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A Machine-Learning Approach to Modeling Cognitive Flexibility, Stress Reactivity, and Executive Function in Clinical Populations

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ABSTRACT

Objective: The objective of this study was to develop a machine-learning model integrating behavioral measures of executive function, cognitive flexibility, and psychophysiological stress reactivity to predict and classify clinical symptomatology in individuals with Major Depressive Disorder, Generalized Anxiety Disorder, and Post-Traumatic Stress Disorder.

Methods and Materials: A cross-sectional design was utilized with a sample of $N = 352$ participants, comprising Healthy Controls ($n = 95$) and individuals diagnosed with Major Depressive Disorder ($n = 88$), Generalized Anxiety Disorder ($n = 84$), and Post-Traumatic Stress Disorder ($n = 85$). Participants completed a comprehensive three-hour assessment protocol including neurocognitive tasks (Wisconsin Card Sorting Test, Stroop Color-Word Test, Trail Making Test), a modified social-evaluative stress task with concurrent psychophysiological recordings (electrocardiography for heart rate variability [HRV], salivary cortisol), and clinical self-report questionnaires. Machine learning models (Random Forest, Support Vector Machine, and XGBoost) were trained on 80%of the data to classify clinical versus control groups, utilizing hyperparameter tuning and SHAP (SHapley Additive exPlanations) values for feature interpretation.

Findings: The XGBoost algorithm achieved the highest predictive performance in classifying clinical versus control groups, yielding an AUC-ROC of 0.91. Traditional linear analyses indicated that clinical cohorts exhibited significantly greater symptom severity and poorer cognitive performance, including elevated perseverative errors on the WCST and compromised Trail Making Test performance. Physiologically, cortisol reactivity (AUC_I) was blunted in the PTSD group and exaggerated in the MDD group, while baseline HRV was significantly lower across all clinical cohorts. SHAP feature importance analysis revealed that the TMT Part B-A difference score was the most crucial predictor of clinical classification, followed closely by cortisol reactivity (AUC_I), baseline anxiety, and baseline HRV.

Conclusion: Advanced machine-learning algorithms effectively capture the complex, non-linear interactions between cognitive flexibility and autonomic stress dysregulation, underscoring the necessity of integrated, multidimensional approaches for accurate psychiatric classification.

Keywords: *Cognitive Flexibility; Executive Function; Stress Reactivity; Major Depressive Disorder; Post-Traumatic Stress Disorder; Generalized Anxiety Disorder*

1. Introduction

Executive functions are widely recognized as a complex and dynamic system of higher-order cognitive processes that enable individuals to regulate their thoughts, emotions, and behaviors in pursuit of goal-directed outcomes. These top-down processes are indispensable when automatic or instinctual responses are insufficient for navigating novel or demanding situations (Miller & Taylor, 2024). At the core of this cognitive architecture lie several interdependent components, most notably working memory, inhibitory control, and cognitive flexibility. Together, these elements facilitate higher-level reasoning and complex problem-solving abilities across various contexts (Schäfer et al., 2024). Cognitive flexibility, in particular, represents the mental agility required to transition seamlessly between differing concepts, adapt to evolving environmental contingencies, and consider multiple perspectives simultaneously. This capacity is fundamentally dependent on an individual's ability to hold information in mind while effectively inhibiting prepotent but irrelevant responses (Corbo et al., 2024). The developmental trajectory of these executive functions begins in early childhood, laying the crucial groundwork for subsequent cognitive milestones. For instance, robust verbal working memory and cognitive flexibility uniquely contribute to the maturation of advanced language skills in preschool-aged children (Filipe et al., 2023). Moreover, the overall intellectual capacity and chronological age of school children heavily dictate the ongoing refinement of these executive processes, especially in populations grappling with intellectual disabilities (Erostarbe-Pérez et al., 2022). Importantly, lifestyle factors such as regular physical activity have been shown to positively differentiate working memory and general executive functioning in early development, underscoring the plasticity of these cognitive domains (Baniasadi, 2024).

Conversely, pronounced impairments in executive functioning and cognitive flexibility serve as hallmark characteristics of numerous neurodevelopmental and learning disorders. In children with attention-deficit/hyperactivity disorder (ADHD), severe deficits in behavioral inhibition and cognitive flexibility precipitate significant academic and social dysfunction. However, targeted clinical interventions, such as transcranial electrical stimulation combined with cognitive rehabilitation, have demonstrated substantial efficacy in ameliorating these specific executive deficits (Arshadi et al., 2022). Furthermore, cognitive empowerment strategies directly targeting emotional regulation and decision-making can yield significant functional improvements in ADHD populations, highlighting the therapeutic potential of addressing cognitive flexibility (Yavaribarha et al., 2022). Similar neurocognitive interventions, such as neurofeedback training, have emerged as highly effective mechanisms for enhancing attention and broader executive capacities in students diagnosed with specific learning disorders (Shari et al., 2021). The reverberations of these executive deficits extend far beyond the individual child, often placing an immense psychological burden on the familial system. Parents of children with autism spectrum disorder, for example, frequently report profound levels of parenting stress. Encouragingly, the implementation of executive function-based parenting training packages has proven highly effective in mitigating this stress (Granmayeh et al., 2023). By focusing on executive principles, these parenting programs not only alleviate parental burden but simultaneously foster significant improvements in the inhibitory control and cognitive flexibility of their children, thereby establishing a reciprocal pathway of psychological resilience within the household (Ghasemi et al., 2022).

The intricate and bidirectional relationship between psychological stress and executive functioning represents a critical frontier in modern clinical research. It is well-documented that exposure to chronic or acute stress profoundly impairs prefrontal cortex functionality, thereby degrading an individual's working memory and cognitive flexibility. Yet, robust cognitive flexibility can also serve as an endogenous protective buffer, directly moderating the deleterious psychological effects of school-related and occupational stress exposure (Harel et al., 2023). In the face of adversity, perceived stress is intimately tethered to an individual's overarching psychological resilience. In this dynamic, cognitive control and cognitive flexibility function as serial mediators, enabling adaptive coping mechanisms and facilitating psychological recovery (Bacıoğlu & Kocabıyık, 2025). This mediating function of cognitive flexibility is evident across a highly diverse array of human experiences and specialized populations. For instance, in immigrant cohorts navigating the complexities of cultural assimilation, acculturation stress severely threatens general health; however, this destructive pathway is heavily mediated by individual differences in cognitive flexibility and perfectionism (Hasheminejad et al., 2024). Similarly, in high-stakes occupational environments, such as nursing, extreme job demands frequently precipitate burnout and emotional exhaustion. Providing optimal, mindfulness-based models to enhance cognitive flexibility has been identified as a critical strategy for mitigating this occupational distress (Parvaresh et al., 2024).

Stress also deeply permeates interpersonal, familial, and marital ecosystems, further illustrating the fundamental importance of executive functions. External societal stressors, most notably the unprecedented disruptions caused by the COVID-19 lockdowns, significantly amplified parental distress. This heightened distress, in turn, directly and negatively skewed parents' perceptions of their children's developing executive capabilities (Polizzi et al., 2021). Expanding on this familial dynamic, the specific parenting styles adopted within households, alongside the inherent executive functioning of young children, serve as vital mediators bridging the gap between parental stress and the overall quality of parenting provided in two-child families (Qian et al., 2024). In intimate partnerships, preserving marital satisfaction is closely tied to executive abilities; advanced structural modeling indicates that executive functions significantly predict marital burnout, a relationship intricately mediated by the Theory of Mind (Babaei et al., 2024). Similarly, the existential anxiety and deep emotional distress experienced by adolescents—particularly those in high-pressure athletic environments—are substantially regulated by their capacity for distress tolerance and cognitive flexibility, mitigating the damaging cycle of rumination (Esmaeilnejad & Mazraeh, 2025).

Transitioning from general environmental stress to severe clinical psychopathology, profound and pervasive deficits in cognitive flexibility and physiological stress reactivity become central pillars in the etiology and maintenance of major psychiatric disorders. Distress tolerance, defined as the perceived or actual behavioral capacity to withstand negative and aversive emotional states, is frequently shattered alongside core executive functions. In patients suffering from Major Depressive Disorder (MDD), pervasive, rigid referential thoughts dominate the cognitive landscape. Intensive therapeutic modalities, such as cognitive behavioral therapy (CBT) and acceptance and commitment therapy (ACT), are therefore essential to deconstruct these rigid patterns and actively rebuild cognitive flexibility and distress tolerance (Yaqubi et al., 2026). These exact therapeutic frameworks are comparably crucial for adolescent populations suffering from obsessive-compulsive disorder (OCD), where purposefully enhancing cognitive flexibility and resilience directly undermines the severity of compulsive behaviors and intrusive thoughts (Baniasadi et al., 2025). Beyond structured clinical disorders, targeted positive psychotherapy has demonstrated significant efficacy in augmenting cognitive flexibility and distress tolerance in individuals enduring profound life transitions and relational severances, such as divorced women (Khorasani, 2024). It is also critical to note that cognitive dysfunctions extend into conditions defined by profound impulsivity and compulsivity, fundamentally driving the behavioral pathology observed in binge eating disorder and broader food addiction (Iceta et al., 2021).

However, arguably the most extreme alterations in both executive functioning and stress reactivity are observed within the spectrum of trauma-related psychopathology. Post-traumatic stress disorder (PTSD) is fundamentally characterized by an exaggerated, hyperactive physiological stress response paired with severely intrusive cognitive symptomatology. Robust longitudinal mediation models have unequivocally demonstrated that pre-existing or concurrent deficits in executive functioning act as a catalyst, significantly exacerbating the trajectory and severity of post-traumatic stress symptoms over time (Bardeen et al., 2022). The clinical presentation is exponentially more complicated in cases of Complex Post-Traumatic Stress Disorder (CPTSD). In CPTSD, prolonged and repeated interpersonal trauma not only shatters the individual's foundational attachment style but also inflicts pervasive, enduring impairments across all domains of executive function (Paula & Antônio José, 2023). In these severely traumatized clinical populations, the cognitive inability to flexibly disengage attention from trauma-related stimuli, combined inextricably with a highly maladaptive and dysregulated psychophysiological stress response, creates an intractable cycle of debilitating symptomatology.

Despite the expansive body of literature intricately linking executive functions, cognitive flexibility, and stress reactivity to an array of clinical psychiatric outcomes, the vast majority of prior empirical investigations have remained overly reliant on traditional, linear statistical methodologies. These conventional analytical approaches fundamentally isolate individual variables—such as exclusively testing the main effect of working memory on depression severity or tracking the linear impact of stress on inhibitory control. Consequently, they inherently fail to capture the highly complex, multidimensional, and frequently non-linear interactions that truly define human neurocognition and psychophysiological reactivity. Advanced computational methodologies, particularly the deployment of machine learning and artificial intelligence algorithms, offer a profound and necessary methodological evolution. By simultaneously evaluating and cross-referencing dozens or even hundreds of interconnected psychometric and physiological variables, machine-learning algorithms possess the unique capacity to uncover hidden structural patterns and delineate intricate predictive networks that routinely elude standard parametric testing models. The superior utility of these advanced algorithmic models in psychological science has already been clearly demonstrated in contemporary research, such as the successful utilization of artificial neural networks to accurately map the complex, multi-variable etiology of marital burnout (Babaei et al., 2024).

Applying a robust machine-learning framework to the complexities of clinical psychology empowers researchers to transcend rudimentary group-level mean comparisons, advancing toward precise, individualized, and highly accurate predictive modeling. By systematically integrating standardized behavioral cognitive testing—capturing vital metrics such as perseverative errors and set-shifting speeds—with real-time, continuous psychophysiological data collected during acute stress induction protocols, a comprehensive and holistic neurobiological profile can be constructed for each individual patient. Identifying the most heavily weighted and critical features within this multi-domain profile holds the potential to dramatically enhance diagnostic accuracy, reduce clinical misclassification, and directly inform the development of highly individualized, targeted therapeutic interventions. At present, there remains a glaring and significant gap in the scientific literature regarding the application of supervised machine-learning classification models to definitively distinguish between varied, high-severity psychiatric populations based entirely on their hybridized profiles of neuroendocrine stress reactivity and cognitive flexibility. The aim of this study was to develop a machine-learning model that integrates behavioral measures of executive function, cognitive flexibility, and psychophysiological stress reactivity to predict and classify clinical symptomatology in individuals with Major Depressive Disorder, Generalized Anxiety Disorder, and Post-Traumatic Stress Disorder.

2. Methods and Materials

2.1. Study Design and Participants

This study employed a cross-sectional design to investigate the relationships between cognitive performance, stress reactivity, and clinical symptomatology. We recruited a total of 352 participants from clinical and community settings across major metropolitan areas in Canada, including Toronto, Vancouver, and Montreal. Recruitment was facilitated through partnerships with outpatient psychiatric clinics, university health services, and community mental health organizations, supplemented by public advertisements. Inclusion criteria required participants to be between 18 and 65 years of age, fluent in English, and have a primary diagnosis of either Major Depressive Disorder (MDD), Generalized Anxiety Disorder (GAD), or Post-Traumatic Stress Disorder (PTSD), as confirmed by a structured clinical interview. A healthy control group, matched for age and sex, was also recruited from the same communities. Exclusion criteria were applied to minimize confounding variables and ensure participant safety; these included a history of neurological disorders, current substance use disorder within the past six months, unstable medical conditions, or any contraindications to the stress induction protocol. The final sample consisted of 352 individuals with a mean age of 38.7 years ($SD = 11.2$) and was composed of 62% female participants.

2.2. Measures

A comprehensive battery of neurocognitive assessments, psychophysiological recordings, and self-report questionnaires was administered in a single laboratory session lasting approximately three hours. Executive function and cognitive flexibility were assessed using a set of standardized, computer-administered tasks. The Wisconsin Card Sorting Test (WCST) was used to measure abstract reasoning and the ability to shift cognitive sets, with primary outcome variables being the number of categories completed and the rate of perseverative errors. The Stroop Color-Word Test was administered to evaluate response inhibition and selective attention, measuring the interference effect calculated from reaction times on incongruent versus congruent trials. The Trail Making Test (TMT), Parts A and B, provided measures of processing speed and task-

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switching ability, with the B-A difference score serving as a key index of cognitive flexibility. To assess stress reactivity, participants underwent a modified, computer-based social-evaluative stress task involving timed, difficult mental arithmetic problems coupled with pre-programmed negative social feedback. Physiological reactivity was captured via continuous monitoring of heart rate variability (HRV) using an electrocardiogram (ECG), and salivary cortisol samples were collected at baseline, immediately post-stressor, and at 10 and 20 minutes post-recovery to map the hypothalamic-pituitary-adrenal (HPA) axis response. Subjective stress was measured using a 100-point visual analog scale (VAS) for state anxiety administered before and after the stressor. Clinical characterization was achieved using the Structured Clinical Interview for DSM-5 (SCID-5) to confirm diagnoses. Symptom severity was quantified using the Beck Depression Inventory-II (BDI-II), the Generalized Anxiety Disorder 7-item (GAD-7) scale, and the PTSD Checklist for DSM-5 (PCL-5).

2.3. Data analysis

Data analysis was conducted using a machine-learning framework in Python with the scikit-learn, XGBoost, and SHAP libraries. Prior to model development, the dataset underwent a rigorous preprocessing pipeline. Missing data, which constituted less than 5% of the total data points, were handled using multiple imputation by chained equations (MICE). All continuous features, such as reaction times from cognitive tasks and physiological measurements, were standardized by converting them to z-scores using the formula $z = (x - \mu)/\sigma$ to ensure that all variables contributed equally to the model performance regardless of their original scale. The primary analytical goal was to develop predictive models capable of classifying individuals into clinical versus healthy control groups based on the multi-domain data. To achieve this, the dataset was randomly partitioned into a training set (80%) and a hold-out testing set (20%). We implemented and compared the performance of three supervised learning algorithms known for their robustness and high performance on complex tabular data: Random Forest, a Support Vector Machine (SVM) with a radial basis function kernel defined as $K(x_i, x_j) = \exp(-\gamma \, || \, x_i - x_j \, ||^2)$, and an Extreme Gradient Boosting (XGBoost) classifier. Hyperparameter tuning for each model was performed on the training data using a 10-fold cross-validation strategy to prevent overfitting and optimize model generalizability. Model performance was evaluated on the unseen testing set using several metrics, including the Area Under the Receiver Operating Characteristic Curve (AUC-ROC), accuracy, precision, recall, and the F1-score. To move beyond simple prediction and gain insight into the underlying mechanisms, we employed SHapley Additive exPlanations (SHAP) to interpret the output of the best-performing model. SHAP values allowed us to quantify the contribution of each feature—such as perseverative errors on the WCST, cortisol reactivity, or HRV suppression—to the model's prediction for each individual participant, thereby identifying the most influential predictors of clinical status and illuminating the complex interplay between cognitive function and stress physiology.

3. Findings and Results

An initial examination of the demographic and clinical profiles of the 352 participants revealed a well-matched sample across the diagnostic and control groups. The sample was divided into four distinct groups: Healthy Controls (HC, $n = 95$), Major Depressive Disorder (MDD, $n = 88$), Generalized Anxiety Disorder (GAD, $n = 84$), and Post-Traumatic Stress Disorder (PTSD, $n = 85$). A one-way analysis of variance (ANOVA) indicated no significant differences in age across the four groups, $F(3{,}348) = 0.84$, $p = .473$. Similarly, a Chi-square test of independence confirmed that the distribution of biological sex did not significantly differ between the groups, $\chi^2(3, N = 352) = 1.25$, $p = .741$. As anticipated, the clinical groups exhibited significantly elevated scores on all psychometric symptom severity scales compared to the healthy control group. Specifically, the MDD group demonstrated the highest mean scores on the Beck Depression Inventory-II (BDI-II), the GAD group scored highest on the GAD-7, and the PTSD group reported the most severe symptoms on the PTSD Checklist for DSM-5 (PCL-5).

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Table 1

Demographic and Clinical Characteristics of the Sample (N=352)

Variable	Healthy Controls ($\boldsymbol{n} = \mathbf{95}$)	MDD ($\boldsymbol{n} = \mathbf{88}$)	GAD ($\boldsymbol{n} = \mathbf{84}$)	PTSD ($\boldsymbol{n} = \mathbf{85}$)
Age ($\boldsymbol{M} \pm \boldsymbol{SD}$)	38.2 ± 10.9	39.5 ± 11.4	37.8 ± 10.5	39.1 ± 12.0
Female Sex ($\boldsymbol{n}$, %)	58(61.1%)	56(63.6%)	52(61.9%)	52(61.2%)
BDI-II ($\boldsymbol{M} \pm \boldsymbol{SD}$)	4.2 ± 2.8	28.7 ± 6.4	15.4 ± 5.1	19.2 ± 6.8
GAD-7 ($\boldsymbol{M} \pm \boldsymbol{SD}$)	2.1 ± 1.5	12.5 ± 4.3	16.8 ± 3.2	14.1 ± 4.5
PCL-5 ($\boldsymbol{M} \pm \boldsymbol{SD}$)	5.5 ± 3.1	18.4 ± 8.2	16.2 ± 7.5	45.6 ± 9.4

In the domains of executive function and cognitive flexibility, significant between-group differences emerged across all standardized tasks. The clinical cohorts consistently demonstrated poorer performance relative to the healthy controls. For the Wisconsin Card Sorting Test (WCST), an ANOVA revealed a significant main effect of group on the number of perseverative errors, $F(3,348) = 14.62, p < .001, \eta_p^2 = 0.11$. Post-hoc Tukey tests indicated that the MDD and PTSD groups committed significantly more perseverative errors than the HC group ($p < .01$). The Stroop interference effect, measured in milliseconds, also varied significantly by group, $F(3,348) = 18.35, p < .001$, $\eta_p^2 = 0.14$, with the GAD group showing the greatest impairment in response inhibition. Furthermore, cognitive flexibility, as indexed by the Trail Making Test (TMT) Part B minus Part A difference score, was significantly compromised in all clinical groups compared to controls, $F(3,348) = 22.41, p < .001, \eta_p^2 = 0.16$. A comprehensive summary of the cognitive and executive function performance metrics is provided in Table 2.

Table 2

Descriptive Statistics for Cognitive and Executive Function Measures by Group

Cognitive Measure	Healthy Controls	MDD	GAD	PTSD
WCST Categories Completed	5.4 ± 0.8	4.1 ± 1.3	4.5 ± 1.1	3.9 ± 1.4
WCST Perseverative Errors	12.1 ± 4.5	18.5 ± 6.2	15.2 ± 5.4	19.4 ± 7.1
Stroop Interference ($\boldsymbol{ms}$)	110.5 ± 35.2	155.2 ± 48.1	175.4 ± 52.3	162.8 ± 50.6
TMT Part A ($\boldsymbol{sec}$)	28.4 ± 6.2	35.1 ± 8.4	33.2 ± 7.5	36.4 ± 9.1
TMT Part B-A Difference ($\boldsymbol{sec}$)	32.5 ± 10.4	52.4 ± 18.6	48.5 ± 15.2	58.1 ± 20.3

Analysis of the physiological and subjective responses to the computerized social-evaluative stress task revealed altered stress reactivity profiles among the clinical populations. While baseline cortisol levels did not significantly differ between groups, $F(3,348) = 1.12, p = .341$, the cortisol area under the curve with respect to increase (AUC_I) was significantly blunted in the PTSD group and exaggerated in the MDD group compared to healthy controls, $F(3,348) = 11.28$, $p < .001$, $\eta_p^2 = 0.09$. Heart Rate Variability (HRV), specifically the root mean square of successive differences (RMSSD), showed a sharp decrease during the stressor for all groups. However, the recovery of HRV back to baseline at 20minutes post-stress was significantly delayed in the GAD and PTSD groups. Subjectively, the Visual Analog Scale (VAS) for state anxiety indicated that all clinical groups experienced a more profound psychological reaction to the stressor than the control group. These reactivity data are systematically presented in Table 3.

Table 3

Physiological and Subjective Stress Reactivity Indicators

Reactivity Measure	Healthy Controls	MDD	GAD	PTSD
Baseline Cortisol ($\boldsymbol{nmol/L}$)	12.4 ± 3.1	13.1 ± 3.5	12.8 ± 3.2	11.9 ± 2.8
Cortisol Reactivity ($\boldsymbol{AUC_I}$)	45.2 ± 15.4	62.1 ± 21.3	50.4 ± 18.2	28.5 ± 14.1
Baseline HRV (RMSSD, $\boldsymbol{ms}$)	48.5 ± 12.1	36.2 ± 10.5	32.4 ± 9.8	34.1 ± 11.2
Stress HRV (RMSSD, $\boldsymbol{ms}$)	35.1 ± 9.4	28.4 ± 8.2	22.1 ± 7.5	25.3 ± 8.8
VAS Anxiety Increase ($\boldsymbol{\Delta}$)	22.4 ± 10.1	38.5 ± 14.2	45.2 ± 15.6	42.1 ± 16.4

Following the univariate analyses, we evaluated the performance of three machine-learning algorithms (Random Forest, Support Vector Machine, and XGBoost) in classifying individuals into clinical versus healthy control categories using the combined cognitive, physiological, and subjective data features (71 total features post-preprocessing). Evaluation on the 20%hold-out testing set ($n = 71$) demonstrated that the XGBoost classifier achieved the highest predictive performance across all evaluated metrics. The XGBoost model yielded an Area Under the Receiver Operating Characteristic Curve (AUC-ROC) of 0.91, signifying excellent discriminative capacity. The Support Vector Machine (SVM) performed adequately but struggled with the non-linear relationships inherent in the psychophysiological data, resulting in a lower recall rate for clinical cases. Random Forest demonstrated robust performance but was marginally outperformed by the gradient boosting approach of XGBoost. Table 4 provides a comprehensive comparison of the predictive metrics for each machine-learning model.

Table 4

Machine Learning Model Performance Metrics for Classifying Clinical vs. Healthy Participants

Model	Accuracy	Precision	Recall	F1-Score	AUC-ROC
Random Forest	0.83	0.85	0.81	0.83	0.87
Support Vector Machine	0.79	0.82	0.75	0.78	0.82
XGBoost	0.89	0.90	0.88	0.89	0.91

To interpret the driving forces behind the superior performance of the XGBoost classifier, SHAP values were calculated to determine global feature importance. This analysis moves beyond black-box prediction, offering a nuanced understanding of how specific cognitive and stress-related variables contribute to the likelihood of clinical classification. The SHAP summary plot revealed that the TMT Part B-A difference score was the single most impactful predictor, with higher difference scores strongly pushing the model toward a clinical prediction. Cortisol reactivity (AUC_I) emerged as the second most important feature, demonstrating a complex, non-linear relationship where both severe blunting (characteristic of PTSD) and hyper-reactivity (characteristic of MDD) increased the probability of clinical classification. Interestingly, subjective baseline anxiety and baseline HRV were more predictive than several primary cognitive outcomes, underscoring the vital role of autonomic nervous system baseline states in mental health classifications. The top ten features and their mean absolute SHAP values, representing their average impact on model output magnitude, are detailed in Table 5.

Table 5

Top 10 Predictors Identified by SHAP Value Analysis in the XGBoost Model

Rank	Feature	Domain	Mean |SHAP| Value
1	TMT Part B-A Difference	Cognitive Flexibility	0.842
2	Cortisol Reactivity (AUC_I)	Endocrine Stress	0.715
3	Baseline HRV (RMSSD)	Autonomic Baseline	0.680
4	Stroop Interference	Response Inhibition	0.594
5	VAS Anxiety Increase	Subjective Stress	0.521
6	WCST Perseverative Errors	Executive Function	0.488
7	Stress HRV (RMSSD)	Autonomic Stress	0.412
8	Baseline Cortisol	Endocrine Baseline	0.355
9	TMT Part A	Processing Speed	0.290
10	WCST Categories Completed	Executive Function	0.215

4. Discussion

The primary objective of this study was to model the complex interplay between cognitive flexibility, executive function, and stress reactivity in diverse clinical populations using an advanced machine-learning framework. The results demonstrated that the XGBoost classifier could accurately discriminate between individuals with Major Depressive Disorder (MDD), Generalized Anxiety Disorder (GAD), Post-Traumatic Stress Disorder (PTSD), and healthy controls, yielding a high AUC-ROC of 0.91. Traditional linear analyses revealed significant between-group

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differences across all cognitive tasks and physiological stress responses. However, the machine-learning approach provided a more nuanced, multidimensional perspective. Through SHAP value analysis, the Trail Making Test (TMT) Part B-A difference score emerged as the most powerful predictor of clinical status, closely followed by cortisol reactivity (AUC_I) and baseline Heart Rate Variability (HRV). These findings strongly validate the shift toward utilizing computational models like artificial neural networks and gradient boosting to capture non-linear, multi-variable interactions in psychological research, as similarly demonstrated in the effective modeling of marital burnout (Babaei et al., 2024).

The prominent predictive power of cognitive flexibility, particularly the TMT B-A difference score and the WCST perseverative errors, aligns robustly with the broader literature emphasizing executive functions as foundational for adaptive behavioral regulation. Executive functions are essential for complex problem-solving and adapting to novel, unpredictable demands across the lifespan (Miller & Taylor, 2024; Schäfer et al., 2024). When these top-down regulatory mechanisms are compromised, individuals exhibit increased vulnerability to psychopathology. Our findings that MDD, GAD, and PTSD groups exhibited pronounced deficits in cognitive flexibility are corroborated by longitudinal evidence demonstrating that pre-existing impairments in executive functioning critically exacerbate post-traumatic stress symptoms (Bardeen et al., 2022). This phenomenon is even more pronounced in instances of Complex PTSD, where trauma fundamentally disrupts both attachment security and executive capacities (Paula & Antônio José, 2023). Conversely, the preservation of cognitive flexibility is heavily implicated as a protective factor across the developmental spectrum, spanning from the maturation of language skills and working memory in preschool children (Filipe et al., 2023) to maintaining higher-level cognitive performance in healthy older adults versus those with mild cognitive impairment (Corbo et al., 2024). Furthermore, cognitive capacity and chronological age remain critical determinants of executive functioning, especially in populations managing intellectual disabilities (Erostarbe-Pérez et al., 2022). Physical lifestyle factors, such as high levels of physical activity, also significantly enhance these foundational executive and working memory functions in early childhood (Baniasadi, 2024), suggesting that neurocognitive resilience can be behaviorally fostered.

Our physiological findings, wherein the clinical groups exhibited maladaptive stress reactivity profiles—such as the blunted cortisol response in PTSD, hyper-reactivity in MDD, and delayed HRV recovery across all clinical cohorts—underscore the profound dysregulation of the autonomic and endocrine systems in psychiatric disorders. In our SHAP analysis, both cortisol reactivity and baseline HRV ranked among the top three predictors of clinical classification. This directly reflects the reality that psychological stress is inextricably linked to cognitive control and resilience. Consistent with previous research, perceived stress severely threatens psychological resilience, but this threat is serially mediated by an individual's cognitive control and cognitive flexibility (Bacıoğlu & Kocabıyık, 2025). For example, robust cognitive flexibility can effectively buffer against the negative impacts of school-related stress exposure (Harel et al., 2023) and significantly mediate the relationship between acculturation stress and general health in immigrant populations (Hasheminejad et al., 2024). Distress tolerance and cognitive flexibility also play a pivotal role in mediating emotional distress and existential anxiety among adolescent populations (Esmaeilnejad & Mazraeh, 2025).

The pervasive impact of stress on executive functioning is profoundly evident within family and social systems, providing critical context for our findings. Increased stress, such as the distress experienced by parents during the COVID-19 lockdowns, negatively distorts parental perceptions of their children's executive functioning (Polizzi et al., 2021). Furthermore, parenting stress is deeply interconnected with the quality of parenting, a relationship mediated by both parenting style and the inherent executive functioning of young children (Qian et al., 2024). Consequently, interventions that target executive functions yield systemic benefits. Providing executive function-based parenting training not only improves children's inhibitory control and cognitive flexibility (Ghasemi et al., 2022) but also effectively diminishes parenting stress, particularly in households managing neurodevelopmental challenges like autism spectrum disorder (Granmayeh et al., 2023).

The diagnostic classification success achieved in this study highlights the immense therapeutic potential of directly targeting cognitive flexibility and distress tolerance within clinical settings. Because cognitive flexibility was identified as a paramount feature distinguishing healthy individuals from those with psychiatric conditions, therapeutic modalities aimed at rehabilitating these domains are essential. Extant literature supports this approach; for instance, combining cognitive rehabilitation with transcranial electrical stimulation significantly improves

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behavioral inhibition and cognitive flexibility in children with ADHD (Arshadi et al., 2022), while cognitive empowerment protocols yield similar enhancements in emotional control for this population (Yavaribarha et al., 2022). Additionally, neurofeedback training has proven successful in rectifying executive and attentional deficits in students with learning disorders (Shari et al., 2021). Cognitive deficits also manifest in compulsive behavioral loops, mediating the pathology seen in binge eating disorder and food addiction (Iceta et al., 2021). Thus, intensive psychological interventions are required for severe psychopathology. Therapies such as Acceptance and Commitment Therapy (ACT) and Cognitive Behavioral Therapy (CBT) have proven vital for dismantling rigid referential thoughts and rebuilding cognitive flexibility and distress tolerance in patients with MDD (Yaqubi et al., 2026). These exact therapies similarly enhance resilience and distress tolerance in adolescents battling obsessive-compulsive disorder (Baniasadi et al., 2025). Positive psychotherapy also offers a robust mechanism for improving cognitive flexibility in individuals navigating profound life distress, such as divorced women (Khorasani, 2024). Finally, fostering cognitive flexibility through targeted mindfulness models serves as an essential protective strategy against burnout and psychological distress in demanding occupational environments, such as nursing (Parvaresh et al., 2024). By integrating physiological reactivity with cognitive performance, our machine-learning model reinforces the necessity of these multimodal, transdiagnostic clinical interventions.

5. Conclusion

This study demonstrates the superior utility of machine-learning algorithms in modeling the intricate, multi-dimensional relationships between cognitive flexibility, executive function, and psychophysiological stress reactivity across distinct clinical populations. By moving beyond traditional linear analyses, the XGBoost classification model successfully identified the Trail Making Test B-A difference score and cortisol reactivity as the most critical features for distinguishing individuals with Major Depressive Disorder, Generalized Anxiety Disorder, and Post-Traumatic Stress Disorder from healthy controls. The findings provide compelling empirical evidence that psychiatric vulnerabilities are heavily tethered to measurable deficits in cognitive adaptability and autonomic nervous system dysregulation. Ultimately, this research underscores the necessity of adopting holistic, multivariate approaches to psychiatric research, paving the way for more precise diagnostic profiling and an integrated understanding of how the mind and body jointly respond to psychological distress.

6. Limitations & Suggestions

Despite the robust findings, several limitations must be acknowledged. First, the cross-sectional design of the study precludes the ability to draw definitive causal inferences regarding the directionality between cognitive flexibility deficits, stress reactivity, and the onset of clinical psychopathology. It remains unclear whether neurocognitive inflexibility is a precursor to these disorders or a consequence of chronic psychiatric distress. Second, while the laboratory-based social-evaluative stress task provides a highly controlled environment to measure acute physiological reactivity, it may not adequately replicate the complex, multifaceted, and often chronic stressors individuals experience in their daily lives, potentially limiting the ecological validity of the physiological data. Furthermore, while the sample was diverse across diagnoses, it was restricted to specific urban metropolitan areas, which may limit the generalizability of the findings to rural populations or individuals from differing socioeconomic and cultural backgrounds.

Future research should prioritize longitudinal study designs to track the developmental trajectory of executive functions and psychophysiological reactivity across the lifespan, particularly observing how these variables interact before and after the onset of clinical symptoms. Incorporating ecological momentary assessment (EMA) and advanced wearable biosensors would allow researchers to continuously monitor heart rate variability and subjective stress in naturalistic, real-world environments, overcoming the limitations of artificial laboratory stressors. Additionally, future machine-learning models should aim to integrate an even broader array of biomarkers, such as neuroimaging data (fMRI or EEG) and genetic profiles, to construct highly comprehensive, multi-omics predictive models. Investigating the specific effects of various psychopharmacological and psychotherapeutic interventions on altering these machine-learning feature importances over time would also provide invaluable insights into mechanisms of treatment efficacy.

The findings from this study have direct implications for modern clinical practice and psychiatric assessment. Clinicians are strongly encouraged to move beyond reliance

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on purely subjective self-report questionnaires by routinely incorporating standardized behavioral measures of executive function and baseline autonomic metrics, such as heart rate variability, into standard psychiatric intake protocols. Because cognitive flexibility emerged as a dominant predictor of clinical psychopathology, transdiagnostic therapeutic approaches that explicitly target the enhancement of cognitive agility—such as Acceptance and Commitment Therapy and specialized cognitive remediation protocols—should be prioritized in treatment planning. Furthermore, mental health practitioners should conceptualize stress reactivity and neurocognition as inextricably linked domains, advocating for integrated treatment models that combine psychological therapies with physiological regulation techniques, such as biofeedback and structured mindfulness training, to build holistic patient resilience.

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Declaration of Interest

The authors of this article declared no conflict of interest.

Ethical Considerations

The study protocol adhered to the principles outlined in the Helsinki Declaration, which provides guidelines for ethical research involving human participants.

Transparency of Data

In accordance with the principles of transparency and open research, we declare that all data and materials used in this study are available upon request.

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Authors' Contributions

All authors equally contributed in this article.

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In order to correct and improve the academic writing of our paper, we have used the language model ChatGPT.

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