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AN EXPLAINABLE MACHINE LEARNING FRAMEWORK FOR EARLY DRUG-ABUSE RISK ASSESSMENT AND STRATIFICATION

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ABSTRACT

Drug abuse and substance use disorders are major public-health concerns that require effective approaches for the early identification of elevated risk and for preventive intervention. Existing risk-assessment approaches often rely on single risk factors, specific populations, clinical evaluations, or isolated psychological and behavioral indicators and they frequently lack interpretable, multidimensional risk stratification. This study addresses this gap by proposing an explainable machine-learning framework that integrates psychological, behavioural, social, familial, lifestyle, academic/work, and exposure-related predictors for early drug-abuse risk assessment. The dataset comprises approximately 5,000 observations; following data-quality review, leakage assessment, and feature selection, 35 multidimensional predictors were retained. Six supervised machine-learning algorithms, namely Logistic Regression, Decision Tree, Random Forest, Support Vector Machine, XGBoost, and LightGBM, were compared for three-level risk classification into Low, Moderate, and High Risk, using leakage-aware feature selection, pipeline-based preprocessing, and an 80:20 train-test split. SHAP-based explainability was applied to identify which variables contributed to model predictions. In the held-out evaluation, Logistic Regression achieved the highest accuracy (70.5%), Macro F1-score (70.0%), and ROC-AUC (0.863) and was selected as the final model. The framework is intended to support early identification of elevated risk among individuals assessed at a given time, including those who may already have a history of substance exposure, rather than to predict first exposure or to provide a clinical diagnosis. SHAP findings are presented as model-based feature attribution, not as causal evidence. The results provide a basis for external validation, fairness and calibration analysis, longitudinal evaluation, and responsible deployment in drug-abuse prevention and public-health settings.

Keywords: Drug Abuse, Risk Assessment, Early Warning System, Machine Learning, Explainable AI, Risk Stratification.

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1. INTRODUCTION

Substance and drug abuse represent multidimensional public-health problems shaped by the interaction of psychological, behavioural, social, familial, lifestyle, academic/work, and exposure-related factors. Because elevated risk rarely arises from a single cause, early preventive action requires assessment approaches that combine information across these domains rather than relying on isolated indicators. Prior work reviewed in this paper has identified risk and protective factors spanning individual, family, peer, and community levels [11, 12], and structured screening instruments have been validated for assessing such factors in adolescent populations [13]. This evidence motivates a multidimensional view of drug-abuse risk.

Machine-learning methods are well suited to this problem because they can identify patterns across multiple interacting predictors that are difficult to evaluate consistently through manual assessment alone. Previous studies have used a range of algorithms to predict substance-use risk from demographic, psychological, and behavioural variables [1-7], and comparative evaluations have shown that performance depends on the dataset, predictor set, and population studied rather than on any single universally optimal method [3, 8, 9]. Machine learning therefore provides a practical tool for structuring multidimensional information into a risk-assessment output.

Nevertheless, existing approaches present several limitations. Many studies rely on predictors from a single domain, focus on a binary outcome or a single substance, target restricted age groups, or are validated on a narrowly defined dataset [1-9]. In addition, models that return only a risk label without an explanation may be difficult for educators, counsellors, and public-health stakeholders to interpret and use responsibly. The absence of an interpretable, multidimensional, and validated risk-stratification framework remains a clear gap [8, 11-13].

Explainable Artificial Intelligence (XAI), and in particular SHapley Additive exPlanations (SHAP) [10], addresses part of this gap by assigning feature-attribution values to individual model predictions. Global SHAP analyses summarize which variables most influence predictions across the dataset, while local explanations show how features contribute to a specific prediction. Interpretability of this kind matters because it helps stakeholders understand which variables contribute to a risk assessment; it does not establish causal relationships.

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Building on the reviewed literature, the present study addresses the research gap of combining multidimensional psychosocial predictors with three-level risk stratification and model explanations. Specifically, most prior work has evaluated a narrow set of predictors or a binary outcome, whereas the proposed framework integrates psychological, behavioural, social,

familial, lifestyle, academic/work, and exposure-related variables into a single interpretable classification pipeline [8, 11-13].

The proposed framework comprises leakage-aware feature selection, pipeline-based preprocessing, comparative evaluation of six supervised machine-learning models (Logistic Regression, Decision Tree, Random Forest, Support Vector Machine, XGBoost, and LightGBM), three-level risk classification into Low, Moderate, and High Risk, and SHAP-based interpretation. The framework was evaluated on a held-out test set using an 80:20 train-test split; the reported results are specific to this dataset and require external validation before deployment.

Throughout this paper, early risk refers to early identification of elevated risk among individuals assessed at a given time, including individuals who may already have a history of substance exposure, and not to prediction of first exposure before any substance use has occurred. Because Previous Substance Exposure is included as a predictor, the framework is positioned as an early risk-assessment and decision-support tool rather than a pre-exposure prediction model. The remainder of this paper is organized as follows: Section 2 reviews related work, Section 3 describes the methodology, Section 4 presents the results, Section 5 discusses the findings and Section 6 concludes with future enhancements.

2. RELATED WORK

2.1 Machine learning for substance-use risk assessment

Earlier machine-learning studies explored whether demographic, psychological, and behavioural variables can help classify students and adolescents as ones who might be at elevated risk of substance abuse. Bulut and Bucak developed a system to identify such students who may benefit from preventive support [1]. Nath, Kilam, and Swetapadma applied artificial neural networks to predict volatile-substance abuse using demographic and personality variables [2]. These early works have shown that machine-learning techniques can identify patterns that could indicate a substance-use vulnerability and assist in preventive assessment.

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Subsequent studies examined algorithm comparison and the inclusion of diverse predictors. Qiao et al. compared Random Forest, XGBoost, and LightGBM for the purpose of predicting potential central-stimulant use and estimating the time-since-last-use [3]. Their analysis shows the value of exploring different algorithms and the informative nature of features. Jing et al. used longitudinal psychological, health, and contextual data to discover substance-use risk factors and reported variations in indicators of relevance in distinct developmental stages [4]. Han et al. evaluated relevant machine-learning models for predicting opioid misuse among adolescents and noted the need for precision and recall given the low prevalence of positive outcomes [5]. Wadekar incorporated individual and environmental influences in a psychosocial framework [6]. Islam et al. explored socioeconomic and environmental predictors and identified that logistic regression was superior after reducing the dimensionality of features [7].

More recent studies have examined the prediction of substance-use outcomes across distinct populations and settings. A multinational adolescent study used cohort-specific analyses as well as SHapley Additive exPlanations (SHAP) to explore model performance and influential features while emphasizing the need for external validation [8]. A Finnish survey compared traditional machine-learning and deep-learning approaches and reported the presence of differing feature importance across substances [9]. Overall, these works illustrate that the performance of models and the identification of influential features depend on the population, the substance-use outcome, how features are represented, and how models are evaluated. They also suggest the need for transparency in model interpretation and appropriate validation procedures.

In addition, research on substance-use risk factors explores the role of multiple individual and contextual dimensions. A systematic review of adolescent drug abuse identified risk and protective factors with a focus on individual, family, peer, and community factors [11]. Similarly, Brook et al. identified risk and protective factors that influence different stages of substance-use development [12]. The EU-Dap questionnaire has been validated for assessing relevant risk and protective factors among early adolescents in Chile [13]. Overall, these studies provide valuable insights about psychological, behavioural, familial, social, and environmental indicators relevant for substance-use risk assessment.

Recent works have examined different outcomes across distinct populations. Some analyses have explored the prediction of substance-use outcomes among children and adolescents [14]

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or the factors associated with early-adult substance-use initiation [15]. Others have focused on the prediction of individual risk for cannabis-use disorder using Bayesian machine learning [16]. While these works have focused on different prediction goals, they illustrate the range of applications of machine learning in the domain of substance use. However, their analysis must be considered in conjunction with the targeted outcome, available features, study population, and evaluation strategy.

While these studies illustrate the potential of machine learning for analysing and predicting substance-use risk, the comparison and interpretation of findings rely on the presence of clearly defined outcomes or validation strategies, as well as an understanding of how individual studies have identified risk factors. This work contributes to this line of research by examining three-class operational risk stratification into Low Risk, Moderate Risk, and High Risk categories based on multiple psychosocial, behavioural, social, familial, lifestyle, and exposure-related predictors subject to the final set of features chosen for constructing models. The analysis makes use of supervised classification and SHAP-based interpretation to examine model predictions and the contribution of features. The assigned categories constitute operational labels for the purpose of classification, and should not be considered as a diagnosis or a confirmed prediction of future substance-use disorder.

This work is thus devoted to explainable, multidimensional machine-learning risk stratification, and does not examine models for EEG-based detection, laboratory drug testing, wearable sensing, recovery monitoring, or other measurement or intervention-related goals [17], [18]. The following section discusses Explainable Artificial Intelligence and the importance of the SHAP approach in interpreting machine-learning predictions.

2.2 Explainable Artificial Intelligence

SHAP provides a framework for explaining model predictions by assigning feature-attribution values to individual observations [10]. Global SHAP analyses summarize the variables that most influence predictions across the dataset, whereas local explanations show how features contribute to a specific prediction. In the present study, explainability is used to improve transparency and support interpretation of model behaviour; it is not used to establish causal relationships.

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2.3 Research gap and Objective

Existing research indicates that machine learning can support substance-use prediction, but many studies use binary outcomes, focus on a single substance, target restricted age groups, or rely on narrowly defined datasets. The present study addresses these limitations by combining multidimensional predictors, three-level risk categorization and model explanations. The objective is to determine whether an interpretable machine-learning framework can integrate psychological, behavioural, social, familial, lifestyle, school/work, and exposure-related information to produce Low, Moderate, or High drug-abuse risk classifications.

3. METHODOLOGY

3.1 Study Design

The dataset contains approximately 5,000 records and 87 raw columns. The target variable, Drug_Abuse_Risk, has three operational classes: Low Risk (2,000 observations), Moderate Risk (1,500) and High Risk (1,500). After data-quality review, leakage assessment and feature selection, 35 predictors were retained for the final workflow.

The predictors span several risk domains. Psychological variables include depression, anxiety, stress, psychological distress, impulsivity, self-esteem, emotional regulation, hopelessness, loneliness and self-control. Social and peer variables include peer influence, peer substance exposure, social isolation, social support and social pressure. Family variables include family conflict, family support and family stability. Behavioural variables include general behavioural problems, decision-making control, intention to use substances, attitude towards substance use and school or work absenteeism. Lifestyle, academic and work variables include sleep duration and quality, screen time, night-time device usage, academic performance, academic or work-related stress, workload, job satisfaction, financial stress and previous substance exposure.

3.2 Dataset

The dataset has about 5,000 records and 87 raw columns. The main outcome variable, Drug_Abuse_Risk, has three categories: Low Risk (2,000 cases), Moderate Risk (1,500), and High Risk (1,500). After reviewing data quality, checking for leakage, and trimming features, 35 predictors made it into the final workflow.

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These features cover a wide range of risk areas. On the psychological side, you've got things like depression, anxiety, stress, distress, impulsivity, self-esteem, emotional regulation, hopelessness, loneliness, and self-control. Social and peer factors include things like peer influence, exposure to substances through peers, social isolation, social support, and social pressure. For family, there's conflict, support, and stability. Behavioral predictors look at things like general behavioral problems, issues with decision-making, intent to use substances, attitudes about use, and missing school or work. On the lifestyle and academic/work front, the model considers sleep (how long, how well), screen time, using devices at night, academic performance, academic or work-related stress, workload, satisfaction with work, financial stress, and prior substance exposure.

3.3 Leakage-aware feature selection

Feature selection was based on domain knowledge, descriptive statistics, correlation analysis, redundancy assessment, missingness patterns, model-based importance and interpretability considerations. To reduce target leakage, predictors that could directly reveal an established problem were excluded, including craving, withdrawal symptoms, use frequency, rehabilitation history and multiple-substance exposure. Age_First_Substance_Exposure was also excluded because it had substantial missingness and because the missingness pattern was directly associated with whether an individual had ever used substances.

Accordingly, the final feature set was intended to support early identification of elevated risk rather than prediction before initial substance exposure. Previous Substance Exposure was retained as a predictor; therefore, the framework is applicable to individuals who may have exposure histories and should not be described as a pre-exposure prediction model.

3.4 Data preprocessing

For numeric data missing values, we filled in with the median; for missing categories, we used the mode. All numeric features were scaled to a standard range (using StandardScaler), and categorical ones got one-hot encoded. All preprocessing happened inside a pipeline, so whether the system was in training or live deployment, it always treated new data the same way, preventing weird mismatches between what the model learned and what it sees in practice.

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3.5 Train-test split and candidate models

The dataset was divided into 4,000 training observations and 1,000 held-out test observations, corresponding to an 80:20 split. All fitting, preprocessing, cross-validation and hyperparameter tuning were performed on the training set; the test set was reserved exclusively for final performance estimation on unseen observations.

Six supervised algorithms were evaluated: Logistic Regression, Decision Tree, Random Forest, Support Vector Machine, XGBoost and LightGBM. This set represents linear, tree-based, ensemble, margin-based and gradient-boosting approaches. Hyperparameter tuning was conducted on the training data; the exact search method and parameter grid are marked for verification in Section 8 parameter ranges and scoring metric]. The cross-validation procedure and number of folds are also marked for verification .The random state is marked for verification .A class-balancing method is not separately documented; because the target classes are approximately balanced (40:30:30), training proceeded on the original class distribution. Macro F1-score was used for model selection because it weights the three risk classes equally.

3.6 Evaluation Metrics

We looked at accuracy, Macro F1-score, and ROC-AUC. Accuracy is just the raw percent correct, but Macro F1 means we balance things out so each class (Low, Moderate, High) gets equal attention. Precision and recall explain how well positive predictions match reality and how many real positives the model catches. F1 is their balance point. Macro F1 means calculating F1 for each class, then averaging the scores so the majorities don’t crowd out the minorities. ROC-AUC gives a big-picture view across thresholds, but it’s no replacement for class-level details.

3.7 Explainability and Application deployment

For interpretability, SHAP analysis was applied to identify which variables influenced the final model output. SHAP values indicate how feature values contribute to a model prediction for a given observation; they describe model behaviour and do not establish causal relationships.

The trained preprocessing and prediction pipeline was serialized and integrated into a Streamlit application. The application accepts the 35 required predictor inputs, applies the saved preprocessing operations, produces a Low, Moderate, or High Risk classification together with class probabilities and presents explanatory information about the factors that contributed to

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the prediction. Additional pages display model performance, feature importance and model details.

4. RESULTS

4.1 Comparative model performance

Table 1 summarizes the reported test-set performance of the six candidate models. Logistic Regression achieved the highest Accuracy and Macro F1-score and was selected as the final model under the study's primary evaluation criterion. Its ROC-AUC was also the highest among the reported models. The corresponding model-comparison charts and detailed metrics report are presented in Figures 1–5.

Table 1. Test-set comparison of candidate models.

Model	Accuracy	Macro F1	ROC-AUC
Logistic Regression	70.5%	70.0%	0.863
Support Vector Machine	69.9%	68.7%	0.862
Random Forest	68.2%	67.2%	0.847
XGBoost	67.7%	65.8%	0.853
LightGBM	67.6%	65.9%	0.842
Decision Tree	57.9%	57.6%	0.704

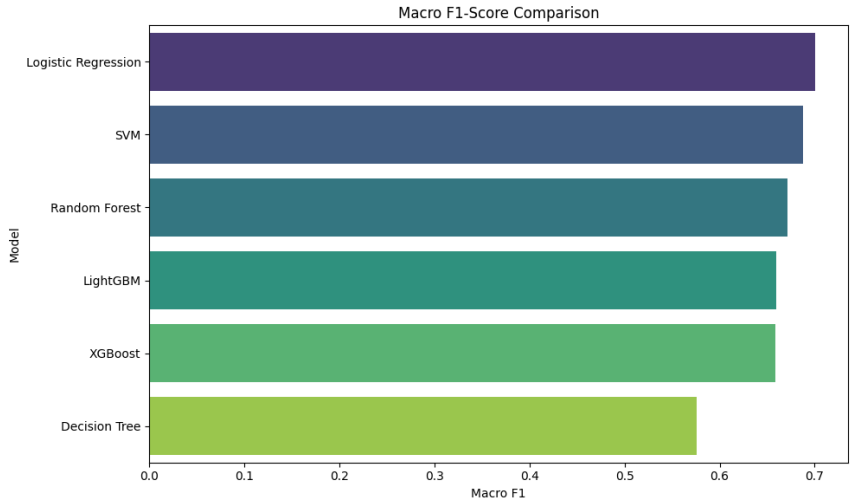


Figure 1. Macro F1-score comparison of the six candidate models.

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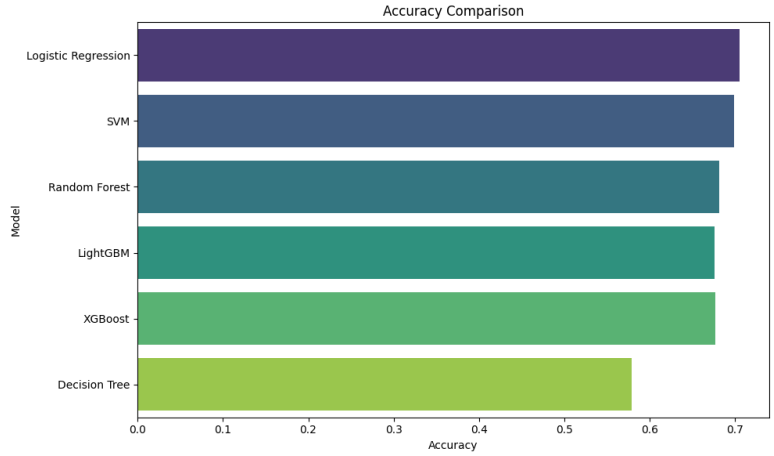


Figure 2. Overall accuracy comparison of the six candidate models.

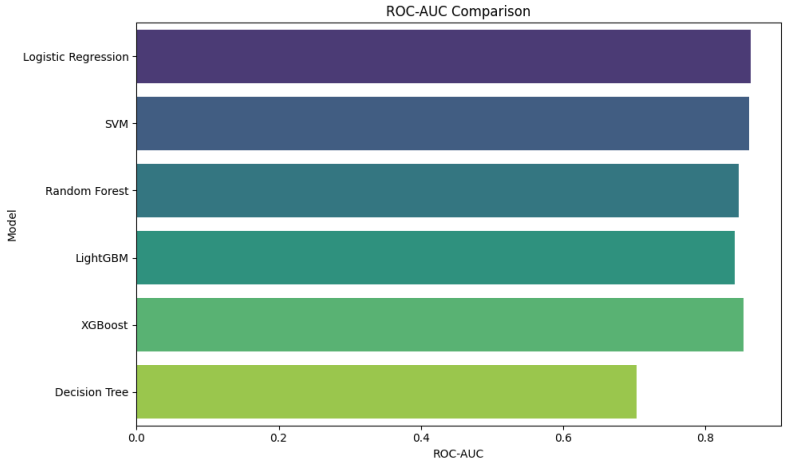


Figure 3. Multiclass ROC-AUC comparison of the six candidate models.

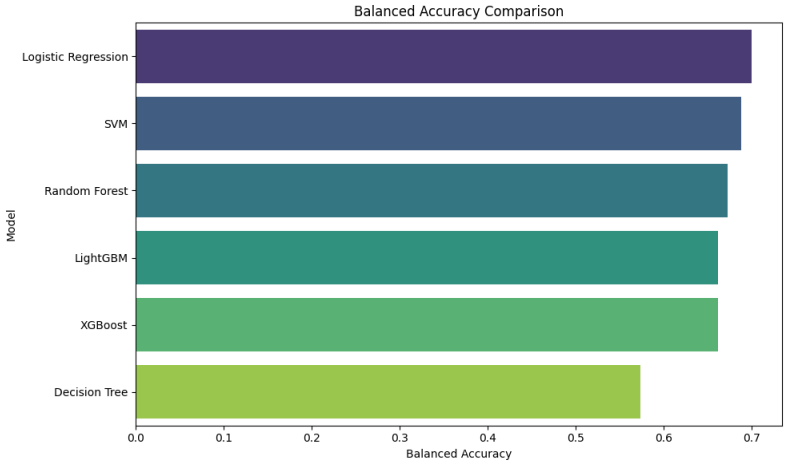


Figure 4. Balanced accuracy comparison of the six candidate models.

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Model	Accuracy	Macro Precision	Macro Recall	Macro F1	Balanced Accuracy	ROC-AUC	Training Time	Prediction Time
Logistic Regression	0.7050	0.7030	0.6994	0.7001	0.6994	0.8631	0.0525	0.0080
SVM	0.6990	0.6873	0.6878	0.6875	0.6878	0.8619	3.3507	0.1014
Random Forest	0.6820	0.6710	0.6725	0.6717	0.6725	0.8471	0.9548	0.0531
LightGBM	0.6760	0.6582	0.6619	0.6593	0.6619	0.8415	0.1411	0.0150
XGBoost	0.6770	0.6578	0.6614	0.6584	0.6614	0.8535	0.2096	0.0130
Decision Tree	0.5790	0.5831	0.5739	0.5762	0.5739	0.7037	0.0531	0.0080

Figure 5. Detailed held-out test-set metrics report including precision, recall, Macro F1, balanced accuracy, ROC-AUC and training/prediction times.

4.2 Confusion Matrix Analysis

To examine class-specific performance, multiclass confusion matrices were calculated for the 1,000 test observations. They show correct and incorrect classifications for the High, Low and Moderate Risk categories. For Logistic Regression, 6 of 300 High-Risk cases were classified as Low Risk (2.0%) and 8 of 400 Low-Risk cases were classified as High Risk (2.0%). Because these errors may be operationally important in a screening context, they warrant attention when defining review thresholds. However, the confusion matrices do not establish clinical consequences; the results should therefore be interpreted as model-classification errors rather than demonstrated clinical harm. Most errors occurred between adjacent risk levels. Tree-based models identified Low Risk cases more effectively but produced more errors in the Moderate Risk class, whereas the Decision Tree distributed errors more broadly.

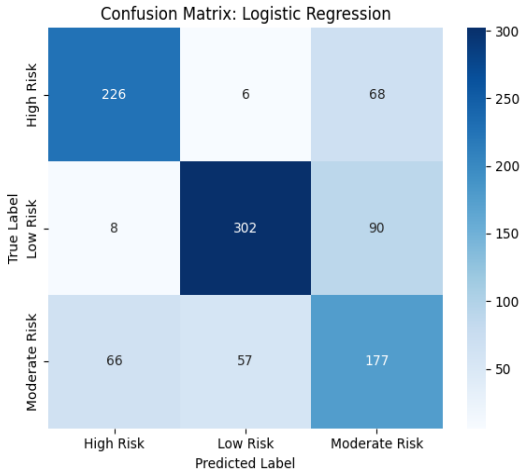


Figure 6. Confusion matrix of Logistic Regression (final model).

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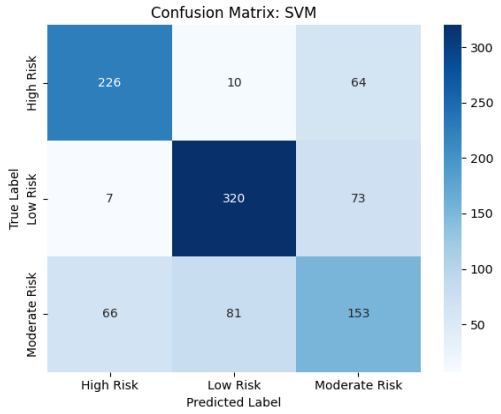


Figure 7. Confusion matrix of Support Vector Machine.

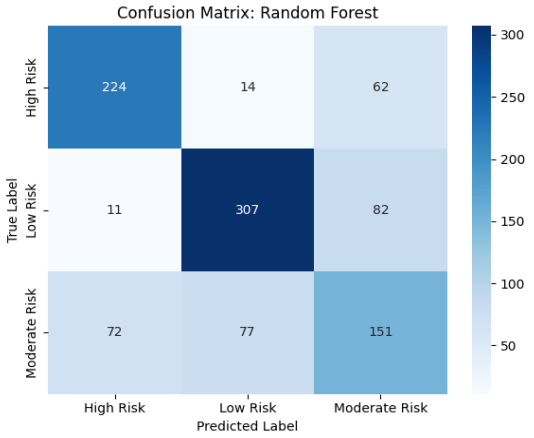


Figure 8. Confusion matrix of Random Forest.

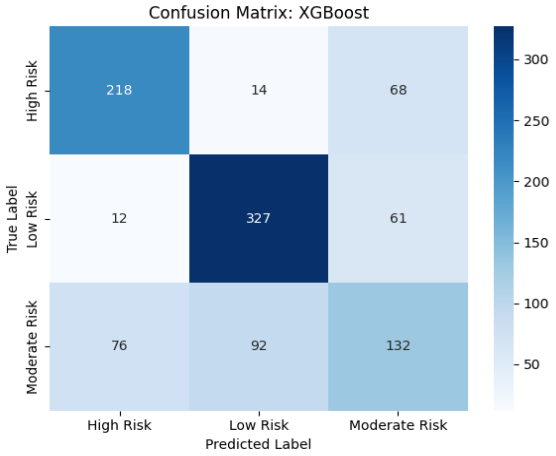


Figure 9. Confusion matrix of XGBoost.

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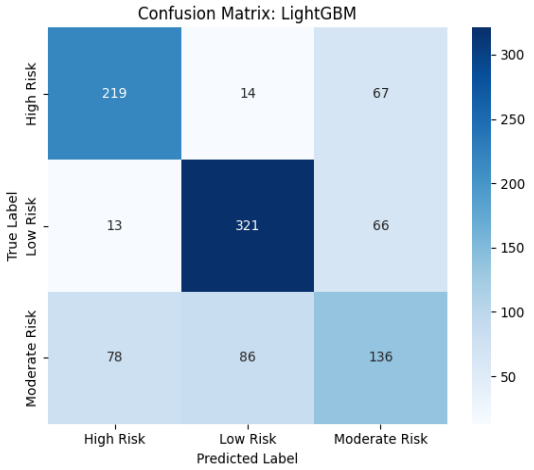


Figure 10. Confusion matrix of LightGBM.

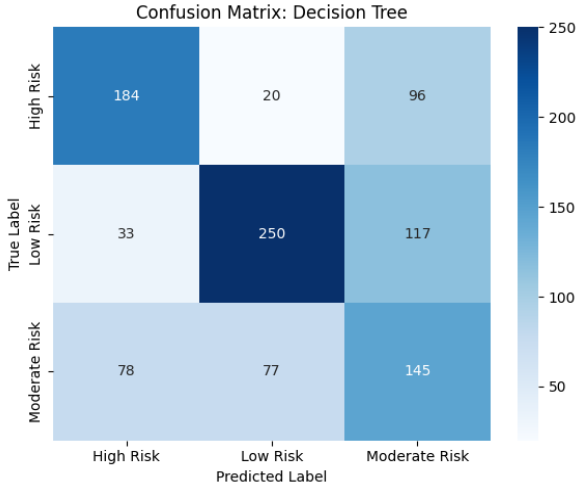


Figure 11. Confusion matrix of Decision Tree.

4.3 Selected model and interpretation of performance

Logistic Regression was selected because it achieved the highest Macro F1-score, accuracy and ROC-AUC in this evaluation. This selection is specific to the present dataset, predictor set and operational target; it does not imply that Logistic Regression consistently outperforms tree-based ensembles or gradient-boosting methods. Under these conditions, the simpler model performed better on the held-out test set than the more complex alternatives

4.4 SHAP-based feature contributions

SHAP analysis identified the following among the most influential features in the model predictions: Previous Substance Exposure, Peer Substance Exposure, Depression Score, Stress

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Level, Impulsivity, Psychological Distress, Anxiety Level, Peer Influence, Family Conflict and Social Isolation. These features represent history, psychological, social and familial dimensions of risk. SHAP values indicate how feature values contribute to a model prediction for a given observation; they do not demonstrate that the features directly cause substance abuse or replace professional judgment

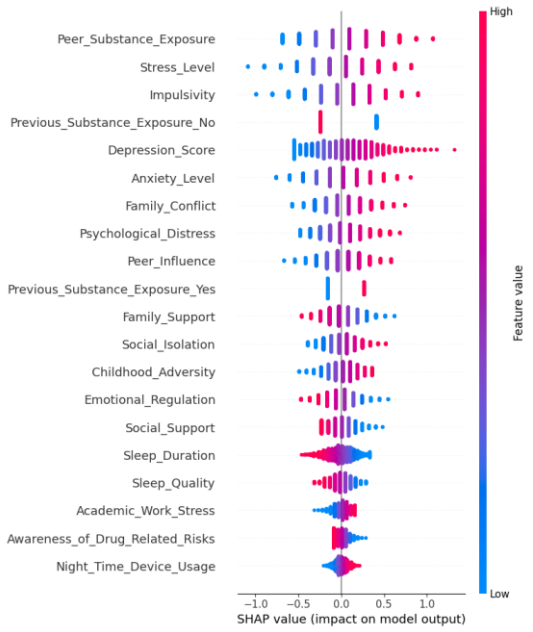


Figure 12. Global SHAP beeswarm summary plot showing the impact of influential features on the risk-assessment output.

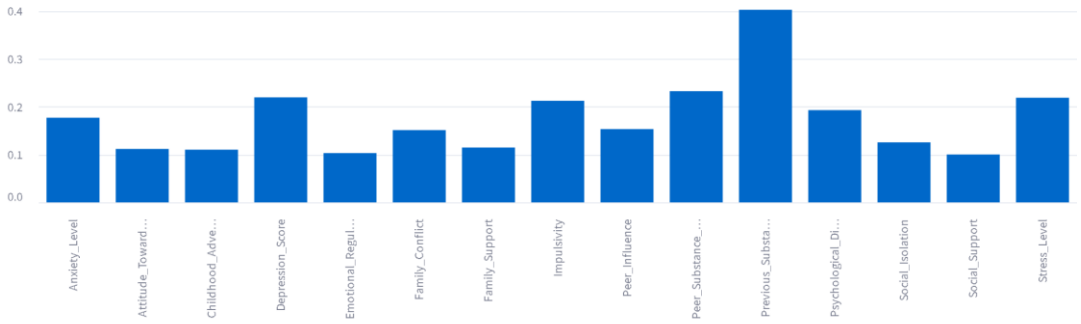


Figure 13. Top 15 most influential features ranked by mean absolute SHAP value.

4.5 Application Workflow

The application workflow is as follows: a user enters the 35 predictor values, the system constructs a DataFrame, applies the saved preprocessing pipeline and passes the transformed data to Logistic Regression. The model returns class probabilities and a Low, Moderate, or

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High Risk classification, together with an explanation of the prediction. The application is therefore a user-facing implementation of the evaluated model and should be regarded as a decision-support interface rather than a clinical decision system.

5. DISCUSSION

Comparison of the candidate models shows that model complexity alone did not determine performance. Logistic Regression achieved the strongest Macro F1-score in this evaluation, while the other models provided useful benchmarks. This result is consistent with the broader literature, in which performance varies according to the dataset, predictor set, study population and operational definition of the outcome.

The feature design is a central aspect of the framework. It integrates psychological distress, impulsivity, family and peer conditions, social isolation, previous exposure and lifestyle variables. This structure is consistent with research indicating that substance-use risk reflects the interaction of individual, familial and environmental factors rather than a single determinant. The framework incorporates these domains within a unified prediction and explanation pipeline.

A three-level target provides greater resolution than a binary outcome by distinguishing Low, Moderate and High Risk categories. These operational categories may help prioritize preventive attention, but they are not guarantees of future substance-use disorder or addiction. The framework is intended to support early awareness, structured discussion, prevention planning and referral decisions rather than to determine an individual’s clinical future.

The explainability component provides information about the variables associated with each risk prediction and may improve the interpretability of the system. SHAP summarizes both global patterns and local contributions. Nevertheless, these explanations describe model behaviour, may reflect artefacts of the data and should not be interpreted as clinical advice or evidence of causation.

Reliable machine-learning research also requires transparent reporting and systematic assessment of methodological limitations. The TRIPOD+AI reporting guideline provides recommendations for reporting prediction models developed using regression or artificial intelligence methods [17]. PROBAST+AI provides a framework for assessing the quality, risk of bias, and applicability of such prediction models [18]. These resources are relevant to future

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evaluation of the proposed framework, particularly with respect to data selection, predictor definition, model validation, and applicability to populations beyond the development dataset. The present results should therefore be regarded as an initial evaluation rather than evidence of clinical validity or generalizability.

6. CONCLUSION AND FUTURE ENHANCEMENTS

This study developed an explainable machine learning framework to classify individuals at risk of drug abuse, into Low, Moderate or High Risk groups. From the six different classifiers used, the Logistic Regression model achieved the best results with an accuracy of 70.5%, Macro F1 score of 70.0% and a ROC-AUC of 0.863. Key variables identified from the SHAP analysis include previous exposure to substances, peer pressure, psychological issues, depression and stress. While the framework provides greater clarity to the model, it does not identify causality or provide any diagnosis. Overall, this provides some initial evidence that can be used to increase risk awareness and make informed decisions for prevention.

The next steps to this project will be to externally validate the framework using larger and more varied sets of data. This will aim to improve calibration of probabilities, evaluate fairness between different groups of people in the population and investigate other models and ways of feature selection. Further studies will also look to investigate stability of explanations, data security and how applicable the model is to real world scenarios. This can help provide a more reliable and responsible framework for assessing individuals at risk of drug abuse.

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