learning approaches by providing a theoretical framework for learning patterns from data with the goal of making accurate predictions (Luxburg & Schoelkopf, 2008). As a foundational concept in machine learning, SLT is particularly relevant to supervised learning, a paradigm that trains models on labeled data to map predictor variables to a response variable. The focus in supervised learning is typically on maximizing predictive accuracy rather than uncovering causal relationship (Shmueli, 2011). Predictive modeling is a core application of supervised learning that involves training probabilistic or algorithmic models to identify patterns in data. These models rely on loss functions, which are mathematical tools used to measure the difference between the model's predicted output and the actual outcome. By minimizing the value of the loss function, the model improves its prediction accuracy and generalizes better to new, unseen data. In clinical neuroscience and neuroimaging, such machine learning methods are increasingly used to associate brain imaging data with predefined categories, such as diagnostic groups. This approach enables the identification of discriminative features that may serve as potential biomarkers for psychiatric or neurological conditions (Enrico et al., 2021).

Learning methods

Linear Model

Linear regressions provide a simple technique for analyzing data by assuming a linear relationship between input variables (X) and an output variable (Y) and typically estimates parameters using the least squares method. While effective for straightforward linear relationships, they are limited with complex data, which has led to advanced adaptations such as generalized linear models and support vector machines, offering broader applicability and improved modeling techniques for diverse patterns.

Decision Trees

Decision trees provide a significant advancement to linear models by effectively handling non-linear relationships and interactions between variables. Tree models operate under the assumption that the interaction between the response variable and the predictors can be modeled through locally constant fits (Breiman, 2017). Unlike the simplicity of linear models, decision trees dynamically segment the feature space through recursive binary splits, adeptly addressing both classification and regression tasks (James et al., 2021). The feature space refers to the set of possible values the predictors can have. In classification tasks, this is achieved by creating subsets with a dominant output class, whereas in regression, it involves reducing the variability of target values within each subset. As illustrated in Figure 1, each node of the tree serves as a decision point, directing data further down branches or reaching leaf nodes where predictions are determined by metrics such as class majority or mean values. Thus, when used for regression the aim is to split the data into subsets that minimize the resulting mean squared error, mean absolute error, or the variance of the target variable within these subsets (Ryan, 2025). Although they are effective in capturing complex patterns, they are also prone to overfitting, which occurs when the model captures noise rather than the underlying pattern. Thus, it crucial to balance bias and variance for accuracy and generalizability.

**Figure 1**

*Example of a Decision Tree Model Predicting Severity Scores Based on Demographic Features*

A diagram of a family

AI-generated content may be incorrect.*Note:* Example of a decision tree used for predicting severity scores based on individual and socioeconomic factors. The root node begins with the condition Age ≥ 16. If this condition is met, the model predicts a severity score of 4. If the condition is not met, the decision process continues down to the next node. Each non-leaf node represents a decision based on a feature threshold, while the leaf nodes indicate the predicted severity score (Y). This hierarchical structure illustrates how different combinations of age, income, and education contribute to the final prediction. Adapted from Machine Learning for Tabular Data (1st ed., by M. Ryan & L. Massaron, 2025, Shelter Island, NY: Manning Publications Co. LLC. Copyright 2025 by Manning Publications Co. LLC. Adapted under fair use.

Boosting

Boosting, as illustrated in Figure 2, is an ensemble method used to enhance predictive accuracy (Schapire & Freund, 2012). An ensemble combines multiple models to make more accurate predictions than a single model. Boosting iteratively adds simpler models, like decision trees, that improve the overall fit by addressing errors from previous models. Figure 2 demonstrates how training error decreases as more trees are added, with the ensemble prediction formed by summing tree outputs for improved accuracy. Gradient Boosting optimizes individual trees to reduce error and minimizes the ensemble's collective error by correcting residuals with each added tree (Friedman, 2001). This approach allows diverse loss functions for error minimization, enhancing the alignment of predictions with true outcomes (Ryan, 2025). Adjusting observation weights in boosting means assigning more importance to certain training examples, typically those that are harder to predict or where previous models have made larger errors. This process helps the model focus on challenging cases, ensuring that these harder-to-fit data points receive more attention in future iterations. In boosting algorithms, this reweighting strategy is central: after each round of learning, the model increases the weight of misclassified or poorly predicted observations so that the next model in the sequence tries harder to get them right. By doing so, the model iteratively corrects errors while maintaining the overall flexibility and robustness of the ensemble. XGBoost, or extreme gradient boosting, is a particularly efficient algorithm for fitting boosting models (Ren et al., 2019).

**Figure 2**

A diagram of a tree

AI-generated content may be incorrect.*Boosting Process in Ensemble Learning*

***Note:*** Illustration of the boosting process used in ensemble learning methods. Training error decreases over successive iterations as additional decision trees are added. Initially, a single tree is trained, followed by subsequent trees that correct the errors of the previous ones. The ensemble prediction is formed by summing the outputs of multiple trees, leading to improved accuracy and reduced training error over time. Adapted from Machine Learning for Tabular Data (1st ed., by M. Ryan & L. Massaron, 2025, Shelter Island, NY: Manning Publications Co. LLC. Copyright 2025 by Manning Publications Co. LLC. Adapted under fair use.

Tuning Parameters

When applying XGBoost to multiclass classification tasks, model performance can be significantly enhanced by fine-tuning key hyperparameters (XGBoost Developers, 2022). While many configurable settings are available, a few are particularly important to highlight due to their influence on the model’s ability to distinguish between multiple categories accurately. The learning rate controls how quickly the model learns patterns in the data; smaller values slow learning but often improve generalization. The depth of each tree affects how complex each decision tree is by limiting the number of splits, with deeper trees capturing more intricate patterns but risking overfitting. Additional parameters govern how the training data and predictor variables are sampled during each iteration, and how splits are determined based on data distribution and predictive gain. These settings help manage the trade-off between model flexibility and robustness, ensuring that the classifier can generalize well across all classes. Together, these parameters help balance the model's ability to learn complex patterns with its ability to generalize well to new, unseen data.

In conclusion, the application of machine learning techniques, particularly XGBoost, offers a powerful methodology for modeling complex interactions between variables to predict an outcome of interest. This approach provides a robust framework for integrating diverse data types, such as neuroimaging, behavioral, and demographic variables. By using the collective strengths of multiple models, boosted ensembles surpass the predictive capabilities of single decision trees and linear models, effectively managing intricate relationships in high-dimensional data. This integration of computational tools with clinical insights holds promise for refining diagnostic criteria and enhancing personalized intervention strategies for OCD, paving the way for more precise and effective treatment approaches.

The present study

This thesis examines the relationship between structural brain features and OCD symptomatology in adolescents, with particular emphasis on the role of informant discrepancies in symptom reporting. The primary objective of this study was to determine whether structural neuroimaging data can reliably predict the severity of OCD symptoms in youth, based on reports from both the youths themselves and their parents. In addition to assessing overall model accuracy, the analysis aimed to examine whether predictive performance systematically varied by informant. To that end, two supplementary questions were addressed: (1) Is predictive accuracy higher for youth-reported internalizing symptoms? and (2) Is predictive accuracy higher for parent-reported externalizing symptoms?

Parcellated brain volume features were extracted from sMRI scans and used as input variables in supervised machine learning models, implemented using the XGBoost algorithm. The internalizing symptom domain was selected as the predictive target because it is assessed using parallel items across youth and parent reports, thus enabling a direct comparison of informant-specific prediction performance. This focus on informant-related variation is motivated by prior findings indicating that internalizing symptoms are more likely to be reported inconsistently and subjectively across sources. By integrating these components, the study seeks to elucidate the relationship between brain structure and subjective symptom expression across informants, thereby contributing to the development of individualized, informant-sensitive predictive models for OCD assessment in adolescent populations.

Methods

Data Source and Acquisition

The Adolescent Brain and Cognitive Development (ABCD) Study is a comprehensive decade-long research initiative in the United States designed to enhance our understanding of physical and mental health and risk factors during adolescence. The study tracks children from ages 9-10 through late adolescence and into early adulthood. This age range includes a crucial developmental stage, when exposure to substance use, and the start of several mental health conditions take place. The repository includes around 12,000 children at baseline, recruited from 21 research sites (Karcher & Barch, 2021). To ensure the cohort is diverse and representative, the ABCD study employs a multi-stage probability sampling technique to minimize selection bias, thus increasing the generalizability of the findings (Garavan et al., 2018). The ABCD comprises a wide range of behavioral (Barch et al., 2018), multimodal brain imaging (Casey et al., 2018), and other evaluations (Zucker et al., 2018). It conducts annual lab-based evaluations and biannual imaging scans to assess mental and physical health metrics (Saragosa-Harris et al., 2022). The data utilized in this thesis is sourced from the ABCD Data Release 5.1 (Haist & Jernigan, 2023). To ensure consistency in data analysis, this thesis utilizes only the year two follow-up time point, as it provided the most comprehensive available data across all key variables of interest, including, neuroimaging data and questionnaire responses.

REK stuff hereeeee and ethical considerations informed consent

Structural MRI

The ABCD study collects MRI data from three different scanner platforms located at 21 collection sites across the United States: Siemens Prisma, General Electric 750, and Philips scanners (Casey et al., 2018). T1-weighted (T1w) images are acquired using a 3D T1w inversion-prepared RF-spoiled gradient echo sequence with 1 mm isotropic resolution (Casey et al., 2018). Prospective motion correction is applied when available (currently only on Siemens and GE scanners; (Tisdall et al., 2012; White et al., 2010)). The Siemens scanner, acquisition parameters are TR = 2500 ms, TE = 2.88 ms, TI = 1060 ms, flip angle = 8°, with a 256 × 256 matrix, 176 slices, and a 256 mm FOV (acquisition time ~6:08). The Philips scanner used TR = 6.6 ms, TE = 3.1 ms, TI = 950 ms, flip angle = 9°, matrix size 256 × 256, 225 slices, and a FOV of 256 × 240 mm (acquisition time ~5:38). And, the GE scanner, parameters included TR = 2500 ms, TE = 2.0 ms, TI = 1060 ms, flip angle = 8°, with 208 slices and the same resolution and matrix size (acquisition time ~6:09).

The ABCD MRI acquisition protocol utilizes high-density phased array head coils, which can lead to significant variations in image intensity. Additionally, head motion presents a significant challenge, especially in adolescent populations where increased movement is more common, since it can degrade image quality and distort derived metrics (Reuter et al., 2015; Satterthwaite et al., 2012). Therefore, although prospective motion correction techniques are implemented to mitigate the effects of motion in sMRI scans, excessive head movement can still introduce substantial artefacts, hindering accurate brain segmentation (Tisdall et al., 2016). If these discrepancies are not adequately addressed, they may lead to inaccuracies in cortical surface reconstruction and brain segmentation (ref).

Due to the potential artifacts in MRI images, T1w quality control during the MRI acquisition includes three checks (ABCD Study, 2025; Hagler et al., 2019). Firstly, (1) automated checks for protocol compliance assess the completeness of the imaging series and ensure that they meet the specified parameters; these criteria include verifying whether key imaging characteristics such as voxel size and repetition time align with the expected values for each scanner. (2) Automated quality control procedures involve calculating signal-to-noise ratio and head motion statistics. Lastly, this is complemented by (3) a manual quality control process where trained technicians visually assess image quality, identifying and flagging significant artefacts. Series that fail to meet quality standards are excluded from further processing and analysis, and reviewers are required to document observable artefacts using standardized notations.

Preprocessing sMRI

All sMRI images used in this study were preprocessed and subjected to quality control by the ABCD Study prior to public data release using their standardized in-house image processing pipeline (ABCD Study, 2025). While the ABCD team provides a set of recommended inclusion criteria—accounting for factors such as image quality, protocol compliance—it is the responsibility of the data user to select criteria that are appropriate for their specific analyses. In this thesis, a subset of these criteria was applied based on their relevance to the research objectives. Preprocessing T1w images involves steps to ensure the accuracy and reliability of the data, including (1) Correction for Gradient Nonlinearity Distortions, which addresses distortions in the MRI images introduced by the scanner's gradient system (Jovicich et al., 2006; Wald et al., 2001). These corrections are specific to each scanner model and are provided by MRI manufacturers to enhance image fidelity. (2) Bias Field Correction involves correcting brightness variations across the brain images, a phenomenon known as intensity non-uniformity. This distortion is often caused by the proximity of brain tissue to the MRI coils, leading to areas with extremely high-intensity values that may be erroneously identified as non-brain tissue (i.e., skull). To address this issue, T2-w images are registered to T1-w images using a technique called mutual information, which facilitates accurate alignment and overlay of the different scan types (Wells et al., 1996). Following this registration, the procedure includes tissue segmentation and the application of smoothly varying estimated B1-bias fields to adjust brightness levels, ensuring that each tissue type is represented consistently across the images (Sled et al., 1998). Lastly, (3) Resample to Isotropic: The final image preprocessing step standardizes the viewing and analysis of brain structures. The images are resized and aligned with an internally generated reference brain that features isotropic voxels of 1.0 mm and is approximately aligned with the anterior commissure/posterior commissure (AC/PC) axis (Friston et al., 1995).

Brain Segmentation

Cortical surface reconstruction and subcortical segmentation are conducted by the ABCD Study team using FreeSurfer version 7.1.1 (https://surfer.nmr.mgh.harvard.edu). FreeSurfer has been validated in adolescent samples (Biffen et al., 2020). The process begins with skull-stripping, which removes the skull and non-brain tissues from the MRI images (Ségonne et al., 2004). Simultaneously, white matter segmentation is conducted to identify white matter regions, while initial mesh creation produces a preliminary three-dimensional representation of the brain's surface (Dale et al., 1999). Following this, the correction of topological defects on the surface model is applied to address errors or irregularities (Fischl et al., 2001; Segonne et al., 2007). The surface model is optimized and refined (Dale et al., 1999; Dale & Sereno, 1993; Fischl & Dale, 2000). Lastly, the reconstructed brain surface undergoes nonlinear registration to a spherical atlas, aligning it with a standardized spherical model to facilitate consistent comparisons across different subjects (Fischl et al., 1999).

Regions of Interest

After completing cortical reconstruction, specific brain regions are labelled by two atlases. Cortical areas are labeled using the Destrieux atlas-based classification (Destrieux et al., 2010). This atlas is widely used in sMRI studies to analyze cortical volume in neurodevelopmental research ref. This atlas uses a sulco-gyral classification, distinguishing between exposed gyri and buried sulci based on mean curvature and convexity, thus providing 74 bilateral regions (148 total). Subcortical structures are labeled using the Automated Segmentation of the Subcortical Structures (ASEG) provided by FreeSurfer (Fischl et al., 2002). This atlas allows the segmentation and volume measurement of subcortical areas and other intracranial structures, providing 46 regions in total. Combining these atlases facilitates a comprehensive analysis of cortical and subcortical regions. Once both cortical and subcortical structures are labeled, a total of 194 parcellated brain volumes are generated per individual. These data are provided by the ABCD Study in tabulated format and made accessible for downstream analyses by independent researchers. An overview of the cortical and subcortical parcellation is presented in Figure 3, which illustrates the spatial distribution of labeled regions across both hemispheres and views.

**A screenshot of a computer screen

AI-generated content may be incorrect.Figure 3**

*Parcellation of Cortical and Subcortical Brain Structures Using the Destrieux and ASEG Atlases*

*Note:* Visualization of tabulated cortical and subcortical regions was produced using the ggseg packages in R (Mowinckel & Vidal-Piñeiro, 2020). Cortical surfaces (top two rows) are segmented using the Destrieux atlas, which identifies 148 sulcal and gyral regions based on curvature and convexity features. The first row illustrates the right hemisphere in lateral and medial views, while the second row presents the corresponding views of the left hemisphere. Subcortical structures (bottom row) are segmented using FreeSurfer’s Automated Segmentation of Subcortical Structures (ASEG) atlas, displayed in sagittal (left) and coronal (right) views.

Categorical Psychopathology Assessment

Present psychiatric diagnoses were determined using the Kiddie Schedule for Affective Disorders and Schizophrenia – Computerized Version (KSADS-COMP), a self-administered, computerized instrument aligned with DSM-5 diagnostic criteria and used in the ABCD Study (J. Kaufman et al., 1997; *KSADS-COMP*, n.d.). The KSADS-COMP evaluates over 50 common childhood and adolescent psychiatric disorders and also provides corresponding ICD-10 codes (Barch et al., 2018). The assessment begins with a structured introductory interview that collects contextual information on family environment, treatment history, gender identity, school functioning, peer relationships (including bullying), and the presence of firearms in the home. This information supports interpretation of mood symptoms and assessment of impairment and risk.

The symptom assessment consists of an initial screening interview, presenting 2–4 key items per disorder. Endorsed symptoms trigger full diagnostic supplements, administered via automated branching logic. Diagnoses are algorithmically assigned as “present,” or “not present” based on DSM-5 symptom criteria, duration, and functional impairment. The system also facilitates differential diagnosis, using automated probes to clarify overlapping symptom domains (e.g., mood vs. substance-related conditions). While not administered by a clinician, the KSADS-COMP is clinically designed and validated for use in large-scale studies, offering reliable and scalable mental health phenotyping (J. Kaufman et al., 2017). Demographics, including age, sex, race, and ethnicity, are also retrieved from the KSADS-COMP.

Dimensional Psychopathology Assessment

The Achenbach System of Empirically Based Assessment (ASEBA) is a comprehensive evaluation tool that captures continuous symptom severity and behavioral, emotional and social functioning across various domains (*ASEBA*, 2019). ASEBA is widely applied in diverse areas such as mental health services, education, healthcare, research, and more. The Child Behavior Checklist (CBCL) and Brief Problem Monitor (BPM), two components of the ASEBA, provides a dimensional assessment approach that places behaviors along a continuum of frequency and/or severity. Raw scores from these instruments are converted into standardized scores using ASEBA-defined algorithms, which account for informant type, age, sex, and ethnicity (Achenbach et al., n.d.). These normed scores are expressed as T-scores, with a mean of 50 and a standard deviation of 10.

Parent-Reported Child Behavior Checklist

The CBCL is a component of the ASEBA first published in 2001, and is used to assess children's behavioral, emotional, or social problems (Achenbach, 2001). It is a 112-item parent-reported survey, which uses a 3-point Likert scale for responses: "Very True," "Somewhat True," or "Not True," where parents are asked to rate each item based on their child's behavior "now or within the past six months." As depicted in Figure 4, the CBCL consists of several dimensions categorized into Syndrome Scales and DSM-Oriented Scales (American Psychiatric Association, 2013; Nelson et al., 2001). The eight syndrome scales are established through factor analysis. They encompass clusters of common behaviors or symptoms. Furthermore, these scales are grouped into three high-level domains Internalizing, Externalizing, and Total Problems scales. These dimensions offer a detailed assessment of a child's emotional, social, and behavioral functioning, aiding in identifying areas that may benefit from therapeutic or educational interventions. The Internalizing Problems scale specifically captures emotional difficulties such as anxiety, depression, withdrawal, and somatic complaints—making it a key indicator of inwardly directed psychological distress in children. The CBCL/6–18 shows high reliability (α = 0.83–0.94; r = 0.88–0.92) and strong clinical validity (Achenbach, 2018).

Self-Reported Brief Problem Monitor

The BPM, another component of the ASEBA, was first published in 2011 (Achenbach et al., 2011). Developed to complement parental assessments, adolescents provide self-reports on higher-level domains and attention. It is a 19-item self-reported survey used to assess children's behavioral and emotional functioning and their responses to interventions (RTIs). It also uses a 3-point Likert scale for responses: "Very True", "Somewhat True," or "Not True." Children are instructed to rate each item based on their behavior "currently or within the past six months." As illustrated in Figure 4, the BPM assesses four domains—Internalizing, Attention Problems, Externalizing, and Total Problems—mirroring the structure of the CBCL/6–18 (Achenbach et al., 2017). Of particular relevance, the Internalizing scale captures symptoms of anxiety, depression, and withdrawal. Recent validation in a Norwegian sample confirmed good internal consistency for this domain (α = .76–.88) and supported the original three-factor structure, affirming its utility as a brief and valid tool for identifying internalizing problems in at-risk children (Pedersen et al., 2021).

**Figure 4**

*The Structure of the ASEBA: Specifically Focusing on the Parallel Between CBCL and the BPM*

***Note:*** The CBCL consists of Syndrome Scales including clusters of symptoms, which are further grouped into three high-level domains known as (1) Internalizing Problems, (2) Externalizing, and (3) Total Problems score that sums all problem items. The BPM is a shorter version that provides a rapid assessment parallel to dimensions in CBCL for monitoring behavioral and emotional functioning over time. Adapted from “Psychometric Properties of the ASEBA Child Behaviour Checklist and Youth Self-Report in Sub-Saharan Africa—A Systematic Review,” by M. R. Zieff, C. Fourie, M. Hoogenhout, and K. A. Donald, 2022, *Acta Neuropsychiatrica*, 34(4), 167–190. <https://doi.org/10.1017/neu.2022.5>. Copyright 2022 by Cambridge University Press. Adapted under fair use.

Sample

Several criteria were applied to determine the final sample for inclusion in the study. Figure 5 illustrates the participant selection process. Beginning with the full ABCD Year 2 dataset (N = 10,730), participants were excluded if they lacked an MRI scan (n = 2,757) or if their imaging data did not meet quality control standards (n = 193). Of those with usable MRI data, additional exclusions were made for missing self- and/or parent-reported data on internalizing symptoms (n = 314). Moreover, to ensure that medication effects did not confound brain structure findings, participants who were currently prescribed common psychotropic medications (e.g., SSRIs, SNRIs, antipsychotics, stimulants) were excluded (n = 169). Participants who met criteria for a current psychiatric diagnosis unrelated to OCD were excluded from the sample (n = 837). In contrast, individuals with a current OCD diagnosis were retained regardless of comorbid conditions, reflecting the high rates of psychiatric comorbidity commonly observed in adolescent OCD (Geller & March, 2012). As a result, healthy control participants were defined as those who did not meet criteria for any current or past psychiatric disorder, based on the KSADS-COMP assessment.

**Figure 5**

*Flowchart of Participant Selection and Subgroup Classification at 2-Year Follow-Up*



The final study sample consisted of 6,460 participants, including 6,054 healthy controls and 406 individuals with OCD. Among those with OCD, 227 were classified as having OCD without comorbidities, while 179 presented with at least one comorbid psychiatric condition. Demographic and clinical characteristics for each group are summarized in Table 1. The mean age was comparable across groups: 9.47 years (SD = 0.51) in the healthy control group and 9.46 years (SD = 0.50) in the OCD group. Sex distribution was identical across groups, with 47.5% female and 52.5% male participants. One individual in the healthy control group identified as intersex male; no intersex participants were present in the OCD group. Regarding race and ethnicity, the healthy control group comprised 2.2% Asian, 13.3% Black, 19.2% Hispanic, 9.8% Other, and 55.6% White participants. The OCD group included 1.0% Asian, 15.3% Black, 19.5% Hispanic, 14.3% Other, and 50.0% White participants. Among individuals with OCD, the most common comorbid diagnoses were ADHD (n = 71), anxiety disorders (n = 46), oppositional defiant/conduct disorder (n = 62), and bipolar disorder (n = 49), with smaller numbers reporting suicidality (n = 39), eating disorders (n = 14), depressive disorders (n = 5), or substance use disorder (n = 2).

**Table 1**

*Characteristics of The Study Sample by Group*

|  |  |  |
| --- | --- | --- |
| Demographics | Healthy Control (n=6,054) | OCD (n=406) |
| Mean Age (SD) | 9.47(0.51) | 9.46(0.50) |
| Sex |  |  |
| Female | 47,5% (n=2,877) | 47.5% (n=193) |
| Intersex Male | 0% (n=1) | - |
| Male | 52.5% (n=3,176) | 52.5% (n=213) |
| Race/Ethnicity |  |  |
| Asian | 2.2% (n=131) | 1.0% (n=4) |
| Black | 13.3% (n=806) | 15.3% (n=62) |
| Hispanic | 19.2% (n=1,160) | 19.5% (n=79) |
| Other | 9.8% (n=593) | 14.3% (n=58) |
| White | 55.6% (n=3,364) | 50.0% (n=203) |
| Clinical |  |  |
| Depressive Disorders |  | n=5 |
| Anxiety Disorders |  | n=46 |
| Attention-Deficit / Hyperactivity Disorder |  | n=71 |
| Oppositional Defiant / Conduct Disorder |  | n=62 |
| Bipolar Disorder |  | n=49 |
| Substance Use Disorder |  | n=2 |
| Suicidality |  | n=39 |
| Eating Disorders |  | n=14 |

Modelling approach

All analyses were conducted in R (version 4.3.3), and all models were implemented using the XGBoost 3.0 package. Under the XGBoost framework, model performance is optimized by minimizing a specified loss function which defines the objective of the model. The objective function serves as a core component of model specification, as it directly reflects the type of prediction task being addressed (Brownlee, 2021). To prevent data leakage, the dataset was stratified and split into three subsets prior to any model building or feature selection. As illustrated in Figure 6, 70% (n=4522) of the data was allocated for training and tuning the hyperparameters of the model, 15% (n=969) for threshold calibration, and the remaining 15% (n=969) for model evaluation. Stratified sampling was applied to maintain proportional representation of the target classes across all subsets, ensuring that each set included a similar distribution of symptom severity levels. Full details of the data partitioning procedure are provided in Appendix II. The data split ensured that information from the evaluation set did not inadvertently influence model training or parameter tuning (S. Kaufman et al., 2012).

**Figure 6**

*Flowchart Illustrating the Machine Learning Pipeline*



*Note:* The full sample was split into three subsets. In the training phase, hyperparameter optimization was performed on the training set using grid search and 5-fold cross-validation. In the threshold calibration phase, here a threshold grid search for class-specific probability cutoffs was used. Finally, in the evaluation phase, the calibrated model was applied to the held-out test set to assess final performance metrics.

Exploratory Modeling and Predictor Selection

As an initial step, simpler linear regression models were tested to evaluate the predictive utility of different sets of variables. These models included demographic predictors (age, sex, and race/ethnicity), latent psychosocial factors (socioeconomic status, social risk, and perinatal risk), and sMRI. The goal of these preliminary models was to assess the individual and combined contributions of each predictor domain and to establish a baseline for comparison. Full details and model summaries are provided in Appendix I (see Tables 1 and 2). Subsequent analyses focused exclusively on structural brain features. This decision was guided by the primary aim of the study (to investigate brain-based prediction of OCD-related internalizing symptoms), as well as by practical constraints associated with the high dimensionality of neuroimaging data relative to sample size, which necessitated dimensionality reduction to prevent overfitting.

Initial Regression Approach

The prediction of the internalizing symptoms was initially formulated as a regression task, using the continuous T-score derived from the Achenbach scale ref. The model was trained to minimize the squared error loss function. However, the distribution of symptom severity was found to be highly skewed, with relatively few individuals classified within the clinical range. This imbalance in the outcome variable resulted in suboptimal model performance and limited interpretability, as the squared error loss function assumes equal importance across all prediction errors, irrespective of class prevalence (Hastie et al., 2009). In contrast, classification models are better equipped to handle imbalanced outcome distributions, particularly when combined with class weighting strategies that adjust for disparities in group sizes (He & Garcia, 2009).

Redefining the Task as Multiclass Classification

To improve clinical interpretability and model performance, the task was reframed as a multiclass classification problem by mapping T-scores to established clinical categories (Achenbach, 2009): normal (<65), borderline (65–69), and clinical (≥70).

The model was trained using the multiclass log-loss (cross-entropy) objective, which provides a probabilistic output across all categories (*XGBoost*, 2022). This approach, mathematically equivalent to multinomial logistic regression, enables a symmetric and interpretable estimation of class membership probabilities (James et al., 2021). Multiclass log-loss is particularly suited for imbalanced classification settings, as it penalizes confident but incorrect predictions more heavily than uncertain ones. This results in a more informative loss signal than traditional accuracy metrics, which may obscure poor performance on minority classes (Niculescu-Mizil & Caruana, 2005).

Addressing Class Imbalance with Cost-Sensitive Learning

To enhance classification performance in the context of unequal class distributions, both data-level and algorithm-level strategies were employed. A commonly used approach for addressing class imbalance involves assigning greater weights to minority class samples during model training, thereby mitigating the tendency of the model to prioritize the majority class (Kuhn & Johnson, 2013; Ting, 2002). In this study, class weights were applied to increase the influence of participants categorized in the borderline and clinical symptom groups, relative to those in the normal range. This strategy was particularly important given the disproportionately smaller size of the clinically significant group and the high dimensionality of the neuroimaging feature space, both of which increase the risk of model bias, variance inflation, and overfitting. Weighting the minority classes ensured that the model remained sensitive to clinically meaningful patterns, even when those patterns were underrepresented in the training data.

Hyperparameter Tuning and Validation

Hyperparameter optimization was conducted using a grid search across a predefined set of key tuning parameters, including maximum tree depth, learning rate, regularization strength, and row and column sampling ratios (Xgboost Grid Search - R, n.d.). To evaluate model performance, a five-fold cross-validation procedure was implemented on the training dataset, with early stopping employed to prevent overfitting and reduce computational burden. Early stopping is a regularization technique that terminates model training when performance on a validation set ceases to improve after 10 iterations, thereby preventing overfitting and reducing training time (Prechelt, 1998). The grid search explored 864 unique parameter combinations, each evaluated across five validation folds, resulting in a total of 4,320 model fits. The configuration that achieved the lowest average multiclass log-loss across validation folds was selected as the final model. This tailored tuning procedure enabled the application of stronger regularization, controlled model complexity, and optimized sampling strategies, collectively contributing to a more robust, stable, and generalizable classifier suitable for high-dimensional neuroimaging data (James et al., 2021; Kuhn & Johnson, 2013).

Threshold Calibration

To improve classification performance and ensure that predicted labels aligned more closely with clinically meaningful groupings, a post-hoc threshold calibration was performed using the class probabilities generated by the XGBoost model (*3.3. Tuning the Decision Threshold for Class Prediction*, n.d.). In standard multiclass classification, labels are assigned using the argmax rule, which selects the class with the highest predicted probability. However, this default strategy can introduce bias toward the majority class, particularly in imbalanced datasets, which are common in clinical research contexts (Van Calster et al., 2019). To address this issue, a class-specific threshold calibration approach was implemented. Using a one-vs-rest (OvR) framework on a held-out validation set, the model evaluated the decision threshold for each class independently (Rifkin & Klautau, 2004). Accordingly, each category—normal, borderline, and clinical—was assessed independently during threshold calibration. For each binary classification (e.g., Class A vs. not Class A), the optimal decision threshold was determined by maximizing balanced accuracy, which accounts for both sensitivity (true positive rate) and specificity (true negative rate), providing a more equitable measure of performance in imbalanced datasets (Brodersen et al., 2010). This process yielded individualized decision thresholds for each class, providing a more flexible alternative to the standard argmax-based decision rule. It addresses the model's inherent tendency to underrepresent minority classes—an effect rooted in the objective function of most machine learning classifiers, including XGBoost, which typically aim to minimize overall loss (e.g., log-loss) across all samples. In imbalanced datasets, this global loss is disproportionately influenced by the majority class, causing the model to prioritize accuracy on the more prevalent classes while neglecting performance on underrepresented ones (He & Garcia, 2009). As a result, the default argmax rule systematically favors majority class predictions, even when the minority class probabilities are clinically meaningful.

Evaluation Metrics

The final tuned and calibrated models’ performance was assessed on a held-out test set. The performance was assessed using a comprehensive set of evaluation metrics selected to address the imbalanced nature of the outcome classes, particularly the underrepresentation of individuals with clinically significant OCD symptoms. Overall accuracy was not used as the sole performance indicator, as it can obscure poor detection of minority classes in imbalanced datasets (Saito & Rehmsmeier, 2015).

Instead, a multidimensional evaluation strategy was implemented. The caret package was used to compute confusion matrices and extract key metrics, including balanced accuracy, sensitivity, specificity, and positive predictive value for each class (Kuhn, 2008). Balanced accuracy was used to account for class imbalance by averaging sensitivity and specificity (true negative rate) for each class, providing a more equitable evaluation of performance (Brodersen et al., 2010). Precision, recall, and F1 scores were calculated for each class using the MLmetrics package (Yan, 2016). Precision reflects the proportion of true positives among all positive predictions, while recall captures the proportion of actual positives correctly identified. The F1 score, defined as the harmonic mean of precision and recall, offers a balanced measure of classification performance that is particularly valuable when the costs of false positives and false negatives are asymmetric. To assess the model's ability to discriminate between classes, the Area Under the Receiver Operating Characteristic Curve (AUC-ROC) was computed using a OvR approach with the pROC package (Robin et al., 2011). These metrics visualize and quantify the trade-off between sensitivity and specificity across thresholds and offer insight into the model’s separability across all classes.

Permutation Based Significance Testing

To evaluate whether the model's performance exceeded what could be expected by chance, a permutation test was conducted following established methods for assessing statistical significance in predictive modeling (Good, 2000; Ojala & Garriga, 2009). This non-parametric approach involves disrupting the relationship between input features and class labels while preserving the underlying feature distributions. For computational efficiency, hyperparameter tuning was performed once using the original labels and fixed for all permutation iterations. This approach may slightly underestimate the variance in the null distribution (Ojala & Garriga, 2009).

To simulate the null hypothesis of no association between features and target labels, class labels in the held-out test set were randomly permuted 1,000 times. For each permutation, the trained XGBoost model was used to generate predicted class probabilities, which were thresholded using the previously calibrated class-specific thresholds. These thresholded outputs were then converted into class predictions. The classification accuracy was computed for each of the 1,000 permutations, producing a null distribution of accuracies expected under chance. The observed accuracy, obtained using the true (non-permuted) labels, was then compared against this null distribution. A permutation-based p-value was calculated as the proportion of permuted accuracies that were greater than or equal to the observed accuracy, providing a robust estimate of statistical significance without assuming distributional properties of the data. A density plot was generated to visualize the null distribution, with the observed accuracy overlaid as a vertical reference line, highlighting its deviation from the permutation-based baseline.

Results

Symptom Score Distribution and Baseline Models

The distribution of internalizing symptom scores was examined for both the CBCL and BPM scales, see Figure 7. Both measures exhibited strong positive skew, with the majority of participants falling within the normal range (T < 65) and relatively few classified in the borderline (65–69) or clinical (≥70) ranges. This skew was more pronounced in the BPM distribution, which demonstrated a sharp mode near the normative threshold, highlighting the low prevalence of clinical internalizing symptoms in the sample. Youth-reported internalizing scores had a mean of 53.10 (SD = 5.13), ranging from 50 to 75. Parent-reported scores had a mean of 46.37 (SD = 9.87), with a wider range of 33 to 90.

**Figure 7**

*Distribution of Outcome Variable: Internalizing Symptom T-Scores for Parent- and Child-Reported Measures*

1. *b)*



*Note:* Density plots showing the distribution of internalizing T-scores derived from the (a) parent-reported CBCL (green) and (b) child-reported BPM (purple). N=6560

As summarized in Table 2, model performance under the default configuration—without class weighting, hyperparameter tuning, or threshold calibration—was near chance level for both models. Overall accuracy was low (CBCL: 33.3%; BPM: 31.4%), closely mirroring the expected performance of a model making random predictions across three categories (healthy, borderline, clinical). Cohen’s kappa values were negative or near zero (CBCL: –0.0074; BPM: –0.0136), indicating no meaningful agreement between predicted and actual classifications. Balanced accuracy was similarly poor (CBCL: 49.4%; BPM: 47.5%), and class-level sensitivity for the borderline (CBCL: 28.6%; BPM: 22.7%) and clinical groups (CBCL: 41.7%; BPM: 38.9%) remained limited. These findings suggest that the base models lacked both discriminative ability and clinical utility.

Applying class weights yielded only modest improvements. Accuracy remained nearly identical to the default models, and while Cohen’s kappa improved slightly, it still indicated minimal agreement beyond chance. Balanced accuracy increased marginally, with some gains in sensitivity for borderline and clinical cases. However, these changes were insufficient to enable reliable classification of minority classes, suggesting that class reweighting alone could not compensate for the effects of class imbalance or overlapping symptom profiles.

**Table 2**

*Classification Performance Metrics for Parent- and Self-Reported Internalizing Symptom Models Across Four XGBoost Configurations*

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | CBCL | | | | BPM | | | |
| Model Configuration | Default | With Weights | Tuned + Argmax | Tuned + Threshold-Cal. | Default | With Weights | Tuned + Argmax | Tuned + Threshold-Cal. |
| Overall Performance | | | | | | | | |
| Accuracy | 0.3333 | 0.3323 | 0.9505 | 0.6801 | 0.3137 | 0.3158 | 0.934 | 0.9247 |
| 95% CI | 0.3037–0.364 | 0.3027–0.363 | 0.9349–0.9633 | 0.6497-0.7094 | 0.2846–0.344 | 0.2866–0.3461 | 0.9164–0.9488 | 0.9062–0.9405 |
| Cohen’s Kappa | -0.0074 | 0.0224 | -0.0016 | -0.0289 | -0.0136 | -0.009 | 0.0 | -0.0168 |
| Class Balance | | | | | | | | |
| Balanced Accuracy | 0.4942 | 0.5687 | 0.4997 | 0.465 | 0.4745 | 0.4795 | 0.5 | 0.4966 |
| Sensitivity (Borderline) | 0.2857 | 0.4524 | 0.0 | 0.048 | 0.2273 | 0.2955 | 0.0 | 0.0 |
| Sensitivity (Clinical) | 0.4166 | 0.5417 | 0.0 | 0.083 | 0.3889 | 0.3334 | 0.0 | 0.0 |
| Specificity (Borderline) | 0.6505 | 0.6440 | 0.9989 | 0.865 | 0.6605 | 0.6681 | 1.0 | 0.9881 |
| Specificity (Clinical) | 0.6878 | 0.6804 | 1.0 | 0.859 | 0.6572 | 0.6509 | 1.0 | 1.0 |
| Class-Level Discrimination | | | | | | | | |
| Precision (Borderline) | 0.0357 | 0.0544 | 0.0 | 0.016 | 0.0309 | 0.0407 | NaN | 0.0 |
| Precision (Clinical) | 0.0327 | 0.0413 | NaN | 0.015 | 0.0210 | 0.0178 | NaN | NaN |
| F1 Score (Borderline) | 0.0634 | 0.0967 | 0.0 | 0.0236 | 0.0538 | 0.0723 | 0.0 | 0.0 |
| F1 Score (Clinical) | 0.061 | 0.0763 | 0.0 | 0.0248 | 0.0382 | 0.0334 | 0.0 | 0.0 |

*Note:* Accuracy refers to the overall proportion of correct predictions. 95% CI indicates the range in which the true accuracy likely falls with 95% confidence. Cohen’s kappa adjusts accuracy for chance agreement, with values near zero indicating chance-level performance. Balanced Accuracy averages sensitivity and specificity across all classes, providing a more informative metric under class imbalance. Sensitivity (also called recall) measures how well the model identifies true positives within each class. Specificity reflects the model’s ability to correctly identify true negatives. Precision is the proportion of predicted cases that are actually correct. F1 Score combines precision and sensitivity, offering a balanced measure of class-specific performance, particularly useful when class distributions are skewed. While argmax models showed high overall accuracy, this reflected overprediction of the healthy class. Class-specific metrics revealed poor detection of minority classes, with only modest gains after threshold calibration for parent reports and persistently low performance for self-reports, underscoring the impact of class imbalance and limited signal in the input data.

Tuning Parameter Exploration and Loss Minimization Across Configurations

As shown in Table 3, both models reached optimal performance at 50 boosting rounds. While core parameters such as learning rate and max depth were consistent, the parent reported model used a lower minimum child weight (1 vs. 5), higher gamma (2 vs. 0), and differed in subsampling strategies (subsample: 0.6 vs. 0.9; colsample by tree: 0.9 vs. 0.6). Hyperparameter tuning revealed variation in model performance across the parameter space, see Figure 8. For both the CBCL (Figure 8a) and BPM (Figure 8b) models, log loss values ranged from approximately 1.090 to 1.108, indicating sensitivity to tuning configurations. Performance was most strongly influenced by tree depth and learning rate, with lower log loss achieved under shallower trees and moderate learning rates. Despite the broad search space, both models converged on similar optimal configurations, yielding final multiclass log-loss values of 1.090 (CBCL) and 1.093 (BPM). Class weighting contributed to improved classification of underrepresented borderline and clinical categories.

**Table 3**

*Optimal Tuning Parameters for Internalizing Symptom Prediction Models*

|  |  |  |
| --- | --- | --- |
| Parameter | CBCL | BPM |
| Booster | Gbtree | Gbtree |
| Objective | Multi:softprob | Multi:softprob |
| Evaluation Metric | mlogloss | mlogloss |
| Max Depth | 3 | 3 |
| Min Child Weight | 1 | 5 |
| Eta | 0.1 | 0.1 |
| Gamma | 2 | 0 |
| Subsample | 0.6 | 0.9 |
| Colsample by Tree | 0.9 | 0.6 |
| Number of Classes | 3 | 3 |
| Best number of rounds | 50 | 50 |
| Best multiclass Log Loss | 1.090 | 1.093 |

**Figure 8**

*Hyperparameter Optimization Results for Internalizing Symptom Prediction Models*

A diagram of a graph

AI-generated content may be incorrect.a)

A graph with lines and numbers

AI-generated content may be incorrect.b)

*Note:* Parallel coordinate plots illustrating how performance varies across the hyperparameter space. Each line represents a unique combination of tuning parameters across the grid search, with axes corresponding to individual hyperparameters and the resulting multiclass log loss on the y axis. (a) . Parent-reported symptoms (CBCL); line color indicating yellow as lower loss and blue as higher loss. (b) Child-reported symptoms (BPM); line color indicates log loss, with red representing lower loss and purple representing higher loss.

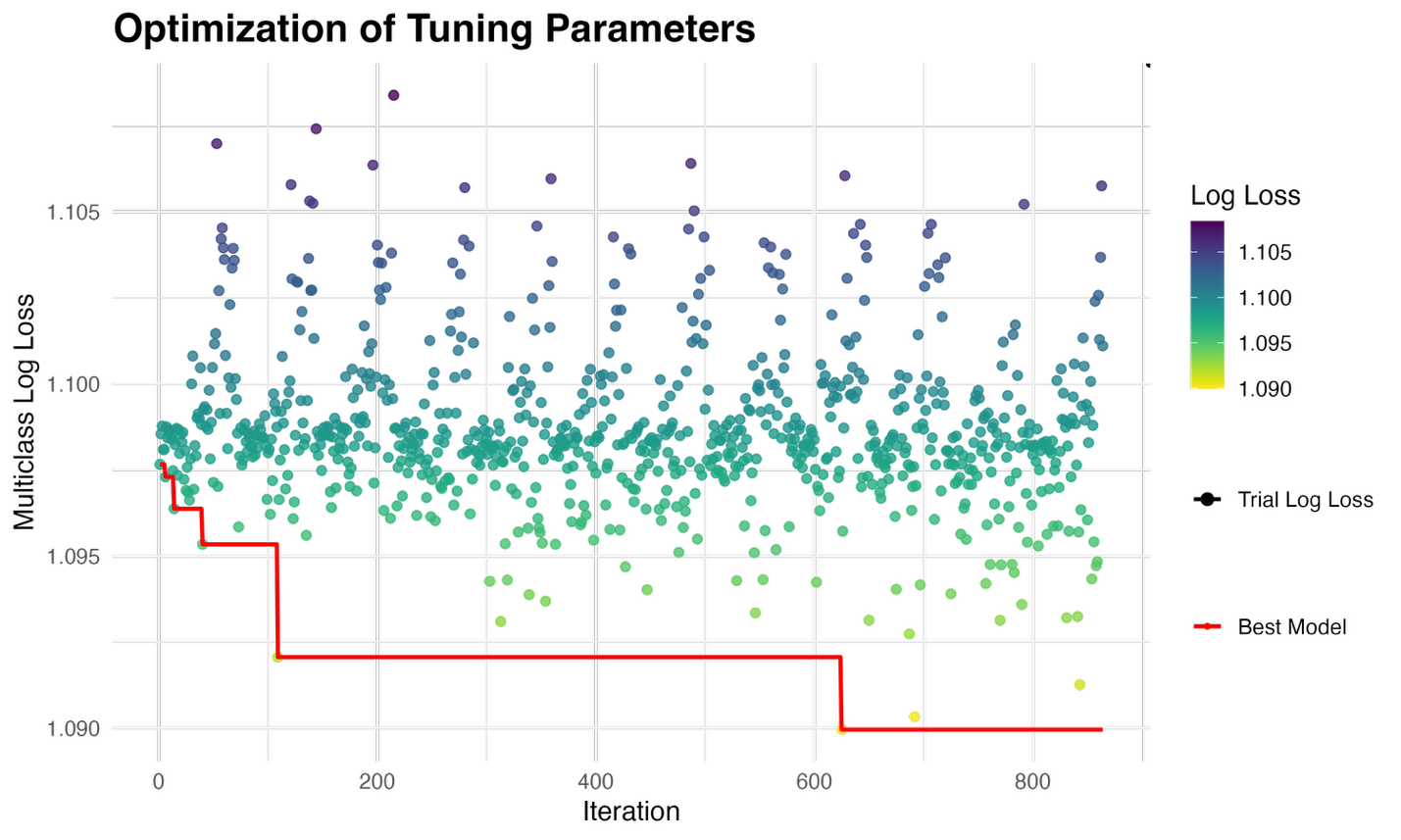
Optimization history across the 864 hyperparameter configurations is visualized in Figure 9. Each point represents a unique parameter combination evaluated during the grid search, with color indicating the resulting multiclass log loss. Performance, as indicated by the minimum multiclass log loss, showed distinct patterns across models. For the CBCL model (Figure 9a) achieved its lowest log loss earlier in the tuning process, after which subsequent configurations showed diminishing returns. In contrast, the BPM model (Figure 9b), performance improved gradually across the tuning process, with the lowest log loss identified near the end of the search.

Notably, as summarized in Table 2 the hyperparameter-tuned models without threshold calibration yielded substantial increases in overall accuracy (CBCL: 95.05%; BPM: 93.4%). Closer inspection revealed that these accuracy gains were primarily due to the models defaulting to the majority (healthy) class. By consistently predicting the most common label, the models correctly classified most healthy individuals but failed to identify any borderline or clinical cases. Thus, Despite the apparent accuracy, Cohen’s kappa values were near zero (CBCL: –0.0016; BPM: 0.000), and balanced accuracy remained at chance (CBCL: 0.4997; BPM: 0.5000), reflecting the models' inability to detect elevated symptom profiles despite tuning efforts.

**Figure 9**

*Tuning Parameter Optimization History Across Iterations*

*a*



*A graph with dots and lines

AI-generated content may be incorrect.b)*

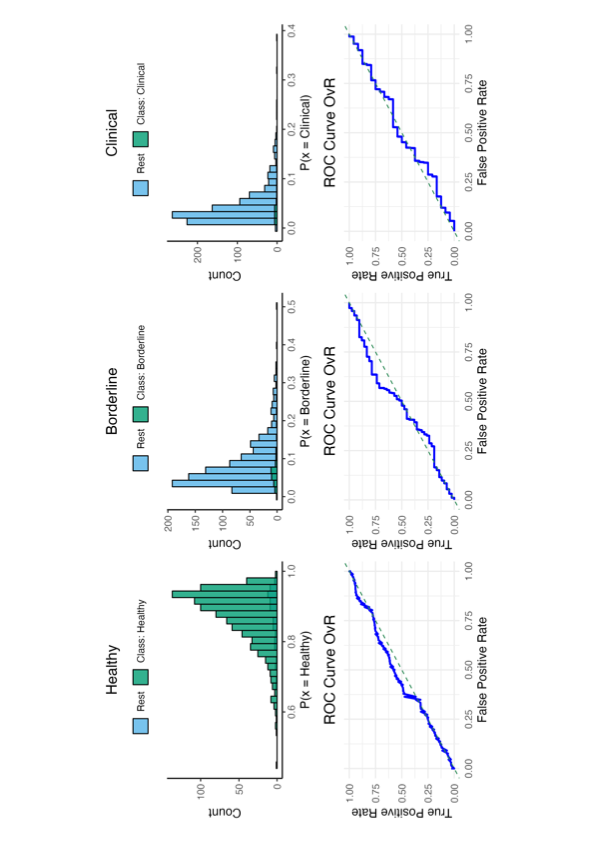
*Note:* Optimization history of multiclass models across hyperparameter configurations. Each point represents a distinct hyperparameter set, with color indicating the corresponding multiclass log loss (lower values shown in red/yellow; higher in purple). The red step line tracks the running minimum log loss, illustrating how increasingly better-performing configurations were identified throughout the tuning process. (a) Optimization trajectory for the model predicting parent-reported (CBCL) internalizing symptom (b) Optimization trajectory for the model predicting child-reported (BPM) internalizing symptom

Threshold Calibration

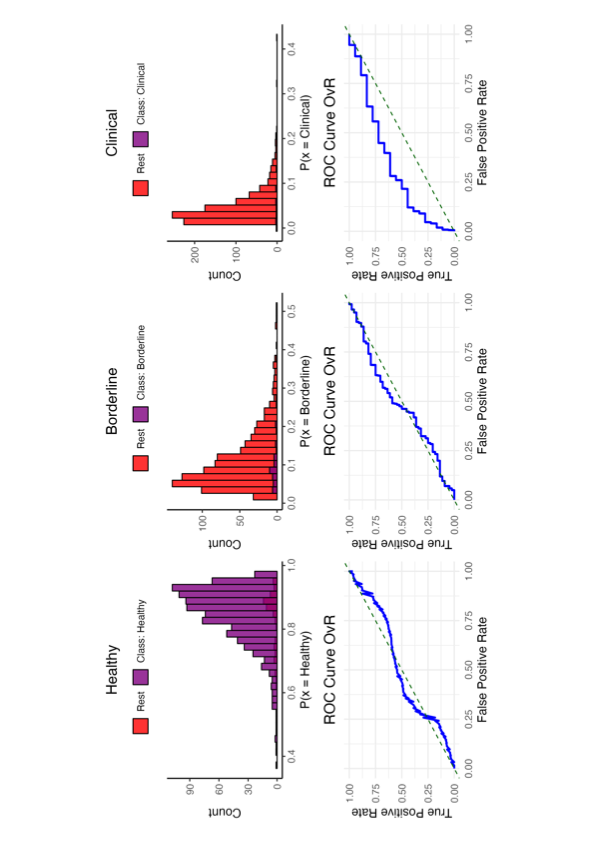
Threshold calibration using a one-vs-rest strategy was implemented to enhance sensitivity for underrepresented classes. As shown in Table 2, this adjustment led to a decline in overall accuracy (CBCL: 68.0%; BPM: 92.5%) and further reductions in Cohen’s kappa (CBCL: –0.0289; BPM: –0.0168). Although calibration redistributed predicted probabilities it did not yield meaningful improvements in minority class detection. Sensitivity for the clinical group remained extremely low (CBCL: 8.3%; BPM: 0.0%), and borderline sensitivity was similarly poor (CBCL: 4.8%; BPM: 0.0%). These findings suggest that threshold calibration, while mitigating some majority-class bias was insufficient to achieve clinically relevant classification performance, particularly in the BPM model where class imbalance was most severe.

Model Performance and Class Discrimination

Overall model classification performance and class discrimination ability were limited, even after threshold calibration, as illustrated by ROC curves and class probability distributions, see Figure 10. The CBCL model, Figure 10a, exhibited near-diagonal ROC curves for both borderline and clinical classes and output probabilities that reflected low certainty and poor separation between classes. This indicates near-random classification and low confidence for minority outcomes. The BPM model, Figure 10b, showed some upward curvature for the clinical group ROC curve, suggesting limited discriminatory ability, whereas the borderline group remained poorly differentiated. Predicted probabilities for healthy cases were more confidently distributed near 1.0, while minority class probabilities clustered near zero, reflecting poor model certainty. Overall, these findings highlight the persistent difficulty of achieving clinically meaningful classification performance in imbalanced symptom categories, particularly for child-reported outcomes.

**Figure 10**

*ROC Curves and Class Probability Distributions for the Test Set*

*a)*

*b)*

*Note:* Model performance for each class is shown using OvR ROC curves (bottom row) and corresponding predicted probability distributions (top row). (a) Parent-reported model (CBCL): The healthy class shows modest separability, with predicted probabilities skewed toward 1, but the ROC curve remains close to chance. Both the borderline and clinical classes exhibit poor separability, with predicted probabilities near zero and ROC curves that closely follow the diagonal, indicating near-random performance. (b) Child-reported model (BPM): The healthy class is more clearly distinguishable, with higher predicted probabilities and a ROC curve above chance. The borderline and clinical classes also show modest discriminative ability, with ROC curves slightly above the diagonal, indicating better performance than CBCL for minority class classification, though separability remains limited.

These trends are further supported by the confusion matrix, see Figure 11a, showed that only two cases from each minority class were correctly classified for parent-reported internalizing, with most predictions still concentrated in the healthy category. For the child-reported model, threshold calibration produced negligible change. Although there was slight upward curvature in the ROC curve for the clinical group, suggesting some degree of separability; however, as illustrated in Figure 11b, the model failed to predict any clinical cases, highlighting a disconnect between probabilistic output and actual classification performance. While the confusion matrix showed more even distribution across predicted labels post-calibration, true positive rates for borderline and clinical remained zero.

**Figure 11**

*Confusion Matrix for Model Predictions on the Test Set*

1. *A graph of a patient's health

   AI-generated content may be incorrect.*A graph of a health care patient

   AI-generated content may be incorrect.*A graph of a patient's health

   AI-generated content may be incorrect.*A graph of a health care patient

   AI-generated content may be incorrect. *b)*

*Note:* Confusion matrices display true versus predicted class labels for models after threshold calibration. Color intensity indicates the number of cases per cell. (a) The parent-reported model (CBCL) correctly identified a small number of clinical and borderline cases, but most predictions remained in the healthy category. (b) The child-reported model (BPM) showed more accurate identification of borderline cases but never predicted any cases as clinical. Despite a more balanced distribution, both models remain biased toward predicting the majority (healthy) class.

Null Model Validation

To evaluate whether model performance exceeded chance levels, permutation testing was conducted with 1,000 random label shuffles. As shown in Figure 12, the null distribution of accuracy scores is represented by a density curve, with the observed accuracy overlaid as a vertical reference line. The parent-reported model (CBCL; Figure 12a achieved a high raw classification accuracy of 0.68. However, the observed performance closely overlapped with the null distribution, yielding a permutation-based p-value of 0.953. This suggests that the elevated accuracy was likely driven by class imbalance rather than a meaningful predictive signal. These findings align with previous ROC and confusion matrix analyses, which indicated that classification success was largely restricted to the majority (healthy) class. A similar pattern was found for the child-reported model (BPM; Figure 12b). The model trained on true labels achieved a classification accuracy of 0.93. The null distribution, generated via label permutation, had a mean of 0.55 and a standard deviation of 0.03. The observed accuracy was near the center of this distribution, yielding a permutation-based p-value of 1.000, indicating that the model’s performance was not significantly above chance. As shown in Figure 12, the observed accuracy falls well within the range expected under the null hypothesis.

**Figure 12**

*Permutation Test Comparing Model Accuracy to Null Distribution*

1. A graph of a graph

   AI-generated content may be incorrect.*A diagram of a normal distribution

   AI-generated content may be incorrect. b)*

*Note:* Density plots show the null distribution of classification accuracies obtained from 1,000 random permutations of test set labels for the parent-reported model (CBCL; a) and child-reported model (BPM; b). The observed accuracy using the true (non-permuted) labels is marked by a vertical line (red for CBCL, green for BPM). In both models, the observed accuracy falls within the null distribution, indicating that model performance was not significantly better than chance. Pvalue

Discussion

The primary aim of this study was to evaluate whether structural brain features could be used to predict the severity of OCD-related internalizing symptoms, based on reports from both youths and their parents. A secondary aim was to compare the predictive utility of youth- versus parent-reported symptoms. To ensure fairness and consistency in this comparison, all models were developed using identical procedures, including class weighting, threshold calibration, and hyperparameter tuning. Initial model performance appeared promising, with high classification accuracy observed across several outcomes. However, further examination suggested that these results were primarily influenced by class imbalance rather than genuine predictive signal. Consequently, the models were limited in their ability to meaningfully address whether sMRI features could predict internalizing symptoms. Similarly, the secondary hypothesis, which anticipated superior performance from self-report models, received only limited support; although the ROC curve for child-reported symptoms exhibited greater curvature, indicating higher discriminative ability, this did not translate into meaningful improvements in identifying clinically significant cases.

This outcome likely reflects several contributing factors. First, the small proportion of participants with elevated symptom severity may have limited the models' ability to detect meaningful associations. Second, the use of symptom scores as the outcome variable may have lacked sufficient granularity to distinguish varying levels of severity. Alternatively, structural brain differences associated with OCD-related internalizing symptoms in adolescence may be too subtle to detect using current methods and features. These limitations highlight the need for cautious interpretation and suggest that future research may benefit from larger, more balanced samples and the integration of additional neurobiological or behavioral data. Taken together, the findings echo longstanding concerns about the low signal-to-noise ratio in community-based samples and the challenges of deriving clinically actionable insights from neuroimaging data alone. These difficulties are further compounded by well-documented issues such as the poor generalizability of sMRI classifiers and informant discrepancies in youth psychopathology assessment (Arbabshirani et al., 2017).

The Problem of Imbalanced Data

The results of the XGBoost analyses underscore a fundamental challenge in applying machine learning in low-base-rate mental health contexts: imbalanced class distributions can severely distort model evaluation metrics. Although accuracy is often cited as a primary measure of performance, it can be misleading in contexts where one class (typically the healthy or normative group) vastly outnumbers others. In such cases, a model may appear highly accurate simply by consistently predicting the majority class, while failing to identify clinically meaningful cases in underrepresented groups. This issue is particularly consequential in mental health research, where accurate detection of borderline and clinical symptom profiles is crucial for screening, diagnosis, and intervention planning.

Despite the theoretical strengths of algorithms like XGBoost in modeling complex relationships, their performance is constrained when trained on datasets that lack sufficient representation of clinically significant but rare cases. In theory, XGBoost is well-suited to psychiatric research, where symptom patterns may emerge from multifactorial influences spanning behavioral, biological, and demographic domains. However, in practice machine learning algorithms typically require a sufficient number of examples from each class to effectively learn distinctions. With 194 features and three outcome classes, traditional guidelines recommend at least 10 outcome events per predictor variable to avoid overfitting, although more recent research emphasizes context-specific and simulation-based approaches to sample size planning (Peduzzi et al., 1996; Riley et al., 2019). Applying the 10-events-per-variable rule post hoc suggests a minimum of 5,820 observations for balanced class representation (10 × 194 × 3). While our dataset included 6,460 total observations, only 109 were labeled as clinical cases. Using the same logic, the clinical group alone would require at least 1,940 observations (10 × 194) to ensure stable performance. Although the sample did not meet this threshold, several best-practice methods, such as class weighting, threshold calibration, and comprehensive hyperparameter tuning, were applied to mitigate the effects of class imbalance. Nonetheless, the limited size of the clinical group likely constrained the model’s ability to learn robust decision boundaries for that class, contributing to its poor sensitivity.

This limitation stems in part from the nature of the loss function used during model training. XGBoost minimizes log loss, standard loss functions like cross-entropy prioritize the global minimization of prediction error, it aims to reduce average error across all cases (Ng, 2004). Without class rebalancing techniques, they offer minimal learning signal for rare outcomes (He & Garcia, 2009). Consequently, the model learns to be highly confident in classifying healthy cases, while failing to sufficiently learn patterns distinguishing the rarer borderline and clinical groups. This is likely because the underlying representations learned by the model failed to meaningfully differentiate those groups in the first place.

Implications of Limited Resolution in The Outcome Measure

Another constraint may be due to the target variable itself, a symptom checklist score. Instruments such as the CBCL and BPM are widely used in youth mental health research due to their efficiency, standardization, and strong psychometric properties (Achenbach, 2001). However, despite these advantages, such questionnaires may lack the precision needed to capture subtle variations in internalizing symptom severity. This limitation is predominantly salient in non-clinical populations, where symptoms may be subthreshold, situational, or masked by social desirability biases (De Los Reyes & Kazdin, 2005; Youngstrom et al., 2000). Self-report measures are especially vulnerable to underreporting and often show limited agreement with external informants, contributing to high intra-individual variability and reducing the reliability and discriminative power of the symptom data (De Los Reyes et al., 2015).

The findings of Ivankovic et al. (2024) further highlight these concerns. In their study, dimensional ratings of OCD symptoms on the CBCL were compared with clinical OCD diagnoses. While elevated checklist scores were generally associated with diagnosis, they did not reliably differentiate youth with clinically significant OCD from those with subclinical symptoms. Importantly, stronger associations were observed for parent-reported obsessions—a domain that is not included in youth-report versions of the CBCL and was therefore unavailable in the present study. This distinction underscores a key limitation in our dataset and highlights the broader challenge of informant effects in modeling brain–behavior relationships. While our study aimed to evaluate the predictive utility of both youth- and parent-reported symptoms, such asymmetries in questionnaire content may constrain the interpretation of comparative findings.

Implications of Limited Resolution in Input Measures

Insufficient Sensitivity of Neuroimaging-Based Input Features

Another limitation of the current study involves the use of tabulated sMRI features as inputs for predictive modeling.

T1w sMRI does not directly image brain tissue; rather, it captures radio-frequency signals emitted by hydrogen atoms in water and fat, influenced by their surrounding microenvironment (Weinberger & Radulescu, 2016). Anatomical metrics such as gray matter volume are derived from intensity contrasts between tissue types and estimated through segmentation algorithms, not by direct visualization of cellular architecture (Ashburner & Friston, 2000). MRI-derived features reflect a composite of neurons, glia, blood vessels, and extracellular components. The resulting signal is modulated by biophysical factors, such as tissue viscosity, perfusion, and magnetic susceptibility, which can be influenced by non-structural variables including hydration status, psychotropic medication, stress, body weight, and substance use (Amianto et al., 2013; Streitbürger et al., 2012; Wang et al., 2022). These factors can introduce signal variability that does not reflect underlying anatomical integrity. In adolescent samples, systematic confounders, particularly head motion, may produce apparent differences in brain structure, such as “cortical thinning” or “tissue loss,” even when no true pathology exists (Reuter et al., 2015). Furthermore, while sMRI can detect macroscopic structural properties, it cannot resolve the cellular mechanisms, such as synaptic pruning or glial remodeling, that drive these changes. For instance, decreases in grey matter volume are often attributed to synaptic pruning, yet synapses comprise less than 1.5% of cortical volume, and reductions may instead reflect broader processes such as increased intracortical myelination or glial cell loss (Bourgeois & Rakic, 1993; Mills & Tamnes, 2014). Consequently, volumetric sMRI measures may lack the specificity needed to meaningfully link structure to behavior in developing brains.

Brain development during childhood is nonlinear and regionally asynchronous, meaning that structural differences associated with symptom severity may emerge at different rates depending on the developmental stage of the child (Tamnes et al., 2013). These, region-specific developmental trajectories present challenges for sMRI-based ROI analyses, particularly when applying static, adult-derived atlases to pediatric samples. For example, cortical grey matter volume typically follows an inverted-U trajectory, peaking in middle childhood and declining through adolescence, and the onset and rate of grey matter changes vary by region (Gilmore et al., 2012; Mills & Tamnes, 2014). Cortical maturation follows a posterior-to-anterior gradient, with earlier development in sensory and parietal regions and later maturation in prefrontal and temporal areas (Tamnes et al., 2013). Furthermore, gyrification decreases from childhood through adolescence due to cortical flattening, reflecting shifts in sulcal depth and width (Alemán-Gómez et al., 2013; Mutlu et al., 2013). Parcellation schemes like the Destrieux atlas, which depend on sulco-gyral anatomy, may therefore misclassify or inconsistently label cortical regions in children, adding noise to volumetric estimates. Subcortical structures pose similar challenges: despite earlier assumptions of early subcortical maturation, structures such as the amygdala, caudate, and thalamus continue to undergo volumetric change well into adolescence (Herting et al., 2018; Tamnes et al., 2018). These ongoing developmental processes reduce the stability of sMRI-derived subcortical measurements and can lead to misestimation of brain–behavior relationships when relying on single-timepoint, cross-sectional data.

Moreover, structural brain differences associated with internalizing symptoms are often subtle and spatially diffuse, making them difficult to detect using coarse-grained sMRI features like global cortical metrics or regional volumes alone (Albaugh et al., 2017). This challenge is further amplified in non-clinical or subclinical populations, where symptom severity is lower, and neural correlates may lie beneath the detection threshold of conventional structural imaging approaches. Recent studies underscore this complexity; for example, Rozovsky et al. (2024) demonstrated that in a transdiagnostic sample of young adults, both increased and decreased cortical thickness in specific regions, such as the left pars opercularis and left inferior temporal gyrus, were differentially associated with depression, anxiety, and mania/hypomania symptom severity. Moreover, these associations were partially mediated by subcomponents of neuroticism, suggesting that personality traits may modulate how structural brain variation relates to internalizing symptoms. These findings highlight that internalizing symptomatology is linked to complex and region-specific patterns of cortical morphology, and underscore the importance of high-resolution, multivariate approaches to capture these nuanced neurobiological correlates in at-risk but non-clinical populations.

Lack of contextual and behavioral data

Although preliminary models included psychosocial and demographic predictors, the final predictive models focused exclusively on structural brain features. As a result, they did not incorporate contextual or behavioral data that could have enriched the interpretation of internalizing symptom variation. This constitutes another key limitation, given that internalizing symptoms are shaped by ongoing interactions between neurobiological vulnerabilities and environmental exposures, including social stressors, daily routines, and affective response (Insel, 2017). Conventional assessments often fail to capture these influences, relying instead on static, decontextualized symptom ratings obtained in clinical or research settings. This narrow focus can result in an incomplete picture of behavior and mood, particularly in everyday contexts where symptoms may fluctuate in response to situational demands (Insel, 2017). The absence of real-world behavioral data thus limits the ecological validity of the current models and constrains their capacity to reflect the lived experience of internalizing symptomatology.

Implications and Future Directions

This study underscores several key challenges in applying machine learning to psychiatric prediction tasks, particularly when working with imbalanced class distributions, checklist-based outcome measures, and limited contextual representation. Despite the use of established techniques such as class weighting, threshold calibration, and hyperparameter tuning, model sensitivity for clinically significant cases remained poor. These findings suggest that widely used approaches may be inadequate when clinical outcomes are both rare and heterogeneous. Building on the limitations identified in this study, several avenues should be explored to improve the effectiveness of machine learning models in predicting internalizing symptoms in youth.

First, addressing the issue of class imbalance would benefit from incorporating sampling techniques such as synthetic oversampling (e.g., SMOTE) and semi-supervised algorithms (Chawla et al., 2002; Zhu & Goldberg, 2009). These methods can help ensure that minority classes are adequately represented during training and can contribute to more equitable and clinically meaningful classification performance. Additionally, increasing the number of clinically affected cases through targeted recruitment or strategic data augmentation may be necessary to meet the data demands of high-dimensional machine learning models (He & Garcia, 2009). Additionally, future work should explore alternative modeling frameworks that better accommodate the challenges of psychiatric prediction.

Second, studies should consider using longitudinal data to differentiate between transient symptom fluctuations and stable clinical trajectories (Dwyer et al., 2018). Modeling symptom change over time may offer a more informative target than single-timepoint scores. Furthermore, the integration of multiple informants, rather than analyzing youth- and parent-reported symptoms in isolation, could help capture a more comprehensive view of symptomatology and reduce the noise introduced by informant discrepancies (De Los Reyes & Makol, 2022). Where feasible, incorporating clinician-rated measures or structured diagnostic interviews as ground truth outcomes would further enhance model validity (Achenbach et al., 1987). Longitudinal designs are also essential for modeling nonlinear, region-specific brain development and distinguishing transient from persistent changes (Tamnes et al., 2018). And, given the anatomical variability of the developing brain, pediatric-specific or data-driven parcellation schemes should replace static, adult-derived atlases to reduce misclassification and improve measurement.

Third, expanding the range and quality of input features may significantly improve model performance. Future models should consider multimodal data sources, including neurocognitive assessments, behavioral observations, ecological momentary assessment (EMA), wearable sensor data, and digital phenotyping. These richer data types may capture underlying constructs that are not adequately reflected in standardized rating scales and offer more precise signals for detecting internalizing psychopathology (Bzdok & Meyer-Lindenberg, 2018). The integration of such data would also align with emerging trends in digital mental health, where continuous and passive monitoring can provide real-time insights into symptom dynamics (Insel, 2017).

Importantly, model interpretability must remain a central consideration; clinical decision-making depends not only on accuracy but also on transparency and trust in the model’s predictions (Lipton, 2018). Finally, future research must prioritize real-world validation and reproducibility. Many studies, including the present one, rely on curated or preprocessed datasets that may not fully reflect the variability encountered in applied clinical environments. Validation in external, heterogeneous samples, particularly from clinical or hospital-based populations, is essential for assessing generalizability and translational value (Van Calster et al., 2019). Transparent reporting of model parameters, performance metrics, and code, along with data sharing where possible, is equally important to support reproducibility and cumulative progress in the field (Collins et al., 2015).

Conclusion

This study evaluated the potential of stMRI features to predict OCD-related internalizing symptoms in youth, comparing models based on self- and parent-reported data. While classification accuracy was initially high, performance was limited by class imbalance, low symptom prevalence, and the coarse resolution of both imaging and outcome measures. These constraints hindered the detection of clinically meaningful patterns. The findings underscore the limitations of using static sMRI data and checklist-based symptoms for psychiatric prediction in youth and point to the need for richer, longitudinal, and multimodal approaches in future research.

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Appendix I

Summary of Linear Regression Models Predicting Internalizing Symptoms

Linear regression models were conducted to assess the contribution of demographic, psychosocial, and neuroimaging predictors to internalizing symptoms as reported by parents and children. The outcome variables were T-scores from the CBCL for parent reports and the BPM for child self-reports. Model fit statistics for each regression are summarized below.

**Table 1.**

*Summary of Linear Regression Models Predicting Parent Reported Internalizing Symptoms*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Model | Residual SE | | R² | Adjusted R² | F (df) | p-value |
| Age, Sex, Race/Ethnicity | 9.70 | 0.016 | | 0.014 | 12.07 (6, 4515) | < .001 |
| Latent SES, Social Risk, Perinatal Risk | 9.73 | 0.010 | | 0.009 | 14.56 (3, 4518) | < .001 |
| sMRI | 9.68 | 0.060 | | 0.019 | 1.45 (191, 4330) | < .001 |
| All Predictors | 9.62 | 0.073 | | 0.031 | 1.73 (196, 4325) | < .001 |

*Note.* Residual SE = Residual Standard Error. R² = Coefficient of Determination. All models used CBCL Internalizing T-score as the outcome variable. This table presents a summary of four linear regression models examining predictors of internalizing symptoms as measured by the CBCL T-scores. Each model includes a different combination of demographic, latent psychosocial, and neuroimaging variables. Key model fit indices are reported, including residual standard error, R², adjusted R², F-statistics, and associated p-values.

**Table 2.**

*Summary of Linear Regression Models Predicting Child Reported Internalizing Symptoms*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | Residual SE | R² | Adjusted R² | F (df) | p-value |
| Age, Sex, Race/Ethnicity | 5.11 | 0.005 | 0.004 | 4.13 (6, 4515) | <.001 |
| Latent SES, Social Risk, Perinatal Risk | 5.08 | 0.017 | 0.016 | 25.63 (3, 4518) | <.001 |
| sMRI | 5.07 | 0.060 | 0.018 | 1.44 (191, 4330) | <.001 |
| All Predictors | 5.03 | 0.074 | 0.032 | 1.77 (196, 4325) | <.001 |

Appendix II

Data Splitting and Class Distributions

To ensure appropriate model training and evaluation, the CBCL internalizing dataset was randomly divided into training (70%), calibration (15%), and test (15%) subsets using stratified random sampling via the create DataPartition function from the caret package in R. A fixed seed (set.seed(123)) was used to ensure reproducibility. Stratification was based on internalizing class labels (healthy, borderline, clinical) to maintain class proportions across splits.

**Table 1.**

*Class Distribution Across Dataset Splits for Internalizing Domain*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| CBCL | | | | | |
| Split | Healthy | Borderline | Clinical | Total | Minority % |
| Full | 6126 | 222 | 112 | 6460 | 5.2% |
| Training | 4301 | 152 | 69 | 4522 | 4.9% |
| Calibration | 922 | 28 | 19 | 969 | 4.9% |
| Test | 903 | 42 | 24 | 969 | 6.8% |
| BPM | | | | | |
| Split | Healthy | Borderline | Clinical | Total | Minority % |
| Full | 6043 | 308 | 109 | 6460 | ~2.5% |
| Training | 4231 | 217 | 74 | 4522 | ~2.7% |
| Calibration | 905 | 47 | 17 | 969 | ~2.8% |
| Test | 907 | 44 | 18 | 969 | ~2.3% |

*Note.* Class labels represent internalizing symptom severity. "Minority %" indicates the proportion of samples in the Borderline and Clinical categories combined.

**Table 2.**

*Class Distribution Across Dataset Splits for Externalizing Domain*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| CBCL | | | | | |
| Split | Healthy | Borderline | Clinical | Total | Minority % |
| Full | 6356 | 66 | 38 | 6460 | ~1.6% |
| Training | 4455 | 44 | 23 | 4522 | ~1.5% |
| Calibration | 953 | 12 | 4 | 969 | ~1.7% |
| Test | 948 | 10 | 11 | 969 | ~2.2% |
| BPM | | | | | |
| Split | Healthy | Borderline | Clinical | Total | Minority % |
| Full | 6096 | 144 | 21 | 6261 | ~2.5% |
| Training | 4266 | 102 | 15 | 4383 | ~2.7% |
| Calibration | 913 | 24 | 2 | 939 | ~2.8% |
| Test | 917 | 18 | 4 | 939 | ~2.3% |

*Note.* Children missing externalizing I forgot, Need to run externalizing again with matching parent and child?

|  |
| --- |

Appendix III

Externalizing Symptoms

The externalizing symptoms outcome variable exhibited similar class imbalance issues as the internalizing symptoms, with a predominance of participants classified as "normal," and comparatively fewer in "borderline" and "clinical" categories. These results are provided here for transparency and reproducibility.

**Figure 1**

*Distribution of Externalizing Outcomes*

A graph of a number of symptom scores

AI-generated content may be incorrect.*a) b)*

*Note:* This figure shows the class distribution (Normal, Borderline, Clinical) for externalizing symptoms. The outcome variable was highly imbalanced, with the majority of participants classified as “Normal,” and relatively few classified as “Borderline” or “Clinical.” N, SD, MEAN

**Table A.**

*Best Tuning Parameters for Externalizing Symptoms – XGBoost Models*

|  |  |  |
| --- | --- | --- |
| Parameter | CBCL | BPM |
| Booster | Gbtree | Gbtree |
| Objective | Multi:softprob | Multi:softprob |
| Evaluation Metric | mlogloss | mlogloss |
| Max Depth | 3 | 3 |
| Min Child Weight | 5 | 1 |
| Eta | 0.1 | 0.05 |
| Gamma | 0.5 | 0.5 |
| Subsample | 0.6 | 0.9 |
| Colsample by Tree | 0.9 | 0.9 |
| Number of Classes | 3 | 3 |
| Best number of rounds | 150 | 50 |
| Best multiclass Log Loss | 1.091149 | 1.08137 |

*Note:* These hyperparameters were obtained through cross-validation to minimize multiclass log loss.

**Table B.**

*Model Performance Metrics for Externalizing Symptoms*

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | CBCL | | | | BPM | | | |
| Model Configuration | Default | With Weights | Tuned + Argmax | Tuned + Threshold-Cal. | Default | With Weights | Tuned + Argmax | Tuned + Threshold-Cal. |
| Overall Performance | | | | | | | | |
| Accuracy | 0.3478 | 0.3498 | 0.9835 | 0.9546 | 0.3323 | 0.3365 | 0.9723 | 0.886 |
| 95% CI | 0.3178–0.3787 | 0.3198–0.3808 | 0.9733–0.9905 | 0.9395–0.9668 | 0.3022–0.3634 | 0.3063–0.3678 | 0.9597–0.9818 | 0.864–0.9057 |
| Cohen’s Kappa | 0.0113 | 0.0084 | 0 | -0.0173 | -0.0106 | 0.005 | 0 | -0.0328 |
| Class Balance | | | | | | | | |
| Balanced Accuracy | 0.5524 | 0.5545 | 0.5 | 0.4879 | 0.4248 | 0.5038 | 0.5 | 0.462 |
| Sensitivity (Borderline) | 0.4 | 0.4 | 0.0 | 0.0 | 0.1667 | 0.3333 | 0.0 | 0.0 |
| Sensitivity (Clinical) | 0.7273 | 0.5455 | 0.0 | 0.0 | 0.5 | 0.5 | 0.0 | 0.0 |
| Specificity (Borderline) | 0.6705 | 0.6621 | 1.0 | 0.9875 | 0.683 | 0.6743 | 1.0 | 0.924 |
| Specificity (Clinical) | 0.6754 | 0.6858 | 1.0 | 0.9885 | 0.6545 | 0.6599 | 1.0 | 0.984 |
| Class-Level Discrimination | | | | | | | | |
| Precision (Borderline) | 0.0125 | 0.0122 | NaN | 0.0 | 0.0102 | 0.0196 | NaN | 0.0 |
| Precision (Clinical) | 0.0251 | 0.0195 | NaN | 0.0 | 0.0062 | 0.0063 | NaN | 0.0 |
| F1 Score (Borderline) | 0.0236 | 0.0236 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| F1 Score (Clinical) | 0.0248 | 0.0248 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

*Note:* The calibrated threshold approach improved overall accuracy substantially. However, class-level discrimination for minority classes (borderline and clinical) remained poor. The extreme imbalance appears to have overwhelmed the model’s capacity to generalize effectively across classes, highlighting the difficulty in modeling low-prevalence categories even with calibrated thresholds.