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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% to 3% of individuals worldwide (de Mathis et al., 2013). Up to half of adult patients with OCD indicate that their disease began in childhood or adolescence, and its prevalence rate in these years is between 1 and 4% (Douglass et al., 1995; Rasmussen & Eisen, 1990). The is characterized by the presence of compulsions – ritualized behavioral or mental acts, and obsessions – intrusive and unwanted thoughts and worries (Karno et al., 1988). OCD is unique among mental illnesses in that it exhibits both externalizing and internalizing symptom domains (Guzick et al., 2019). Externalizing symptoms, like compulsivity and repetitive actions, are often outwardly disruptive and are associated with dysfunctions in circuits that govern motor behaviors and reward processing. In contrast, internalizing symptoms, including anxiety and obsessions, often lead to avoidance and withdrawal, and can be closely associated to dysregulation within certain circuits involved in fear response and emotion regulation (Achenbach, 2009; Shephard et al., 2021). Understanding OCD within the dual framework of internalizing and externalizing enhances our grasp of the complexity of its clinical presentation and can informs more effective therapeutic strategies. This framework is therapeutically beneficial and supported by empirical research (Kessler et al., 2011; Slade & Watson, 2006).

Neurobiology of OCD

Advances in neuroimaging, particularly magnetic resonance imaging (MRI), have elucidated the brain's role in OCD, pointing to abnormalities within the cortico-striato-thalamo-cortical (CSTC) circuit and other key regions (de Wit et al., 2014; Hu et al., 2017; Picó-Pérez et al., 2020). OCD is a clinically and etiologically highly heterogeneous disorder, characterized by various overlapping symptom dimensions (Bragdon & Coles, 2017). The CSTC model is the most widely accepted explanation for the neurobiological underpinnings of OCD (Graybiel & Rauch, 2000; van den Heuvel et al., 2016). The traditional neurobiological model of OCD describes the disorder as a dysfunction in within the CSTC circuit. The CSTC consists of the thalamus, basal ganglia, anterior cingulate cortex, and orbitofrontal cortex (OFC) (Brennan & Rauch, 2017). Primarily, the CSTC model attributes compulsive behaviors as failures in inhibitory control, where these distinct neural pathways struggle to suppress unwanted thoughts and actions effectively.

Building upon the CSTC model, a more recent neurocircuit-based approach has developed to account for diverse symptom profiles observed in OCD (Shephard et al., 2021). This expanded model incorporates additional circuits between regions involved in emotion regulation, habit formation, sensory processing, and reward sensitivity. As illustrated in figure 1, the framework described by van den Heuvel et al. (2016) describes OCD as dysfunction within five circuits. OCD symptoms are mediated by partially distinct neural systems (van den Heuvel et al., 2009). Each circuit is associated to a specific symptom dimension. Although each circuit is described as associated to a particular symptom dimension relevant to OCD, it is important to recognize their interconnected nature rather than viewing them in isolation. These circuits offer a more nuanced understanding of how diverse OCD symptoms manifest, highlighting the complexity of interactions between multiple brain regions. This model is especially relevant for adolescents because their brains are still developing, particularly in areas like the prefrontal cortex, which governs impulse control and emotional regulation (Casey et al., 2008).

An overview of the relationship between OCD symptoms and these neural circuits provides insight into how they are connected. For instance, (1) the fronto-limbic circuit is involved in regulating fear and emotional responses. Hyperactivity within this circuit can lead to intrusive thoughts and potentially trigger obsessions due to impaired top-down emotional regulation (Milad et al., 2013). The amygdala-prefrontal connectivity has been found to be predictive of therapy outcomes for OCD in youth (Cyr et al., 2021). Meanwhile, dysfunction in the (2) sensorimotor circuit, involved in integration of motor behavior and sensory input, explains why some OCD symptoms stem from sensory-driven urges, such as "not-just-right" feelings, averse or uncomfortable sensations that drive compulsions like excessive touching or arranging objects (Stern et al., 2025). Additionally, habit formation also implicated in this circuit can cause compulsive behaviors to become automatic, persisting beyond their initial triggers. The (3) ventral cognitive circuit plays a major role in self-regulation, acting as a "braking system" for inhibiting inappropriate actions; dysfunction here may prevent individuals from stopping compulsions even when they recognize them as irrational (van den Heuvel et al., 2016). The (4) ventral affective circuit is involved in reward processing and motivation, where compulsions can become self-reinforcing behaviors, thus may not just alleviate anxiety but become rewarding behaviors themselves, reinforcing habitual and compulsive loops of the sensorimotor circuit. Clinical studies have reported heightened connectivity between the NAcc and other reward-processing regions, such as the OFC during resting-state brain activity, with this increased connectivity correlating with the severity of OCD symptoms (Xie et al., 2017). Lastly, (5) the dorsal cognitive circuit involved in executive functioning and cognitive flexibility, dysfunction in this circuit leads to rigid thinking and challenges in emotional regulation, thus A diagram of a brain

AI-generated content may be incorrect.exacerbating obsessions and repetitive behaviors.

***Figure. 1*** *Neural Circuits Involved in Obsessive-Compulsive Disorder: Brain Regions and Connectivity. (1) The Fronto-Limbic Circuit consisting of the amygdala and ventromedial prefrontal cortex (vmPFC). (2) The Sensorimotor Circuit consisting of the supplementary motor area, putamen, pallidum, and thalamus. (3) The Ventral Cognitive Circuit consisting of the inferior frontal gyrus (IFG), ventrolateral prefrontal cortex, subthalamic nucleus (STN), and ventral caudate. (4) The Ventral Affective Circuit consisting of the orbitofrontal cortex (OFC) and nucleus accumbens (NAcc). (5) The Dorsal Cognitive Circuit consisting of the dorsolateral prefrontal cortex (dlPFC) and dorsomedial prefrontal cortex (dmPFC). This visual representation is taken from Shephard et al. (2021).*

Structural Brain Abnormalities

Structural abnormalities in individuals with OCD have been identified across a range of neuroimaging studies, revealing notable differences in several key brain regions. Generally, adolescents with OCD tend to exhibit a reduction in cortical thickness and volume, specifically in the parietal and frontal regions, such as the inferior and superior parietal cortices and certain frontal gyri (Pagliaccio et al., 2021; Wu et al., 2022). In contrast, the thalamus generally shows increased volume in these individuals, although the degree of enlargement and involvement of specific subnuclei seem to vary across studies (van den Heuvel et al., 2022).

Apart from global measurements, investigations into subcortical structures have uncovered distinct alterations that further delineate the neural landscape of OCD. Structural deviations in several subcortical regions including the caudate nucleus, putamen, and pallidum, are implicated in OCD pathology (Wang et al., 2022). Notably, Wang et al. (2022) identified specific structural changes in the nucleus accumbens (NAcc), amygdala, and pallidum among individuals diagnosed with OCD. Adolescents exhibited more pronounced structural deviations in the NAcc and pallidum than adults, with the NAcc being of particular interest due to its potential role as a biomarker for OCD development. Meanwhile in adults, amygdala alterations, characterized by inward deformation, correlated with symptom severity and highlighted the involvement of the fronto-limbic circuit, underscoring the role of fear and emotional dysregulation in OCD. These findings suggest that OCD is not only a disorder of habit formation (as CSTC emphasizes) but also involves dysfunctional emotional regulation and altered motivation systems.

These insights imply a developmental trajectory in OCD symptomatology; younger individuals may present more automatic, sensory-driven compulsions aligned with the sensorimotor circuit, whereas adults may experience heightened emotional dysregulation and cognitive rigidity indicative of fear-based compulsions within the fronto-limbic circuit (Wang et al., 2022).

Informant Discrepancies

Traditionally, clinicians have depended on parents to provide comprehensive information about how an illness and its treatment affect their children. This reliance stems from the perception that children may not possess the cognitive and linguistic skills required to understand and respond to surveys accurately (Vygotsky, 1978). Consider the case of Liam, a 12-year-old having battled severe OCD for several years. After starting therapy, he was showing signs of improvement. According to Liam, he felt he was making excellent progress. He reduced his handwashing rituals from every hour to three times a day and started joining some family meals. He was also beginning to meet his friends for short walks around the neighborhood. However, his parents observed a different reality. While Liam had made some progress, he often became trapped in lengthy rituals that caused him significant distress. He had yet to return to school full-time, attending only partial days if he went at all. Though he started venturing out with friends, it was only to familiar, controlled environments. His parents continued to monitor his progress closely, supporting him in his journey while remaining aware of the continuous obstacles that his OCD presented. 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.

The phenomenon of informant discrepancy has been recognized for nearly 70 years, dating back to Lapouse and Monk's work in 1958. Achenbach, McConaughy, and Howell (1987) conducted a seminal analysis of 119 studies investigating these informant inconsistencies. Their key findings included: (a) reports of the same behavior by different informants generally show low to moderate agreement; (b) the reports of two informants observing children in the same setting are more similar than those of two informants observing children in different settings; (c) there is greater agreement between informants' reports for younger children compared to older ones; and (d) reports of externalizing behaviors like aggression show higher consistency than those of internalizing behaviors such as anxiety. They concluded by stating, "Different informants are needed for different situations. . . there is no royal road or preeminent gold standard for phenomena that are inevitably affected by assessment procedures and other situational variables" (p. 227–228). Consequently, the primary objectives of the informant discrepancies research summarized by Achenbach et al. (1987) were to outline the extent of informant discrepancies, identify the informant pairs (e.g., parent and child, teacher and parent) with the greatest discrepancies, and pinpoint the behavioral domains where these discrepancies were most pronounced. A prominent finding indicated discrepancies and varying accuracy in symptom reporting, with no clear consensus. Additionally important because obsessions (an internalizing symptom) are a distinguishing symptom of OCD.

The issue of informant discrepancies is particularly pertinent when interpreting study findings in the field of developmental psychopathology. A significant portion of the evidence about prevalence rates of psychological disorders, classification of diagnosis, and effectiveness of interventions for children is derived from reports by multiple informants (Weisz et al., 2005). For instance, the prevalence rates of conduct and oppositional defiant disorders in community samples can vary significantly depending on whether assessments are based solely on parental or teacher reports or if both sources are considered simultaneously. According to Offord et al. (1996), these rates range from 1.6% to 10.2%. More recent research by Munkvold et al. (2009) also noted substantial variability in oppositional defiant disorder prevalence, although the reported rates were lower, ranging from 0.2% to 2.6%. Moreover, depending on the informant, it is typical to find inconsistent results from controlled studies evaluating psychological therapies (De Los Reyes & Kazdin, 2005).

First, research shows that parent and youth reports begin to diverge in early adolescence (Grills & Ollendick, 2002; Fisher et al., 2006; Rockhill et al., 2007; Rothen et al., 2009), with worse agreement for internalizing disorders compared to externalizing ones (Rey et al., 1992; Grills & Ollendick, 2002; Foley et al., 2004; Rothen et al., 2009), though not always (Verhulst & van der Ende, 1992). Second, parents' own depression and anxiety can color their reports of their children's mental health (Rothen et al., 2009). Third, youth self-reports may offer predictive insights beyond parental reports in some areas (Sourander et al., 2006a; Sourander et al., 2006b; Rothen et al., 2009). Demographics (Barch, 2021)

While the use of multiple informants in mental health assessment is thought to enhance our understanding of the psychological functioning of children, particularly in the infant population, we are still in the process of discovering how to effectively utilize this wealth of information (Reyes, 2013).

Statistical Learning

Statistical Learning Theory (SLT) is the basis for many modern machine learning algorithms, emphasizing generalization by extracting patterns from data for accurate predictions (Luxburg & Schoelkopf, 2008). It is central to supervised learning, which uses labeled data to train models that relate predictor variables to a response variable, focusing on prediction accuracy rather than causal understanding (Shmueli, 2011).  Predictive modeling prioritizes accuracy, using probabilistic or supervised learning models, and employs loss functions to measure prediction discrepancies and refine models for real-world use. In the context of clinical neuroscience and neuroimaging, the most common machine learning paradigm, learns to associate brain imaging data with specific classifications such as diagnostic groups. This approach can help identify key predictive features that differentiate between these categories (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 et al., 1984). 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). 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 2. 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 2.*** *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.*

Boosting

Boosting, as illustrated in Figure 3, 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, than improve the overall fit by addressing errors from previous models. Figure 3 demonstrates how training error decreases as more trees are added, with the ensemble prediction formed by summing tree outputs for improved accuracy. Gradient Boosting, which operates similarly to gradient descent, 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 helps the models focus on challenging cases, correcting errors while maintaining flexibility. XGBoost, or extreme gradient boosting, is a particularly efficient algorithm for fitting boosting models (Ren et al., 2019).



***Figure 3.*** *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.*

Tuning Parameters

When using XGBoost for regression tasks, several key parameters can be fine-tuned to optimize model performance (XGBoost Developers, 2022). It's important to note that this overview is not exhaustive of all tuning parameters available in XGBoost; rather, it is a short summary of some of the most impactful parameters to consider when optimizing regression models. The learning rate determines how quickly the model learns patterns, with smaller values allowing for more cautious learning to reduce overconfidence and potential overfitting. The maximum depth sets how complex each decision tree can be by limiting the number of splits, with deeper trees capturing more intricate patterns but risking overfitting. “Minimum child weight” sets the amount of data required in a leaf node before further splitting, promoting simpler, less complex trees. For each tree, only a random subset of the predictor variables is made available to the model, and the size of this subset is a tuning parameter denoted colsample\_bytree in XGBoost. Furthermore, a threshold on the magnitude of improvement required for making a new split is controlled by the parameter “gamma”. Finally, only a random subset of the training data is used when fitting each tree, and the size of this subset is controlled by the parameter “subsample”. 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 complex interactions between variables predicting 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

The present study strives to bridge the gap between neuroimaging advancements and the ongoing challenges posed by discrepancies in symptom reporting for adolescent OCD. While MRI studies provide insights into the neurobiological underpinnings of OCD, variations between parent and self-reports often result in inconsistencies in diagnosing and evaluating the disorder's severity, potentially impacting treatment efficacy. Notably, symptom reports of externalizing behaviors, such as compulsions, demonstrate greater consistency compared to internalizing behaviors like obsessions, underscoring the impact of information source on report reliability. To tackle these issues, our study explores the potential of structural brain data in predicting the severity of two higher-level OCD symptom domains—internalizing and externalizing—as reported by adolescents and their parents. Utilizing the XGBoost algorithm, the study aims to develop predictive models that capture the nuanced differences in symptom reporting. This research aims to deepen our understanding of how neuroimaging data can enhance symptom assessments in adolescent OCD, ultimately contributing to improved personalized treatment outcomes.

Research question

Can structural brain data be used to predict the level of OCD symptoms reported by youths and parents?

Supplementary questions:

Is the predictive accuracy of structural brain data for internalizing domain higher for self-reported symptoms than for parent-reported symptoms?

Is the predictive accuracy of structural brain data for externalizing domain higher for parent-reported symptoms than for self-reported symptoms?

Methods

Data Source and Collection Procedures

The Adolescent Brain and Cognitive Development (ABCD) Study is a comprehensive decade-long research initiative in the United States, tracking children from ages 9-10 through late adolescence and into early adulthood. It conducts annual lab-based evaluations and biannual imaging scans to assess various mental and physical health metrics (Saragosa-Harris et al., 2022; Barch et al., 2018). The ABCD Study is designed to enhance our understanding of the behavioral, genetic, neurobiological, and environmental factors influencing health and risk factors for physical and mental health problems during adolescence. The study includes 12,000 children at baseline, recruited from 21 research sites across the United States (Karcher & Barch, 2021). To ensure the cohort is diverse and representative, the ABCD Study employs a multi-stage probability sampling technique, along with weighting methods and stratified sampling within specific regions to minimize selection bias.

Data acquisition

Structural MRI

High-resolution T1-weighted and T2-weighted 3D structural images were acquired using Siemens, Philips, and GE 3T MRI scanners. Preprocessing includes correcting for bias field, distortion, and resampling (Hagler et al., 2019). Images were corrected for gradient nonlinearity distortions (Jovicich et al., 2006), and T2w images were registered to T1w images using a mutual information-based approach (Wells et al., 1996). Intensity non-uniformity was corrected through tissue segmentation and sparse spatial smoothing. All images were resampled to 1 mm isotropic resolution and rigidly aligned to a standard atlas space. Regions of interest (ROIs) were defined using the Destrieux atlas-based classification (Destrieux et al., 2010). 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). It is widely used in structural MRI studies to analyze cortical volume, thickness, and sulcal depth in neurodevelopmental and neurodegenerative research. Subcortical structures were analyzed using the Automated Segmentation of the Subcortical Structures (ASEG) provided by FreeSurfer, developed by Fischl et al. (2002). This atlas allows the segmentation and volume measurement of subcortical areas, cortical white and gray matter, ventricles, and other intracranial structures from T1-weighted MRI scans. The combination of these atlases facilitates a comprehensive analysis of both cortical and subcortical regions.

Demographics and categorical diagnosis

Demographic questionnaire derived primarily from the validated computerized Kiddie Schedule for Affective Disorders and Schizophrenia for DSM-5 (KSADS-5) (Kobak et al., 2013). Demographic variables include age, sex, race and ethnicity. The KSADS-5 is a comprehensive diagnostic tool compatible with DSM-5 criteria, which facilitates the precise categorization of psychiatric diagnoses. Diagnoses may be classified as "certain," "possible," "in remission," or "not present." This categorical diagnostic approach leverages established criteria to determine the presence or absence of disruptive or abnormal behaviors, aligning closely with standards set forth in the Diagnostic and Statistical Manual of Mental Disorders (APA, 2000).

Self and Parental Reports of dimensional diagnosis

The Achenbach System of Empirically Based Assessment (ASEBA) is a comprehensive evaluation tool developed after years of research and practical use (*ASEBA*, 2019). It is designed to assess behavioral, emotional, and social aspects, along with strengths, competencies, and adaptive functioning in individuals ranging from 1½ years old to over 90. 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 diagnostic/assessment approach that places behaviors along a continuum of frequency and/or severity. Moreover, assessments are normed by informant, age, sex, and ethnicity. The resulting scores are reported as z-scores within a full T-score range, 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 5, the CBCL consists of several dimensions categorized into Syndrome Scales and DSM-Oriented Scales. The eight syndrome scales are established through factor analysis. They encompass clusters of common behaviors or symptoms. Meanwhile, the more recently developed seven DSM-Oriented Scales align with diagnostic categories outlined in the DSM-5 (American Psychiatric Association, 2013; Nelson et al., 2001). 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.

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 5, the BPM measures four scales, including Internalizing, Attention Problems, Externalizing, and Total Problems scales, paralleling the items and scales found on the more comprehensive CBCL/6-18 (Achenbach et al., 2017).



***Figure 5.*** *Structure of the ASEBA, specifically focusing on the CBCL and the BPM. The parent-reported CBCL consists of Syndrome Scales and the more recently developed DSM-Oriented Scales. The DSM-Oriented Scales are aligned with diagnostic criteria from the DSM and include categories such as OCD and Anxiety Problems. The syndrome Scales include clusters of symptoms which are further grouped into three high-level domains known as (1) Internalizing Problems, (2) Externalizing, and a (3) Total Problems score that sums all problem items. The child-reported BPM is a shorter version, provides a rapid assessment parallel to dimensions in CBCL for monitoring behavioral and emotional functioning over time.*

Sample

To ensure consistency with data collection, we focused on the Year 2 follow-up time point, during which both MRI data and questionnaire responses were gathered. The process of participant selection and group classification is illustrated in Figure 4. Participants were excluded for the following reasons: lack of MRI data, lack of parental or self-report data, or a diagnosis of any other psychological disorder. The OCD group was defined as having a current diagnosis of OCD based on the KSADS. Notably, individuals with a current diagnosis of OCD are included in the OCD group regardless of any comorbid psychiatric conditions, reflecting the highly comorbid nature of OCD. Conversely, the healthy control group was defined by the absence of any current psychological diagnosis. A total of 6,513 participants were included in the study.



***Figure 4.*** *Flowchart of participant selection and subgroup classification at 2-year follow-up. Considered groups are colored in green.*



For the healthy control group (n= 6079), the mean age of participants was 9.47 years (SD = 0.51). The sex distribution, 47.3% were female (n = 2875), 0% identified as intersex-male (n = 1), and 52.7% were male (n = 3203). The racial and ethnic composition of the group was as follows: 2.2% Asian (n = 136), 13.4% Black (n = 813), 18.9% Hispanic (n = 1150), 9.8% identifying as Other (n = 597), and 55.7% White (n = 3383). For the OCD group (n= 434), the mean age of participants was 9.46 years (SD = 0.50). The sex distribution included 47.5%female (n = 206) and 52.5% male (n = 228). The racial and ethnic composition was 0.9% Asian (n = 4), 14.7% Black (n= 64), 18.7% Hispanic (n = 81), 14.3% identifying as Other (n = 62), and 51.4% White (n = 223).

Modelling approach

All analysis and data handling were done in R version 4.3.3. Mean imputation was used to handle the missing data in the subcortical atlas (n=9). Additionally, two variables related to Aseg lesions in the left and right hemispheres were excluded due to having over 30% missing data. Both BPM and CBCL assessments were standardized using z-score transformation to facilitate transparent comparisons across datasets. Models were built with xgboost package. Separate XGBoost models were trained for each symptom domain resulting in four prediction models: CBCL internalizing score, BPM internalizing score, CBCL externalizing score, and BPM externalizing score. For each model, the predictor sets comprised 194 variables derived from the Destrieux and Aseg brain regions. To prevent bias in predictions, the target variable was not included in the predictor set. The dataset was then partitioned into training and testing subsets, with 70% of the data (n=4,559) allocated for training and the remaining 30% (n=1,954) reserved for testing.

Training

Hyperparameter tuning was achieved through 5-fold cross-validation (CV) using a grid search strategy, exploring parameters such as the number of boosting rounds, tree depth, learning rate, and subsampling ratios. Model selection was optimized by minimizing the root-mean-square error (RMSE), ensuring high predictive accuracy. The cross-validation output is then plotted as the interaction between boosting rounds and CV error across different tree depths and learning rates. These plots visualize how model complexity and iteration affect performance of the model.

Subsample = high class imbalance.

Testing

The hyperparameters yielding the best performance were used to evaluate feature importance. Feature importance plots were generated for each model, allowing identification of the most impactful predictors of symptom severity. Predictions were generated using the trained model with optimized tuning parameters applied to the test dataset. Subsequently, performance metrics including, R-squared and MAE were computed with the caret package. This entailed comparing the model-generated predictions against the actual outcomes, thereby assessing the model's generalization capabilities to unseen data. The final model was also utilized to derive a feature importance analysis, identifying the relative significance of each feature. This matrix is displayed as a graphical representation of the top three features, which elucidates the key variables impacting model predictions. This methodological approach is essential for both evaluating predictive accuracy and discerning the primary factors influencing the model's decision-making process.

Results

Training

Hyperparameter tuning for cbcl:



We tune max\_depth and min\_child\_weight first because they have the highest impact on the model outcome. To start with, let’s set wider ranges, and then we will perform another iteration for smaller ranges.

max\_depth:

Controls the maximum depth of each tree. Increasing max\_depth can help capture complex patterns but may also lead to over fitting. Lower values can prevent over fitting but might oversimplify the model.

min\_child\_weight:

Controls the minimum sum of instance weight needed in a child node. This parameter helps prevent over fitting by making it more difficult for leaf nodes to learn from small amounts of data.

Once optimal max\_depth and min\_child\_weight are found, tune gamma, subsample, and colsample\_bytree.

5. Regularization and Final Model

Finally, you can fine-tune alpha and lambda for regularization.

Optimal parameters

For the CBCL prediction, optimal tuning parameters:

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Nrounds | Max\_depth | Eta | Gamma | Colsample | Minchild weight | subsample |
| Cbcl I | 50 | 2 | 0.05 | 0.1 | 0.8 | 2 | 0.6 |
| Bpm I | 100 | 2 | 0.05 | 1 | 0.8 | 2 | 0.8 |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |

Hyperparameter tuning for bpm:



Optimal parameters

For the BPM prediction, optimal tuning parameters:

Testing

Evaluation

|  |  |  |  |
| --- | --- | --- | --- |
|  | RMSE | Rsquared | MAE |
| CBCL internal | 0.944972416 | 0.001488248 | 0.767723949 |
| BPM internal | 0.94465596 | 0.00018654 | 0.70570213 |
|  |  |  |  |
|  |  |  |  |

CBCL

BPM

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Discussion

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Appendix

A diagram of a sample

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