Title?

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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). The disorder commonly arises in early life and 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 symptoms (Guzick et al., 2019). Externalizing features, like compulsivity and repetitive actions, are often outwardly disruptive and align with disorders such as attention-deficit/hyperactivity disorder (ADHD) and disruptive behavior disorders. In contrast, internalizing aspects, including anxiety, concerns, and obsessions, cause internal distress and align with conditions like depressive and anxiety disorders, often leading to avoidance or withdrawal (T. M. Achenbach, 2001). Understanding OCD within this dual framework enhances our grasp of its complexity and informs more effective therapeutic strategies. This framework is therapeutically beneficial and supported by empirical research (Kessler et al., 2011; Slade & Watson, 2006).

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 (ref). 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. However, 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. Mental health problems can vary across different contexts (Bauducco et al., 2024; Beesdo et al., 2009). Children and adolescents may exhibit mental health concerns in specific environments, such as at home or school, while appearing unaffected in others, like during peer interactions. These contextual variations are evident across various domains, including conduct problems, attention, hyperactivity, and anxiety (Beesdo et al., 2009). This divergence in perspectives introduces complexities in clinical practice, research, and theory regarding child psychiatry and psychopathology (Chen et al., 2017; Salbach-Andrae et al., 2009). These differences have been thoroughly examined and will be covered in more detail below. Furthermore, 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).

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, depending on whether parent or teacher assessments are used to categorize the child's problem or if both are taken into account at the same time, the prevalence rates of conduct and oppositional defiant disorders in community samples vary from 1.6% to 10.2% (Offord et al., 1996). Furthermore, depending on the informant, it is typical to find inconsistent results from controlled studies evaluating psychological therapies (De Los Reyes & Kazdin, 2005). Understanding these discrepancies is crucial for accurately assessing intervention outcomes and advancing research in developmental psychopathology.

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.

Agreement as a test of validity for multiple informant (?) Child reports internalized symptoms more accurately, while parents tend to be more precise in identifying externalized symptoms (Silverman & Eisen, 1992).

MRI

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). Such findings suggest that neuroimaging biomarkers hold promise for enhancing diagnostic accuracy and understanding the neurobiological underpinnings of OCD.

A diagram of a brain

AI-generated content may be incorrect.Neurobiological Theories of OCD

OCD is a clinically and etiologically highly heterogeneous disorder with multiple overlapping symptom dimensions (Bragdon & Coles, 2017). These symptoms are mediated by partially distinct neural systems (van den Heuvel et al., 2009). 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 CTSC model describes how loops between the cortex, striatum, thalamus, and back to the cortex regulate thought patterns and behaviors (Brennan & Rauch, 2017). The neurocircuit-based model of OCD builds upon the traditional CSTC model by incorporating additional brain circuits that contribute to the diverse symptom profiles of the disorder (Shephard et al., 2021). While the CSTC model primarily explains compulsions as failures in inhibitory control, the neurocircuit-based approach expands this by considering how emotional regulation, habit formation, sensory processing, and reward sensitivity play crucial roles in OCD. This model identifies five key circuits: fronto-limbic, sensorimotor, ventral cognitive, ventral affective, and dorsal cognitive circuits, each associated with specific symptom dimensions. It is important to note that these neurocircuits have more complex functions beyond the specific neurocognitive alterations discussed in this short summary. Additionally, these circuits are highly interconnected rather than functioning as isolated systems, despite how they may be presented in the following sections.

Fronto-Limbic Circuit

The fronto-limbic circuit, involving the amygdala and ventromedial prefrontal cortex (vmPFC), regulates fear and emotional responses (Kohn et al., 2014). In OCD, hyperactivity in the amygdala strengthens feelings of fear and anxiety, leading to excessive worry and intrusive thoughts, while impaired top-down regulation by the vmPFC makes it difficult to control these emotions (Milad et al., 2013). Dysregulated fear reactions to intrusive thoughts, controlled by this circuitry, may be the initial cause of obsessions for some patients. Furthermore, studies indicate alterations in amygdala-prefrontal connectivity during the onset of symptoms (Paul et al., 2019). The connectivity within this neural pathway has been found to be predictive of therapy outcomes for OCD in youth (Cyr et al., 2021).

Sensorimotor Circuit

The sensorimotor circuit, which includes the supplementary motor area (SMA), putamen, pallidum, and thalamus, governs motor behaviors and sensory integration (van den Heuvel et al., 2016). Dysfunction in this circuit 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). This is particularly evident in compulsions related to cleanliness, where patients may feel a tactile sensation of dirtiness, prompting excessive washing or cleaning. This circuit is also implicated in habit formation, where repeated compulsions become automatic and disconnected from their original triggers, leading to rigid, motor-driven rituals that persist even when anxiety is no longer present (Gillan & Robbins, 2014).

Ventral Cognitive Circuit

The ventral cognitive circuit includes prefrontal areas such as the inferior frontal gyrus (IFG) and ventrolateral prefrontal cortex, alongside subcortical regions like the subthalamic nucleus (STN), ventral caudate, and thalamus, which are integral to self-regulation functions. The IFG and the ventral caudate function as a "braking system" for response inhibition, facilitating the ability to suppress inappropriate reactions (Shephard et al., 2021). This means dysfunction here prevents individuals from stopping compulsions even when they recognize them as irrational (van den Heuvel et al., 2016).

Ventral Affective Circuit

The ventral affective circuit including the orbitofrontal cortex (OFC) and nucleus accumbens (NAcc), is responsible for reward processing and motivation (van den Heuvel et al., 2016). In some OCD cases, compulsions may not just alleviate anxiety but become rewarding behaviors themselves, reinforcing habitual and compulsive loops. Consistent with these clinical findings, 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).

Dorsal Cognitive Circuit

Lastly, the dorsal cognitive circuit, involving the dorsolateral prefrontal cortex (dlPFC) and dorsomedial prefrontal cortex (dmPFC), is essential for executive functioning and cognitive flexibility (van den Heuvel et al., 2016). Due to this circuit's broad and fundamental role, specific dorsal cognitive dysfunctions are not linked to distinct OCD symptom profiles but rather general impairments that interact with other neurocircuit disruptions (Shephard et al., 2021). When this circuit is impaired, individuals struggle with rigid thinking, difficulty shifting attention, and poor emotional regulation, which can contribute to the persistence of obsessions and repetitive behaviors (Van Schalkwyk et al., 2016).

Adolescent OCD

This expanded 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 (ref). By mapping specific OCD symptoms to these circuits, the neurocircuit-based model provides a more comprehensive understanding of the disorder and allows for the development of targeted interventions (Shephard et al., 2021).

Structural abnormalities

Many studies highlight structural differences in the brains of individuals with OCD, particularly in regions like the thalamus, parietal cortices, striatal regions, and fronto-parietal areas (van den Heuvel et al., 2022; Wang et al., 2022; Wu et al., 2022). Some studies note mixed findings and developmental differences, while others focus more on surface shape alterations, specifically in pediatric samples. Multiple studies agree that adolescents with OCD tend to show a reduction in cortical thickness or volume in parietal and frontal regions (Pagliaccio et al., 2021; Wu et al., 2022). This is particularly noted in areas such as the inferior and superior parietal cortices and certain frontal gyri. There is general agreement that the thalamus may show increased volume in adolescents with OCD; however, the degree of enlargement and the specific subnuclei involved can vary across studies (van den Heuvel et al., 2022). There are consistent findings of structural alterations in several subcortical regions, including the caudate nucleus, putamen, and pallidum, which are implicated in OCD (Wang et al., 2022).

Wang et al. (2022) identified specific structural changes in subcortical brain regions in individuals diagnosed with OCD, noting variations in the NAcc, amygdala, and pallidum.

Importantly, they found structural-developmental variations in the pallidum and accumbens associated with the presence of an OCD diagnosis. Adolescents show more pronounced structural deviations in the NAcc and pallidum surfaces than adults, which relates to the sensorimotor circuit and ventral affective circuit. They noted that the NAcc could potentially serve as a biomarker for OCD development. Additionally, they found an inward deformation of the amygdala, most substantially in adults, which correlated with symptom severity. This aligns with the fronto-limbic circuit, emphasizing 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. Furthermore, these findings in pediatric OCD suggest that OCD symptoms in youth may be more habit-driven and sensory-based, aligning with the sensorimotor circuit in the expanded model. Meanwhile, the amygdala findings in adults suggest a shift toward fear-based compulsions consistent with the fronto-limbic circuit. This supports a developmental progression in OCD, where younger individuals may struggle more with automatic, sensory-driven compulsions, whereas adults may experience more emotional dysregulation and cognitive rigidity (Wang et al., 2022).

Statistical Learning

Statistical Learning Theory (SLT) is the theoretical foundation of many modern machine learning algorithms (Luxburg & Schoelkopf, 2008).  In this context, “learning” refers to the process of deducing general rules from observed examples, with a strong emphasis on generalization; extracting patterns from a dataset that can be accurately applied to new, unseen data for accurate predictions.  This theoretical framework is integral to supervised learning, which focuses on establishing relationships between a response variable Y and a group of predictor variables X, using labeled data to train the model.

In predictive modeling, the goal is to forecast the response variable using the predictor variables as tools for achieving accurate predictions. Unlike explanatory modeling, which seeks to understand causal relationships, predictive modeling emphasizes accuracy without delving into causal theory (Shmueli, 2011). There are two main approaches to predictive modeling: probabilistic models, which assume a specific statistical form for the data, and supervised learning models, which focus on creating functions that map inputs to outputs without necessarily assuming a data generation process. The accuracy of predictions is gauged by a loss function that measures the discrepancy between the predicted and the true or observed outcomes, crucial for refining the model to make accurate predictions in real-world applications.

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). Ina: more background ml in neuro

Learning methods

Linear Model

Linear regressions serve as fundamental tools in statistical learning, offering a straightforward approach to understanding relationships within data sets. Linear regression posits a linear relationship between input variables X and an output variable Y. Linear models use methods like least squares for parameter estimation, offering clarity and ease-of-use in scenarios where linear relationships are fitting.  However, these models have limitations when confronted with complex data patterns, prompting extensions like generalized linear models or support vector machines. These adaptations incorporate various loss functions and statistical methods to broaden applicability and enhance modeling capabilities in more diverse contexts.

A diagram of a tree

AI-generated content may be incorrect.Decision Trees

Decision trees provide a significant advancement 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. 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). This versatile, branching framework enables decision trees to naturally capture intricate patterns and interactions, surpassing the constraints of linear models. Something about overfitting, Bias variance tradeoff.

A diagram of a tree

AI-generated content may be incorrect.Boosting

Boosting is an ensemble method used to improve the predictive accuracy of models (Schapire & Freund, 2012). An ensemble refers to a collection of multiple models that together contribute to making a more accurate and robust prediction than any single model could achieve on its own. This is done by iteratively adding simpler models (otherwise known as base learners), such as decision trees, which enhance the model's fit by focusing on errors made by previous learners. Gradient Boosting combines individual decision trees through a process similar to gradient descent, and involves two layers of optimization: first, decision trees are individually optimized to reduce error using their own criteria; second, the collective error of the entire ensemble is minimized, correcting the residual errors with each new tree added (Friedman, 2001). This layered approach gives gradient boosting flexibility over other tree ensembles by enabling diverse loss functions for error minimization, which helps the summation of predictions align closer with desired or true outcomes (Ryan, 2025). Adjusting observation weights allows these models to focus on more challenging cases, effectively correcting mistakes while maintaining flexibility.

XGBoost, known as an “extreme” gradient boosting algorithm is an implementation of gradient boosting, which frames the boosting challenge as an optimization problem (Ren et al., 2019). It uses a version of gradient descent called Newton descent to fine-tune its models more precisely (Nocedal & Wright, 2006). Also unique because of regularization terms, feature splitting and sparse data handling.

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. Colsample\_bytree decides how many features the model considers when building each tree, allowing for randomness that can enhance generalization. Gamma establishes the required improvement for a split to occur, encouraging simpler models by preventing unnecessary splits. Finally, subsample controls the fraction of the training data used per tree, adding variability and reducing overfitting by preventing the model from relying too heavily on specific data subsets. 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 ability of neuroimaging to identify the neurological underpinnings of OCD has sparked interest in using MRI indices to distinguish between healthy group and OCD patients. XGBoost can model complex interactions within datasets, providing a robust framework for integrating diverse data types, such as neuroimaging data with behavioral and demographic variables. By using the collective strengths of multiple models, boosted models offer superior capabilities to single trees and linear models, effectively managing complex relationships in high-dimensional data.

The present study (?)

Despite advances in neuroimaging that emphasize the potential of structural MRI to uncover neurobiological correlates of OCD, discrepancies between parental and self-reports of OCD symptoms remain a significant challenge. Traditional diagnostic methods often overlook critical nuances in symptom severity and informant variability. Considering these challenges, this study aims to address the research question: Can structural brain data be used to predict the level of OCD symptoms reported by youths and parents? This thesis will focus on predictive modeling of adolescent OCD symptomology as reported by adults vs. self. By using sMRI data as predictor variables, the study will apply the supervised learning algorithm XGBoost to try achieve accurate predictions.

Research question

Focus on predictive model: Can structural brain data be used to predict the level of OCD symptoms reported by youths and parents?

Hypothesis

There will be a significant difference in the prediction accuracy of structural brain data between self-reported and parent-reported OCD symptoms in adolescents with OCD, with an expectation of higher accuracy for self-reported symptoms for the internalizing dimension and higher accuracy for parent-reported symptoms for the externalizing dimension.

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

Questionaries

Kiddie Affective

Demographic variables

Achenbach System and Empirically Based Assessment (ASEBA)

Child Behavior Checklist (CBCL).

The CBCL is a component of the ASEBA 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." It consists of several dimensions categorized into Syndrome Scales and DSM-Oriented Scales. The eight syndrome scales are established through factor analysis (ref). They encompass clusters of common behaviors or symptoms, including (1) Anxious/Depressed, (2) Withdrawn/Depressed, (3) Somatic Complaints, (4) Social Problems, (5) Thought Problems, (6) Attention Problems, (7) Rule-Breaking Behavior, (8) Aggressive Behavior. Meanwhile, the more recently developed seven DSM-Oriented Scales align with diagnostic categories outlined in the Diagnostic and Statistical Manual of Mental Disorders. They include; (1) OCD Problems, (2) Depressive Problems, (3) Anxiety Problems, (4) Somatic Problems, (5) Attention Deficit/Hyperactivity Problems, (6) Oppositional Defiant Problems, (7) Conduct Problems (American Psychiatric Association, 2013; Nelson et al., 2001). Furthermore, these scales are grouped into three high-level domains known as (1) Internalizing Problems (which combines Anxious/Depressed, Withdrawn/Depressed, and Somatic Complaints), (2) Externalizing Problems (which combines Rule-Breaking Behavior and Aggressive Behavior), and a (3) Total Problems score that sums all problem items. 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 Obsessive-Compulsive Symptom (OCS) Scale (?)

**Discrepancy (?)**

small discrepancy = child agrees with parent about OCS score (probably)

high discrepancy = child probably disagrees with the parent about the OCD score

Brief Problem Monitor (BPM).

The BPM 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." 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).

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). While it excludes subcortical structures, it is widely used in structural MRI studies to analyze cortical volume, thickness, and sulcal depth in neurodevelopmental and neurodegenerative research.

Also, subcortical atlas

Sample

Statistical analyses/Preliminary analyses(?)

Modelling approach(?)

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