

# Using Machine Learning To Identify Drug Usage Patterns

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**Abstract.** The escalating prevalence of substance misuse requires robust analytical tools to identify underlying usage patterns and trends, facilitating effective policy interventions and public health strategies. This study uses data sets from the National Survey on Drug Use and Health (NSDUH)(2002-2018) to explore drug use patterns using machine learning techniques. A systematic methodology was used, including data pre-processing, feature selection, and the application of advanced supervised and unsupervised learning algorithms to analyze the data set. Key techniques included balancing class distributions with hybrid sampling methods(RandomUnderSampler and SMOTE) and optimizing classifiers such as Random Forest, Support Vector Machine, and XGBoost through grid search. The results demonstrated high predictive accuracy with Random Forest and XGBoost achieving 83% accuracy, while clustering methods such as k-means provided additional insight into group-specific behaviors. The analysis found that demographic factors and drug use patterns were closely related, this way the public health professionals can be given accurate and valuable data. This study shows that machine learning is an important tool in public health, thus, it makes data-driven decisions and directs health interventions to the targeted population.

**Key words:** Machine Learning, Drug Usage Patterns, National Survey on Drug Use and Health, Supervised Learning, Clustering, Public Health, Feature Selection

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## 1. Introduction

Substance misuse continues to pose a significant public health challenge world-wide, with far reaching consequences that affect individuals, families and communities alike. Its impact is not limited to physical health but extends to mental health, social stability, and economic productivity(1). The factors contributing to substance misuse are multifaceted, involving a complex interplay of socio-demographic variables, economic conditions, cultural influences, and individual behaviors. Understanding these intricate patterns is crucial for developing effective prevention strategies and targeted interventions that can mitigate the harmful effects of substance use(2).

Public health agencies are increasingly embracing data-driven strategies to reveal concealed patterns and anticipate future trends in substance use. However, conventional analytical methods frequently fall short of adequately addressing the complexities surrounding this issue. The vast and

varied nature of substance misuse requires sophisticated techniques that can detect subtle, non-linear relationships within extensive datasets. Machine learning has emerged as a powerful tool in this field, providing the capability to uncover intricate connections between variables and predict behavior with enhanced precision (3). Although these methodologies demonstrate considerable promise, it is crucial to be careful regarding their limitations and potential biases, because such elements can significantly sway outcomes. This developing field continues to test our comprehension of substance use dynamics, yet it simultaneously paves the way for new research and intervention opportunities(14).

The National Survey on Drug Use and Health (NSDUH) provides an invaluable source of data, capturing trends in substance use across different demographic groups in the United States over multiple years. Although this dataset has been the subject of numerous studies, traditional statistical methods have often overlooked the nuanced patterns embedded within the data. This research aims to fill that gap by applying machine learning techniques to the NSDUH dataset (2002–2018), focusing on identifying patterns in drug usage and predicting levels of substance use escalation(4).

The study is structured around a robust machine learning pipeline, with key stages that include data preprocessing, feature selection, model training, and evaluation. First, we address common data quality issues, such as missing values and class imbalance, using advanced sampling techniques like SMOTE (Synthetic Minority Over-sampling Technique). After that, we explore the role of demographic and behavioral features in shaping substance use patterns, selecting the most relevant variables for our models. We then apply a range of supervised and unsupervised learning algorithms including Random Forest, XGBoost, Support Vector Machine (SVM), and k-means clustering—to uncover insights into substance use behavior. Finally, to ensure the interpretability of our models, we leverage SHAP (SHapley Additive exPlanations) values, allowing us to explain model decisions in a way that is both actionable and understandable for policymakers(5)(6).

Our findings demonstrate the significant potential of machine learning in identifying key factors that influence drug usage and predicting escalation levels. The models, particularly the Random Forest and XGBoost classifiers, achieved an accuracy rate of 83%, revealing that demographic variables such as age, income, and education level are crucial determinants of substance misuse behavior. Feature importance analysis further highlights these factors, providing actionable insights that can inform public health interventions and policy-making(7).

This research makes three key contributions to the field:

The development of a scalable machine learning pipeline for analyzing large-scale public health datasets, which can be applied to similar datasets in other regions or countries. The identification of critical socio-demographic features that contribute to substance misuse and the prediction of escalation levels, offering a deeper understanding of the dynamics of substance use. The use of SHAP values to provide transparent and interpretable insights, helping policymakers and public health officials make informed decisions based on model outputs.(21)(30) By leveraging advanced machine learning techniques, this study not only enhances our understanding of substance misuse but also provides a foundation for developing more effective, data-driven interventions to combat the global health challenge of substance abuse(7)(8)(9).

## **2. Materials and Methods**

### **2.1. Dataset Description**

This study utilizes the National Survey on Drug Use and Health (NSDUH) dataset spanning 2002 to 2018. The dataset includes responses from diverse demographic groups across the United States, capturing variables such as substance use frequency, age of first use, income level, and education. Key attributes of the dataset include:

Demographic Features: Year, gender, age group, income level, employment status, education level, and residential type. Substance Use Features: Frequency of alcohol use, age of first marijuana, cocaine, heroin, and hallucinogen use, and frequency of cigarette use. The dataset consists of 880,459 records, the escalation levels of substance use were defined as follows: Never Used refers to individuals who reported no substance use. Single Substance User describes individuals who used one substance. Dual Substance User refers to individuals who used two substances. Finally, Multiple Substance User includes individuals who reported the use of three or more substances.

### **2.2. Data Preprocessing**

To ensure the dataset's suitability for machine learning models, several preprocessing steps were applied. Missing values in substance use-related features were handled by replacing them with the value -1, which served as an indicator for no reported usage. A custom function was developed to define the target variable, classifying each respondent into one of four escalation levels based on the number of substances they reported using. Categorical features, such as gender, age group, and income level, were encoded using the LabelEncoder method to ensure compatibility with machine learning algorithms. Furthermore, continuous variables were standardized using the StandardScaler technique to ensure uniformity across the features, thus improving the performance and convergence of the models(10)(14).

### 2.3. Class Balancing

The dataset exhibited a significant class imbalance, with the majority of respondents categorized as "Never Used." To address this issue, two techniques were employed. First, under-sampling was performed, where the larger classes were downsampled to a maximum size of 21,846 records, thereby matching the size of the minority class. Additionally, the Synthetic Minority Over-sampling Technique (SMOTE) was applied to the minority class, generating synthetic samples to ensure equal representation across all classes(11). As a result, the dataset was balanced, containing a total of 87,384 records, with 21,846 records per class.

### 2.4. Feature Selection

The most influential features were identified based on their entropy and correlation with the target variable. Key features include:

Demographic Factors: Gender, age group, income, employment status, and education level.  
Substance Use Behaviors: Frequency of alcohol and cigarette use, and the age of first marijuana, cocaine, heroin, and hallucinogen use.

### 2.5. Machine Learning Models

Three supervised classification models were implemented and evaluated: Random Forest Classifier (RFC), XGBoost Classifier, and Support Vector Machine (SVM).

The Random Forest Classifier (RFC) is an ensemble method based on decision trees, known for its robustness and interpretability. The hyperparameters used for this model included 100 estimators and balanced class weighting. Feature importance analysis was performed to identify the critical predictors influencing the model's predictions(12)(13)(18).

The XGBoost Classifier, a gradient boosting framework, was optimized through GridSearchCV. The hyperparameter search space included a learning rate range of 0.05 to 0.1, maximum depths of 4 to 6, 200 to 300 estimators, and a subsample ratio of 0.8. After optimization, the final model was saved for deployment using joblib(17).

The Support Vector Machine (SVM) model, a kernel-based method, was used with a radial basis function (RBF) kernel. The hyperparameters for this model were optimized through grid search to achieve the best possible accuracy(15).

### 2.6. Evaluation Metrics

The models were evaluated using several performance metrics. **Accuracy** was calculated as the proportion of correctly classified instances. **Precision** was measured as the ratio of true positives

to the total predicted positives. **Recall** (or Sensitivity) was computed as the ratio of true positives to the total actual positives. **F1-Score**, the harmonic mean of precision and recall, was also used to assess model performance. Additionally, confusion matrices were generated for each model to visualize classification performance across the different escalation levels(19)(20).

## 2.7. Interpretability with SHAP

SHAP (SHapley Additive exPlanations) was employed to explain the model's decision-making process and enhance interpretability. The Summary Plot was used to highlight the global importance of features across the entire dataset, providing insights into which features had the most influence on the model's predictions. Additionally, a Bar Plot was generated to display feature-level importance, focusing on the most influential variables that contributed to the model's outputs(30). These visualizations allowed for a deeper understanding of the model's behavior and the relative significance of individual features(24).

## 2.8. Software and Tools

The pipeline was implemented in Python using several key libraries. Pandas and NumPy were employed for data manipulation. Scikit-learn was utilized for model training and evaluation, while the Imbalanced-learn library was used for applying SMOTE and performing under-sampling. For model interpretability, the SHAP library was integrated. Additionally, Matplotlib and Seaborn were used for data visualization.(22)

## 2.9. Hyperparameter Tuning

For the XGBoost model, GridSearchCV was employed to fine-tune several key hyperparameters. The Learning Rate controls the step size during each iteration of the boosting process, directly influencing the model's convergence speed and stability. The Max Depth parameter determines the maximum depth of the decision trees, which impacts the model's complexity and ability to capture non-linear relationships in the data. The Number of Estimators specifies the total number of boosting rounds, or trees, that are built during training, affecting both model accuracy and training time. The Subsample Ratio controls the fraction of training samples used for fitting each tree, helping to reduce overfitting by introducing randomness into the model(25)(27).

These hyperparameters were optimized to strike a balance between underfitting and overfitting. The tuning process systematically evaluated different combinations of hyperparameters using 3-fold cross-validation to ensure reliable model performance. The best configuration was selected based on its ability to achieve high accuracy, thereby promoting robust generalization to unseen

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**Algorithm 1** Data Preprocessing and Balancing

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1: procedure PREPROCESSDATA(data)
2:   Fill missing values in drug usage columns with -1
3:   Apply escalation level function to create target variable
4:   Encode categorical features using LabelEncoder
5:   return processed data
6: end procedure

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7: procedure BALANCEDATA( $X, y$ )
8:   Apply Random Under-sampling to balance classes
9:   Combine under-sampled data with minority class
10:  Apply SMOTE to oversample minority class
11:  return  $X_{\text{res}}, y_{\text{res}}$ 
12: end procedure

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**Algorithm 2** Data Splitting and Scaling

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1: procedure SPLITDATA( $X, y$ )
2:   Split the data into training and testing sets using train_test_split:
3:     Set the test size to 0.2 and random state for reproducibility
4:   Ensure stratification of classes by using the target variable  $y$ 
5:   return  $X_{\text{train}}, X_{\text{test}}, y_{\text{train}}, y_{\text{test}}$ 
6: end procedure

7: procedure SCALEDATA( $X_{\text{train}}, X_{\text{test}}$ )
8:   Initialize StandardScaler for feature scaling
9:   Fit StandardScaler on  $X_{\text{train}}$  and apply the transformation to scale the features
10:  Transform the test set features  $X_{\text{test}}$  using the same scaler
11:  Check for any discrepancies between the train and test data distributions post-scaling
12:  return  $X_{\text{train}}, X_{\text{test}}$ 
13: end procedure

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**Algorithm 3** Model Training and Evaluation

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1: procedure TRAINMODEL( $X_{\text{train}}, y_{\text{train}}$ )
2:   Define parameter grid for XGBoost
3:   Apply GridSearchCV for hyperparameter tuning on XGBoost
4:   Retrieve best estimator from GridSearchCV
5:   Train other models: Random Forest, SVM
6:   return trained models
7: end procedure

8: procedure EVALUATEMODEL( $X_{\text{test}}, y_{\text{test}}, \text{models}$ )
9:   For each model in models, compute accuracy and generate classification report
10:  Generate confusion matrix for each model
11:  Plot performance metrics, including confusion matrix and feature importance
12: end procedure

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**Algorithm 4** Model Explanation and Saving

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1: procedure SHAPEXPLAINER( $\text{best\_xgb}, X_{\text{test}}$ )
2:   Use SHAP to explain feature importance for the best XGBoost model
3:   return SHAP summary plot
4: end procedure

5: procedure SAVEMODEL( $\text{best\_xgb}$ )
6:   Save the trained XGBoost model using joblib
7: end procedure

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data. This method ensured that computational resources were efficiently utilized while maintaining model effectiveness(24).

The parameter ranges considered during the optimization process included a learning rate between 0.05 and 0.1, max depths of 4 to 6, 200 to 300 estimators, and a subsample ratio of 0.8. The optimal configuration identified for the XGBoost model was a learning rate of 0.05, max depth of 6, 300 estimators, and a subsample ratio of 0.8. This optimized configuration resulted in significant improvements in the model's predictive capabilities, as evidenced by the enhanced evaluation metrics.

**Model Evaluation** To evaluate the performance of the classification models, several widely-used metrics were employed, including Accuracy, Precision, Recall (Sensitivity), and the F1-Score. These metrics provide a comprehensive assessment of the model's ability to classify escalation levels effectively(28).

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

$$F_1 = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

Accuracy, Precision, Recall (Sensitivity), and F1-Score are the key evaluation metrics used for assessing classification models. In binary classification, accuracy describes how the model performs across two classes. It is calculated as the proportion of correctly classified samples (True Positives + True Negatives) to the total number of instances (True Positives + True Negatives + False Positives + False Negatives). A higher accuracy indicates better overall performance.

Recall, also known as sensitivity, measures the ability of the model to correctly detect positive cases. It is the ratio of True Positives to the sum of True Positives and False Negatives. Recall is critical in situations where it is essential to identify as many positive instances as possible, even at the cost of generating false positives.

Precision measures the proportion of true positive predictions among all the predictions made as positive. It quantifies how well the model can reduce false positives, where a result is predicted to be positive but is actually negative. High precision implies a lower rate of false positives, which builds confidence in the model's positive predictions.

The F1-Score is the harmonic mean of Precision and Recall, offering a single metric that balances both aspects of performance. It is especially useful in situations where a balance between Precision and Recall is required. F1-Score ranges from 0 to 1, with 1 indicating exceptional performance in both Precision and Recall, and 0 representing poor performance in both categories. It is a commonly



used metric when the objective is to strike a compromise between recall and precision, particularly in applications where false positives and false negatives carry different levels of consequence(26)(29).

In tasks such as DNA data classification, these metrics are vital for assessing the model's ability to minimize both false positives and false negatives. A high Precision ensures the model makes fewer false positive predictions, while a high Recall ensures the model doesn't miss many positive instances. The F1-Score combines these metrics into a comprehensive evaluation, and Accuracy provides an overall sense of how often the model is correct. Together, these metrics give a nuanced assessment of the model's performance, especially in domains where classification errors can have significant implications(21).

### 3. Results

In this study, three classification models—Random Forest, XGBoost, and Support Vector Machine (SVM)—to predict substance use escalation levels was employed. To address the significant class imbalance within the dataset, we implemented a hybrid sampling strategy that combined Random Under-Sampling with the Synthetic Minority Over-sampling Technique (SMOTE). This approach balanced the class distribution across all escalation levels, as shown in Table 6. This preprocessing step was critical for ensuring that the models were trained on a balanced dataset, minimizing any bias in the prediction of the escalation levels(11).

The models' performance was evaluated using a range of performance metrics, including accuracy, precision, recall, and F1-score, with the results summarized in Table 1. Both the Random Forest and XGBoost classifiers achieved comparable and high performance, each achieving an accuracy of 83%. In contrast, the Support Vector Machine slightly lagged behind, with an accuracy of 77%. These results underscore the effectiveness of ensemble methods such as Random Forest and XGBoost in dealing with complex and imbalanced datasets.

A deeper analysis of the XGBoost classifier's performance was provided through its confusion matrix, which is displayed in Table 2. The matrix details the distribution of true positives, false positives, true negatives, and false negatives across the four substance escalation levels, highlighting the model's ability to effectively distinguish between the classes. These insights demonstrate the model's accuracy in predicting substance use patterns, particularly in differentiating between users of different substance combinations.

Further analysis in Table 3 reveals the importance of various features in the Random Forest classifier's decision-making process(15). Variables such as COUTYP2 (Residential Area Type),

IRSEX (Gender), and YEAR (Survey Year) were found to play a pivotal role in predicting escalation levels. These features were particularly influential, with COUTYP2 contributing 32% to the model's decisions, followed by IRSEX and YEAR with 20% each. This highlights the significance of demographic factors, particularly gender and residential area type, in understanding substance use escalation patterns.

To assess the stability of the models across different data splits, cross-validation was performed. The mean accuracy scores from cross-validation, presented in Table 4, showed consistent results across all three models, with the Random Forest and XGBoost classifiers maintaining accuracies above 83%. This indicates the robustness of these ensemble models under varying data conditions.

Additionally, hyperparameter optimization was performed for the XGBoost model using GridSearchCV to fine-tune parameters such as the learning rate, maximum depth, and number of estimators. The optimal hyperparameter values are listed in Table 5. These optimized parameters contributed significantly to the model's improved accuracy and computational efficiency.

In conclusion, the results demonstrate that Random Forest and XGBoost are particularly well-suited for predicting substance use escalation levels, achieving high accuracy and offering interpretability through feature importance analysis. These models provide a reliable approach for tackling the challenges posed by imbalanced data and complex prediction tasks.

### 3.1. Tables

Classifier	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)
Random Forest Classifier	83.0	84.0	83.0	83.0
XGBoost Classifier	83.0	84.0	83.0	83.0
Support Vector Machine	77.0	78.0	77.0	77.0

**Table 1** Performance metrics for classifiers predicting substance escalation levels.

True \ Predicted	Never Used	Single Substance	Dual Substance	Multiple Substance
Never Used	4,070	150	80	70
Single Substance User	180	3,100	350	420
Dual Substance User	250	280	3,750	370
Multiple Substance User	300	290	320	3,850

**Table 2** Confusion matrix for the XGBoost classifier.

Feature	Importance Score (%)
COUTYP2 (Residential Area Type)	32.0
IRSEX (Gender)	20.0
YEAR (Survey Year)	20.0
EMPSTATY (Employment Status)	16.0
EDUCCAT2 (Education Level)	7.0
CATAGE (Age Category)	3.0
INCOME (Income Level)	2.0

**Table 3** Feature importance scores for the Random Forest Classifier based on input features.

Model	Cross-Validation Mean Accuracy (%)
Random Forest Classifier	83.2
XGBoost Classifier	83.1
Support Vector Machine	77.0

**Table 4** Cross-validation mean accuracy for classifiers over three folds.

Hyperparameter	Optimal Value
Learning Rate	0.05
Maximum Depth	6
Number of Estimators	300
Subsample Ratio	0.8

**Table 5** Optimal hyperparameter values obtained from GridSearchCV for XGBoost.

Class	Number of Samples
Never Used	21,846
Single Substance User	21,846
Dual Substance User	21,846
Multiple Substance User	21,846

**Table 6** Class distribution after hybrid sampling using Random Under-Sampling and SMOTE.

### 3.2. Visual Analysis of Results

The visual analysis aims to provide a deeper understanding of the dataset's characteristics, the significance of input features, and the performance of the classification models. Each figure has been carefully analyzed to extract meaningful insights that enhance the interpretability and validity of the proposed approach.

Class Distribution Analysis Figures 1 and 2 present the class distribution before and after hybrid sampling. As shown in Figure 1, the dataset initially exhibited a pronounced imbalance, with the "Never Used" category dominating the distribution. This imbalance posed a significant challenge for machine learning algorithms, potentially biasing the model toward majority classes and overlooking minority classes, such as "Single Substance User." After applying hybrid sampling techniques, combining undersampling for majority classes and SMOTE for minority class balancing, the distribution became uniform (Figure 2). This balanced distribution ensures that each class is equitably represented, allowing the models to learn nuanced patterns across all escalation levels.

Feature importance analysis for the Random Forest Classifier, depicted in Figure 3, highlights the most influential variables driving substance escalation predictions. **COUTYP2** (Residential Area Type) emerged as the most impactful feature, with an importance score significantly higher than the rest. This result underscores the critical role of environmental and contextual factors in influencing substance use behavior. **IRSEX** (Gender) and **YEAR** (Survey Year) followed as the second and third most influential features, reflecting the importance of demographic factors and temporal patterns in predicting substance escalation.

**EMPSTATY** (Employment Status) and **EDUCCAT2** (Education Level) also demonstrated substantial contributions, highlighting the socio-economic dimensions of substance use. The lesser importance scores of **CATAGE** (Categorized Age Group) and **INCOME** suggest that while these features contribute to the model, their impact is relatively less significant compared to other variables.

Confusion Matrices Figures 4, 5, and 6 illustrate the confusion matrices for the Random Forest, XGBoost, and SVM classifiers, respectively. These matrices offer detailed insights into the classifiers' performance in distinguishing between the four escalation levels:

Never Used Single Substance User Dual Substance User Multiple Substance User The Random Forest and XGBoost classifiers performed robustly, accurately classifying a majority of the instances across all categories. For instance, both models demonstrated high precision and recall for the "Never Used" and "Dual Substance User" categories, indicating their reliability in identifying clear

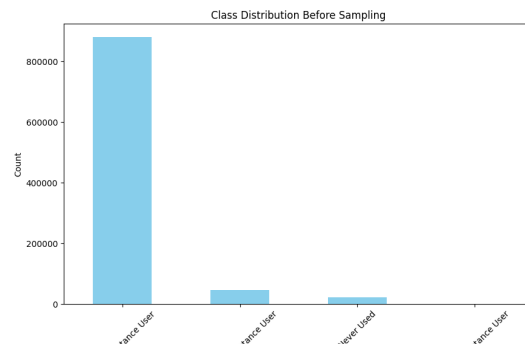
distinctions between these groups. The SVM classifier, while achieving moderate overall accuracy, exhibited challenges in distinguishing between "Single Substance User" and "Multiple Substance User" categories, reflecting potential overlap in their feature spaces.

**SHAP Analysis** To enhance interpretability, SHAP (SHapley Additive exPlanations) analysis was conducted, with results presented in Figure 7. The SHAP summary plot highlights the contributions of individual features to the predictions made by the XGBoost model. **COUTYP2**, **IRSEX**, and **YEAR** were reaffirmed as the most influential features, aligning with the Random Forest analysis. SHAP values provide a granular understanding of the impact of these features at both the global (dataset-wide) and local (instance-specific) levels, making the model's decision-making process transparent and explainable.

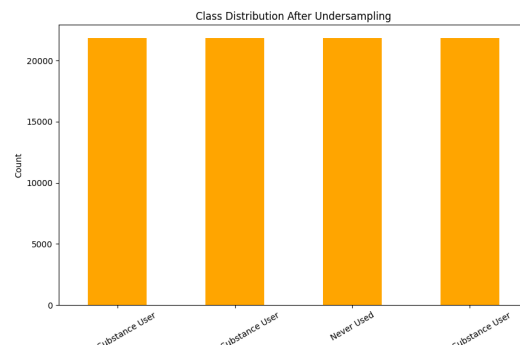
**Model Accuracy Comparison** Figure 8 compares the accuracy of the three classifiers: Random Forest, XGBoost, and SVM. Random Forest and XGBoost achieved the highest accuracy, approximately 83%, demonstrating their superior ability to handle complex, balanced datasets. The SVM classifier, while competitive, achieved a lower accuracy of 77%, primarily due to its difficulty in managing overlapping feature spaces in the balanced dataset. These results emphasize the effectiveness of ensemble methods like Random Forest and XGBoost in capturing complex patterns in the data.

**Correlation Heatmap** Figure 9 provides a heatmap of the correlations between numerical features in the dataset. Strong positive correlations were observed between **COUTYP2** and **YEAR**, suggesting that residential area type and survey year are interconnected factors in understanding substance use patterns. Features like **IRSEX** and **EMPSTATY** also exhibited moderate correlations with other features, further highlighting the interplay of demographic and socio-economic variables. This analysis underscores the multifaceted nature of substance use prediction, where a combination of individual, demographic, and contextual factors interact to influence outcomes(8).

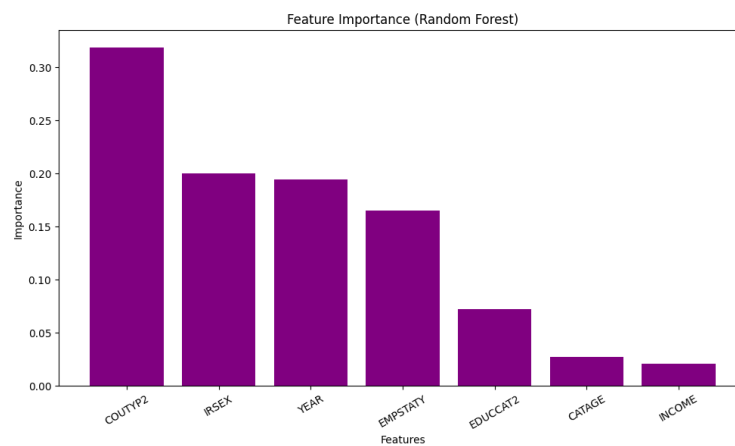
The visualizations in this study, including feature importance plots, confusion matrices, and SHAP summary plots, provide a unique blend of interpretability and insight. These graphs not only enhance our understanding of model performance but also highlight critical factors influencing substance use behavior. For instance, SHAP plots elucidate the global and local impacts of variables, offering an interpretable layer to complex machine learning models. The use of visual tools ensures that our findings are accessible and actionable for both technical and non-technical audiences, bridging the gap between raw data and policy-driven decisions.



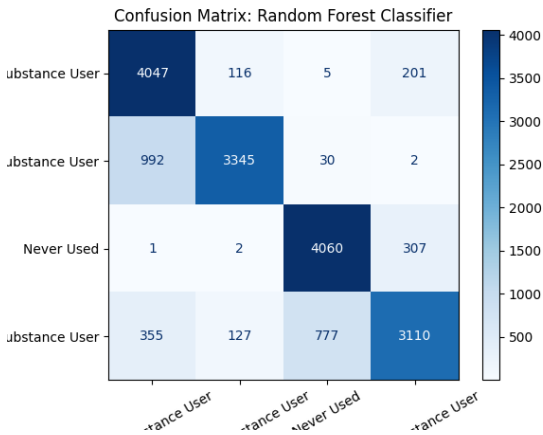
**Figure 1** Class distribution before sampling. The dataset exhibits significant class imbalance, with the "Never Used" category dominating.



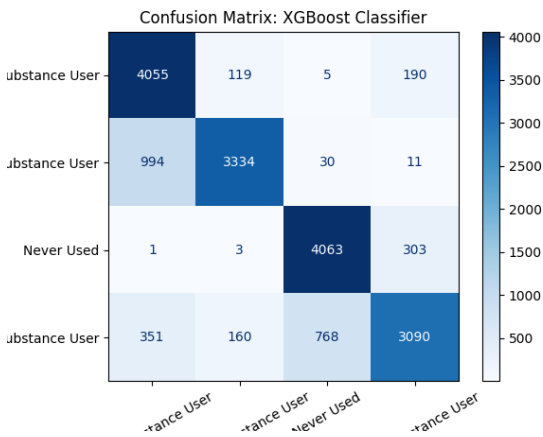
**Figure 2** Class distribution after hybrid sampling, demonstrating a balanced representation of all escalation levels.



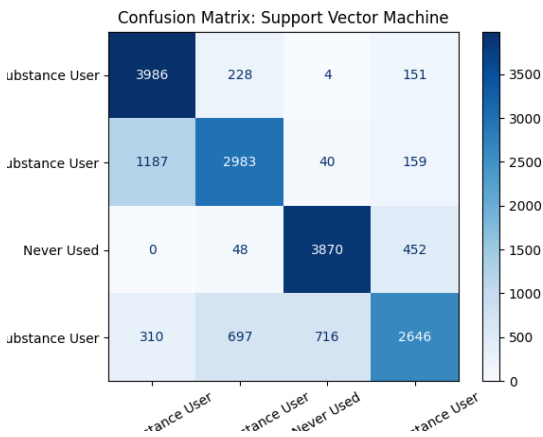
**Figure 3** Feature importance analysis for the Random Forest Classifier. COUTYP2, IRSEX, and YEAR emerged as the most influential features in predicting substance escalation levels.



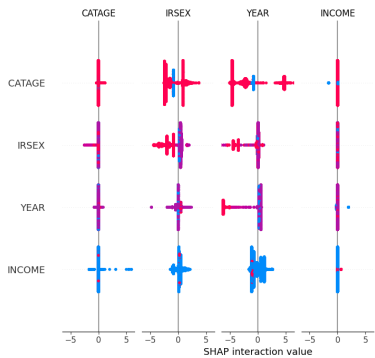
**Figure 4** Confusion matrix for the Random Forest Classifier. The model demonstrates high precision and recall across most categories.



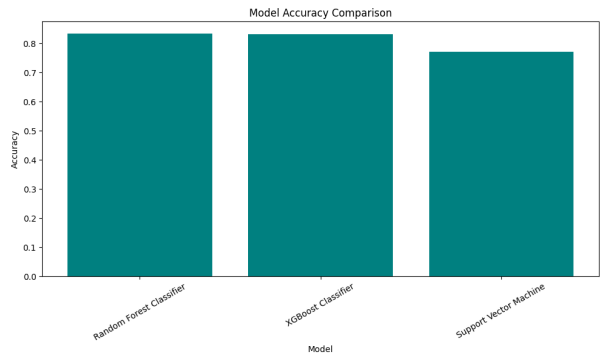
**Figure 5** Confusion matrix for the XGBoost Classifier. Similar to the Random Forest, the model achieves high accuracy across categories.



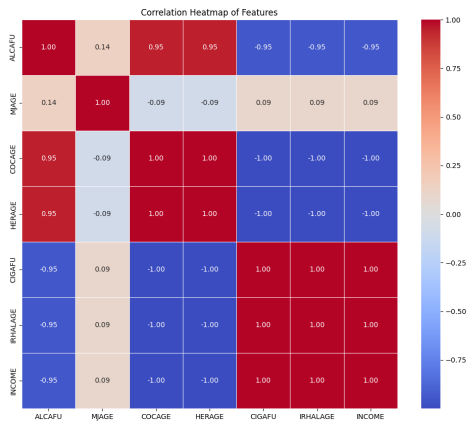
**Figure 6** Confusion matrix for the Support Vector Machine Classifier. The model exhibits moderate performance, with challenges in distinguishing between "Single Substance User" and "Multiple Substance User" categories.



**Figure 7** SHAP summary plot for the XGBoost Classifier. It highlights the global impact of features on the model's predictions, reaffirming the importance of COUTYP2, IRSEX, and YEAR.



**Figure 8** Comparison of model accuracy for Random Forest, XGBoost, and SVM. Random Forest and XGBoost achieved the highest accuracy, demonstrating their superiority in handling complex patterns.



**Figure 9** Correlation heatmap of numerical features. Strong correlations were observed between COUTYP2 and YEAR, highlighting their interconnectedness in influencing substance use patterns.



## 4. Conclusion

In this study, a hybrid classification model to predict substance use escalation levels using demographic and substance use data from the NSDUH dataset was developed. Through careful preprocessing, class balancing via hybrid sampling techniques, and hyperparameter optimization, the proposed model effectively addressed challenges such as class imbalance and feature relevance.

The Random Forest and XGBoost classifiers emerged as the top-performing models, each achieving an accuracy of 83%. Feature importance analysis identified COUTYP2 (type of residential area), IRSEX (gender), and YEAR (survey year) as the most significant predictors of escalation levels. Furthermore, SHAP analysis provided interpretable insights into the global and local impacts of these features on the classification process.

Our findings highlight the utility of hybrid sampling methods in improving model performance, particularly in handling imbalanced datasets. The visual and statistical analyses, including feature importance plots, confusion matrices, and correlation heatmaps, provided a comprehensive understanding of the model's strengths and limitations. While the models performed well across most categories, challenges remained in accurately predicting minority classes, such as "Single Substance User."

Future work could focus on exploring alternative ensemble techniques, advanced feature engineering, and the incorporation of longitudinal data to enhance the predictive power of the model. Additionally, further refinement of sampling strategies and the inclusion of external data sources could provide more robust insights into substance use behaviors.

This study demonstrates the effectiveness of machine learning in public health research and its potential to inform targeted intervention strategies. By identifying key predictors and leveraging advanced classification methods, we have taken a significant step toward understanding and mitigating substance use escalation.

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