Explainable Machine Learning for Predicting 12-Month Relapse in Compulsory Drug Rehabilitation: A Multicenter Study

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Abstract: Relapse following compulsory drug rehabilitation remains a critical barrier to sustained recovery, yet routine discharge assessments often lack the prospective precision required for targeted interventions. This multicenter study developed an interpretable prediction framework using data from 4,697 individuals discharged from four rehabilitation centers in Eastern China (2018–2022). Four supervised machine learning models were evaluated via nested cross-validation. A transparent Logistic Regression model provided the most stable discrimination (AUC = 0.735) and calibration, outperforming complex ensemble algorithms. SHapley Additive exPlanations (SHAP) revealed that relapse risk was primarily driven by modifiable psychosocial factors—specifically elevated impulsivity, emotional dysregulation, and injection drug use history—while stronger family support consistently reduced relapse probability, regardless of addiction chronicity. These findings demonstrate the utility of explainable AI in facilitating risk stratification within resource-constrained correctional settings, promoting a shift from generalized supervision to personalized, evidence-based discharge planning.

Keywords: Substance Use Disorder; Relapse Prediction; Machine Learning; Logistic Regression; SHAP Analysis

1. Introduction

Relapse remains one of the most significant challenges in the treatment of substance use disorders (SUDs). Studies have shown that relapse rates within the first year after treatment range from 40% to 60%, with considerable variation depending on factors such as substance type, treatment setting, and follow-up intensity [1]. In China, research on compulsory rehabilitation centers has revealed a high rate of relapse within 12 months post-discharge, with up to 50% of participants re-entering treatment within a year [2]. These statistics highlight the need for more effective, personalized aftercare strategies, especially given the limited resources available in large-scale rehabilitation facilities. Standardized discharge plans are often insufficient to address the diverse relapse risks across individuals, underscoring the importance of tailored, data-driven intervention tools.

Relapse is influenced by a complex interplay of neurobiological, psychological, and social factors. Chronic substance use alters brain function, impairing executive control and enhancing reward pathways that are sensitive to drug-related stimuli [3]. Psychosocial stressors, such as emotional dysregulation, social isolation, and unstable employment, further increase vulnerability to relapse [4]. These multidimensional factors create intricate, nonlinear risk profiles that traditional models struggle to capture. Machine learning (ML) offers a promising solution to unravel these complex relationships, providing insights for developing more precise relapse prediction strategies [5].

Despite the growing interest in ML for relapse prediction, many existing studies are limited by small sample sizes or lack external validation [6]. Moreover, the "black-box" nature of many advanced ML models limits their clinical utility, as clinicians often require transparent, explainable insights to inform treatment decisions [7]. This study aims to bridge this gap by developing interpretable ML models to predict relapse among individuals in compulsory rehabilitation. By incorporating psychosocial factors such as impulsivity, emotional regulation, and family support, we aim to identify key risk predictors and enhance the individualized care process using SHapley Additive exPlanations (SHAP).

2. Literature Review

Relapse prediction in substance use disorder (SUD) rehabilitation has been a longstanding focus of research, with various methods developed to identify individuals at high risk for relapse. Traditional tools, such as the Addiction Severity Index (ASI), are widely used to assess severity across multiple domains, including medical, employment/social support, and family functioning, and have shown some prognostic value for treatment outcomes and relapse risk. However, the predictive power of ASI is often limited, especially in the areas of social support and employment status, which show moderate correlations with relapse outcomes [8]. These limitations underscore the need for more dynamic tools capable of incorporating a broader range of factors, including behavioral, emotional, and social aspects of recovery.

Recent advancements in machine learning (ML) have opened new avenues for relapse prediction by leveraging large datasets that incorporate diverse clinical and psychosocial factors. ML models have shown promise in various SUD risk prediction contexts. For instance, Alaa (2018) demonstrated that ML models, such as Bayesian optimization and random forests, outperform traditional statistical methods in predicting disease progression, though challenges such as small sample sizes, limited temporal validation, and generalizability remain [9]. Similarly, impulsivity, often measured by the Barratt Impulsiveness Scale (BIS-11), has been found to correlate strongly with relapse risk, as individuals with higher impulsivity scores are more likely to engage in risky behaviors that increase the likelihood of substance use [10].

Similarly, difficulties in emotion regulation, assessed by the Difficulties in Emotion Regulation Scale (DERS), have been identified as a transdiagnostic vulnerability factor for relapse in multiple substance use populations [11]. Incorporating explainable AI (XAI) into relapse prediction models has further enhanced their clinical applicability. SHapley Additive exPlanations (SHAP) have emerged as a powerful tool for interpreting ML models, enabling clinicians to understand the reasons behind a particular prediction. By quantifying feature contributions, SHAP allows for transparent analysis of relapse risk, making it possible to identify modifiable factors such as low family support or poor emotional regulation, which can then be targeted in individualized treatment plans [12]. The integration of SHAP with ML models has shown great promise in improving both predictive accuracy and interpretability, which is crucial for clinicians who need actionable insights to inform clinical decision-making.

However, challenges remain in the adoption of ML-based relapse prediction models in real-world clinical settings. The majority of current studies are limited by small sample sizes or lack of external validation, and the clinical integration of these models is still in its infancy [7]. To address these issues, future research must focus on large-scale, multicenter studies that validate the generalizability and effectiveness of ML models in diverse rehabilitation settings.

3. Methodology

3.1 Study Design and Setting

This multicenter, retrospective observational study aimed to investigate relapse risk among individuals undergoing compulsory drug rehabilitation at four prefecture-level centers in Eastern China. These centers, which are operated under the provincial justice bureau, provide court-mandated treatment for individuals with substance use disorders (SUDs). Located in both urban and semi-urban areas, each center admits approximately 900 to 1,500 individuals annually. The facilities include both male and female centers, treating a diverse range of primary drug use profiles, primarily narcotics and stimulants, thus offering a representative sample of rehabilitation contexts across the region.

3.2 Participant Selection

Participants were selected through a structured screening procedure. Out of 5,432 individuals initially assessed between January 2018 and December 2022, 4,697 met the inclusion criteria and had complete baseline and 12-month administrative outcome data. Key exclusion reasons included age outside the 18–55 years range (n = 247), severe psychiatric illness or neurological trauma (n = 162), missing baseline variables (n = 238), and incomplete 12-month outcome data (n = 88).

3.3 Inclusion/Exclusion Criteria

Inclusion criteria were: (1) age between 18 and 55 years; (2) DSM-5 diagnosis of substance use disorder; and (3) completion of baseline assessments, including psychosocial, behavioral, and clinical evaluations. Exclusion criteria were: (1) severe psychiatric illness or cognitive impairment; (2) history of major neurological trauma; or (3) inability to complete standardized assessments due to literacy or sensory limitations. Informed consent was waived in accordance with regulations, and all data were processed under strict confidentiality and access-control procedures.

3.4 Relapse Definition

Relapse was defined as documented re-entry into compulsory drug rehabilitation (recidivism) within 12 months after discharge, based on official administrative records. Participants meeting this criterion were coded as relapse = 1; all others were coded as relapse = 0. Follow-up contacts were made at 3, 6, and 12 months to collect supplementary behavioral information.

3.5 Participants and Variables

The final analytic cohort included 4,697 individuals, divided into relapse (n = 2,528; 53.8%) and non-relapse (n = 2,169; 46.2%) groups. Key predictor variables were categorized into four domains: demographics, health and social characteristics, substance use history, and psychosocial indicators.

Key psychosocial measures included: (1) Emotional dysregulation, assessed using the 18-item Difficulties in Emotion Regulation Scale (DERS-18) [11], where higher scores indicate greater dysregulation; (2) Impulsivity, measured with the Barratt Impulsiveness Scale (BIS-11) [10]; and (3) Family support, assessed using the Family Support Index (FSI).

3.6 Machine Learning Workflow

Data preprocessing excluded predictors with over 20% missing data. For the remaining variables, missing continuous values were imputed using iterative Bayesian ridge regression. Categorical variables were one-hot encoded, and variables were standardized (Z-score) within each cross-validation fold to prevent data leakage.

Four supervised algorithms were compared: Logistic Regression (LR), Random Forest (RF), XGBoost, and LightGBM. Hyperparameters were optimized via an inner fivefold cross-validation loop using Bayesian optimization with Optuna (v3.5).

3.7 Model Evaluation and Validation

Model performance was evaluated using a nested cross-validation (CV) framework (5-fold outer, 5-fold inner) with metrics including AUC-ROC, F1 score, sensitivity, specificity, and Brier score. Calibration was assessed via Platt sigmoid calibration and Brier scores.

3.8 Model Interpretability (SHAP Analysis)

To improve clinical application, SHapley Additive exPlanations (SHAP) were employed to attribute prediction variance to individual features [13]. Local and global analyses were conducted to interpret feature contributions and identify key risk factors.

3.9 Statistical Analysis

Descriptive statistics compared relapse vs. non-relapse groups using t-tests, Mann–Whitney U tests, or χ^2 tests as appropriate. All analyses were conducted in Python 3.10 (scikit-learn v1.3, SHAP v0.44.1, statsmodels v0.14), adhering to TRIPOD+AI reporting guidelines [14].

4. Results and Discussion

4.1 Descriptive Statistics of the Study Cohort

A total of 4,697 participants met all inclusion criteria and were included in the final analytic cohort. Among these, 2,528 (53.8%) experienced relapse (documented re-entry) within 12 months post-discharge, while 2,169 (46.2%) maintained abstinence. Baseline characteristics of the cohort, stratified by relapse status, are summarized in Table 1. Although there were statistically significant demographic differences, the absolute magnitude of the separation was modest. Participants who relapsed were slightly younger (median age: 38 vs. 40 years; $p < 0.001$) and had a younger age at first drug use (27 vs. 30 years; $p < 0.001$). In contrast, psychosocial and behavioral measures showed pronounced differences between the relapse and non-relapse groups. Individuals who relapsed had significantly lower Family Support Index (FSI) scores (45 [35–55] vs. 53 [43–62]; $p < 0.001$), higher impulsivity (BIS-11: 72 vs. 69; $p < 0.001$), and greater emotional dysregulation (DERS-18: 44 vs. 40; $p < 0.001$). Injection drug use was notably more prevalent among relapse cases (28.2% vs. 17.2%; $p < 0.001$), while stable employment was more common in those who maintained abstinence (30.9% vs. 24.5%; $p < 0.001$). No significant differences were observed for gender, smoking, alcohol use, BMI, or physical inactivity.

Table 1. Baseline Characteristics of Participants Stratified by Relapse Status (n = 4,697)

Variable	Overall, N = 4,697	Relapse Status		Statistic/Test	Effect size	p-value
		No n=2,169(46.2%)	Yes n=2,528(53.8%)			
Age (years)	38[32–45]	40[33–46]	38[32–44]	U=3,014,501.0	r=0.086	<0.001
Gender				χ^2=0.00	V=0.000	0.947
Female	1,019(21.7%)	472(21.8%)	547(21.6%)			
Male	3,678(78.3%)	1,697(78.2%)	1,981(78.4%)			
Smoking history (Yes)	2,831(60.3%)	1,298(59.8%)	1,533(60.6%)	χ^2=0.28	V=0.008	0.598
Alcohol use (Yes)	2,336(49.7%)	1,077(49.7%)	1,259(49.8%)	χ^2=0.01	V=0.001	0.943
BMI (kg/m²)	24.02±3.93	24.01±4.00	24.03±3.88	t=–0.11	d=0.003	0.916
Years of drug use	11[7–14]	10[6–13]	11[7–15]	U=2,355,096.5	r=0.122	<0.001
Age at first drug use	28[21–36]	30[23–37]	27[20–34]	U=3,136,949.0	r=0.124	<0.001
Route of administration (Injection)	1,087(23.1%)	374(17.2%)	713(28.2%)	χ^2=78.24	V=0.129	<0.001
Drug type				χ^2=0.98	V=0.014	0.613
Narcotics	1,996(42.5%)	927(42.7%)	1,069(42.3%)			
Stimulants	2,395(51.0%)	1,109(51.1%)	1,286(50.9%)			
Mixed	306(6.5%)	133(6.1%)	173(6.8%)			
Family Support Index (FSI)	49[38–59]	53[43–62]	45[35–55]	U=3,520,884.5	r=0.245	<0.001
BIS-11 (Impulsivity)	70[64–77]	69[62–75]	72[66–79]	U=2,133,604.5	r=0.191	<0.001
DERS-18 (Emotional Dysregulation)	42[35–49]	40[33–46]	44[37–51]	U=2,072,554.0	r=0.211	<0.001
Employment status				χ^2=25.04	V=0.073	<0.001
Unemployed	1,113(23.7%)	479(22.1%)	634(25.1%)			
Freelance	1,129(24.0%)	509(23.5%)	620(24.5%)			
Stable	1,291(27.5%)	671(30.9%)	620(24.5%)			
Other	1,164(24.8%)	510(23.5%)	654(25.9%)			
Physical inactivity (Yes)	1,888(40.2%)	874(40.3%)	1,014(40.1%)	χ^2=0.01	V=0.001	0.921

4.2 Model Performance

Model discrimination and calibration results are summarized in Table 2 and Figure 1,2. All four models demonstrated acceptable discrimination for 12-month relapse prediction, with AUC values ranging from 0.687 to 0.735. Logistic Regression (LR) demonstrated the best overall performance, achieving the highest mean AUC (0.735 ± 0.019) and F1 score (0.700), outperforming the more complex tree-based algorithms (Random Forest AUC = 0.716, XGBoost AUC = 0.697, LightGBM AUC = 0.687). Statistical comparison using the Friedman test confirmed significant differences in discrimination (*p* = 0.0018), with Nemenyi post-hoc tests ranking LR as the top model.

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Table 2. Model Performance Metrics (Mean ± SD across Outer 5-Fold Cross-Validation)

Model	AUC-ROC (SD)	F1	Sensitivity	Specificity	Brier(uncal)	Brier(cal)
Logistic Regression (LR)	0.735 (0.019)	0.700	0.715	0.617	0.208	0.208
Random Forest (RF)	0.716 (0.012)	0.689	0.702	0.610	0.214	0.213
XGBoost (XGB)	0.697 (0.009)	0.671	0.675	0.607	0.228	0.220
LightGBM (LGBM)	0.687 (0.009)	0.667	0.667	0.614	0.236	0.232

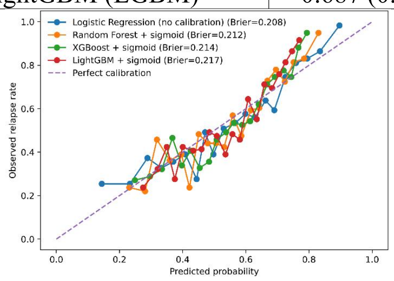

Figure 1. Receiver Operating Characteristic (ROC) Curves of Machine Learning Models for Relapse Prediction

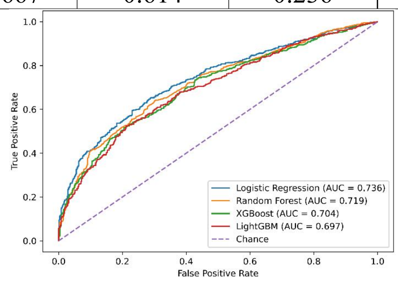

Figure 2. Calibration Plots after Platt Sigmoid Calibration

In terms of probability reliability, LR exhibited superior native calibration with a Brier score of 0.208, compared to the tree-based models, which required Platt sigmoid calibration to achieve comparable reliability (Figure 2). Using a conventional 0.50 probability threshold, the LR model achieved a sensitivity of 0.715 and a specificity of 0.617. In the context of correctional settings, this performance is favorable as it prioritizes the identification of high-risk individuals (higher true positive rate), supporting a "safety-first" approach to risk stratification.

4.3 SHAP-Based Interpretability

To enhance clinical interpretability, we analyzed the feature contributions of the LR model using SHapley Additive exPlanations (SHAP).

(1) Global Feature Importance: The global SHAP summary (Figure 3) revealed that relapse risk was primarily driven by modifiable psychosocial and behavioral factors rather than static demographics. Family support (FSI) exhibited the strongest negative SHAP contribution, indicating it as the most significant protective factor against relapse. In contrast, emotional dysregulation (DERS-18), impulsivity (BIS-11), and injection drug use emerged as dominant risk-enhancing factors.

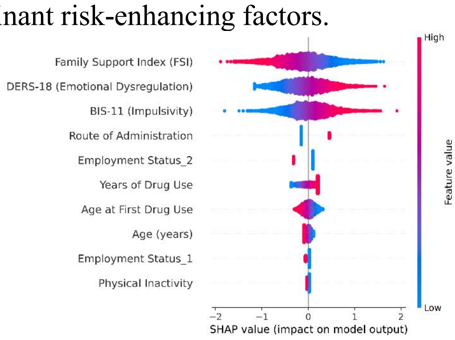

Figure 3. SHAP Summary Plot of Global Feature Importance (Top 10 Predictors, Logistic Regression Model)

(2) Individual Risk Attribution: SHAP waterfall plots (Figure 4) illustrated how the model individualized risk assessment. For a representative high-risk participant (predicted probability = 98.1%), relapse risk was primarily driven by low family support (+1.37 log-odds) and high impulsivity (+0.75). Conversely, a low-risk participant (predicted probability = 3.4%) was protected by robust family support (-0.45) and effective emotion regulation (-0.93).

(3) Additive Protective Effects: We further explored the relationship between addiction chronicity and family support using partial dependence analysis (Figure 5). Although relapse risk naturally increased with longer years of drug use, higher FSI levels consistently reduced this risk. Formal statistical testing revealed no significant multiplicative interaction (p = 0.982), supporting the hypothesis that family support provides a stable protective buffer across varying levels of addiction chronicity.

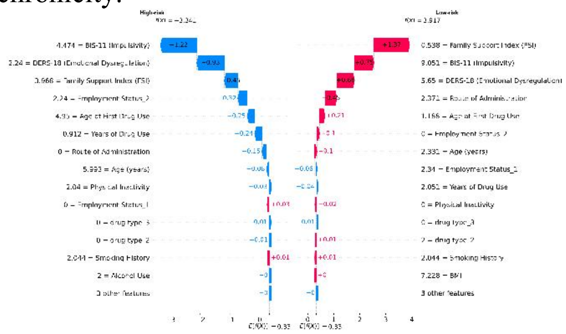

Figure 4. Local SHAP Waterfall Plots for Representative High-and Low-Risk Individuals

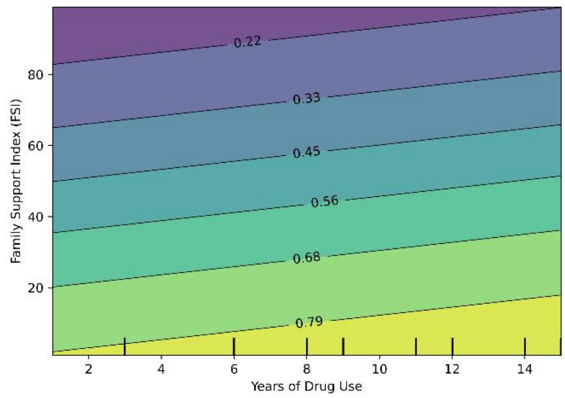

Figure 5. Partial-Dependence Surface of Years of Drug Use × Family Support Index (FSI) Demonstrating Additive Effects on Relapse Probability

5. Discussion

5.1 Principal Findings

This study identified key psychosocial and behavioral factors associated with relapse among individuals in compulsory drug rehabilitation. Our findings highlight that relapse vulnerability is more accurately predicted by modifiable factors such as impulsivity, emotional dysregulation, and family support, rather than basic demographic characteristics. The logistic regression (LR) model demonstrated stable discrimination (AUC = 0.735) and reliable calibration, confirming the utility of interpretable machine learning models in this setting.

Importantly, the LR–SHAP framework not only quantified relapse risk but also provided patient-level explanations, improving clinical interpretability. Elevated impulsivity and emotional dysregulation consistently correlated with relapse risk, aligning with existing literature suggesting that difficulties in emotion regulation are transdiagnostic vulnerabilities for relapse across substance types. Additionally, the protective role of family support was significant, with higher Family Support Index (FSI) scores correlating with lower relapse rates, and this relationship remained stable even for individuals with long drug-use histories.

5.2 Comparison with Previous Literature

Our results support a growing body of biopsychosocial literature suggesting that relapse vulnerability arises from a combination of cognitive-affective dyscontrol and insufficient social-contextual support. This is consistent with prior studies where impulsivity and emotion dysregulation were identified as strong predictors of relapse [6]. The inverse relationship between family support and relapse risk further corroborates findings from Chinese and Vietnamese cohorts, where family functioning significantly impacts relapse outcomes [15].

Methodologically, our findings demonstrate that the interpretable LR model performs comparably to more complex algorithms like Random Forest and XGBoost, which is consistent with previous studies advocating for the use of transparent models in clinical settings. The ability to communicate risk through interpretable models supports the ethical deployment of AI tools in correctional settings, facilitating practical and informed decision-making by clinicians [16].

5.3 Clinical and Policy Implications

The study's findings have direct implications for compulsory drug rehabilitation systems. Incorporating brief psychosocial screenings into routine intake and discharge workflows can support personalized, risk-stratified care planning. High-risk individuals, particularly those with elevated impulsivity or low emotional regulation, could benefit from interventions like Mindfulness-Based Relapse Prevention (MBRP) or Dialectical Behavior Therapy (DBT) [17]. Additionally, strengthening family support during discharge planning can provide a stable protective buffer, even among those with long histories of substance use.

From an operational perspective, risk scores derived from ML models can facilitate stepped care approaches, allowing for more efficient allocation of resources. Correctional systems can prioritize intensive monitoring for high-risk individuals while offering maintenance support for lower-risk cases, improving the overall efficiency of service delivery in resource-constrained settings.

5.4 Mechanistic Interpretation

Our study aligns with contemporary neurobehavioral models of addiction, which emphasize impaired executive regulation and heightened incentive salience as key contributors to relapse susceptibility. The significant role of impulsivity and emotional dysregulation in relapse prediction supports this view, suggesting that deficits in self-regulation increase vulnerability to drug-related cues and stressors. Additionally, the protective influence of family support underscores the importance of social resources in buffering these vulnerabilities [18].

5.5 Strengths and Limitations

This study adheres to best-practice guidelines for clinical prediction modeling, including the use of nested cross-validation and explicit calibration. However, several limitations exist. The study's cohort was confined to Eastern China, limiting generalizability to other settings. Moreover, relapse was defined as re-entry into rehabilitation, which may underestimate the prevalence of relapse events not captured by official records. Finally, the self-reported nature of some psychosocial predictors introduces potential measurement biases.

5.6 Future Directions

Future research should focus on validating this model through longitudinal studies and ecological momentary assessments (EMA), enabling dynamic, real-time risk stratification. Integrating multimodal data, such as text and sensor data, could further enhance the mechanistic understanding of relapse. Additionally, translating predictive models into Just-in-Time Adaptive Interventions (JITAIs) represents an exciting frontier for mobile health tools.

6. Conclusion

This multicenter study demonstrates the feasibility and clinical utility of an interpretable machine learning framework for predicting 12-month relapse (recidivism) following compulsory drug rehabilitation in Eastern China. By utilizing routinely collected psychosocial and behavioral data, we found that a transparent Logistic Regression model provided robust discrimination (AUC = 0.735) and superior calibration compared to more complex "black-box" algorithms. SHAP-based explanations revealed that relapse risk was primarily driven by modifiable psychosocial and behavioral factors. Specifically, deficits in emotional regulation and impulsivity were identified as key risk factors, while strong family support emerged as a consistent protective buffer against relapse.

These findings support a paradigm shift in correctional practice from generalized supervision to a more personalized, risk-stratified, and mechanism-informed approach to aftercare. We recommend integrating brief, validated screenings for emotional regulation and social support into routine discharge planning, enabling more targeted allocation of resources. By identifying individuals at high risk of relapse, tailored interventions can be provided, thus improving treatment outcomes and optimizing resource utilization in correctional settings.

Moving forward, the translation of these analytic prototypes into trustworthy clinical decision support tools will require rigorous external validation, continuous fairness auditing, and the incorporation of human oversight to ensure ethical deployment in justice-administered settings. Future efforts should focus on enhancing the real-time applicability of these models while ensuring their ethical, transparent, and equitable use in rehabilitation contexts.

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