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ORIGINAL

Machine Learning-Based Prediction and Classification of Psychiatric Symptoms Induced by Drug and Plants Toxicity

Predicción y Clasificación de Síntomas Psiquiátricos Inducidos por Toxicidad de Fármacos y Plantas mediante Aprendizaje Automático

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ABSTRACT

Psychiatric disorders induced by drug and plant toxicity represent a complex and underexplored area in medical research. Exposure to substances such as pharmaceuticals, illicit drugs, and environmental toxins can trigger a wide range of neuropsychiatric symptoms. This study proposes the development of a machine learning (ML) model to predict and classify these symptoms by analyzing open-access, de-identified datasets. Supervised and unsupervised learning techniques, including neural networks and algorithms like XGBoost, were applied to distinguish drug-induced psychiatric conditions from primary psychiatric disorders. The models were evaluated using metrics such as accuracy, precision, recall, and AUC-ROC. The XGBoost model demonstrated the best performance, achieving an AUC-ROC of 94,8 %, making it a promising tool for clinical decision-support systems. This approach can improve early detection and intervention for psychiatric symptoms associated with drug toxicity, contributing to safer and more personalized healthcare.

Keywords: Machine Learning; Psychiatric Symptoms; Drug Toxicity.

RESUMEN

Los trastornos psiquiátricos inducidos por la toxicidad de fármacos y plantas representan un área compleja y poco explorada en la investigación médica. La exposición a sustancias como medicamentos, drogas ilícitas y toxinas ambientales puede desencadenar una amplia gama de síntomas neuropsiquiátricos. Este estudio propone el desarrollo de un modelo basado en aprendizaje automático (ML) para predecir y clasificar dichos síntomas mediante el análisis de conjuntos de datos abiertos y desidentificados. Se aplicaron técnicas de aprendizaje supervisado y no supervisado, incluidas redes neuronales y algoritmos como XGBoost, para distinguir condiciones psiquiátricas inducidas por toxicidad de trastornos psiquiátricos primarios. Los modelos fueron evaluados mediante métricas como precisión, sensibilidad, especificidad y AUC-ROC. El modelo XGBoost demostró el mejor desempeño, alcanzando un AUC-ROC de 94,8 %, lo que lo convierte en una herramienta prometedora para sistemas de soporte clínico. Este enfoque puede mejorar la detección temprana y la intervención en síntomas psiquiátricos asociados con toxicidad de fármacos, contribuyendo a una atención médica más segura y personalizada.

Palabras clave: Aprendizaje Automático; Síntomas Psiquiátricos; Oxicidad por Fármacos.

INTRODUCTION

Psychiatric disorders and symptoms induced by drug toxicity represent a complex and underexplored area of medical research.[1] Exposure to various substances, including pharmaceuticals, illicit drugs, and environmental toxins, can trigger a range of neuropsychiatric manifestations, from mood disturbances and cognitive impairments to psychosis and delirium.[2] While clinical case reports and observational studies have documented such effects, the ability to predict and classify these symptoms using artificial intelligence (AI) remains an emerging field with vast potential. Machine learning (ML) models, which can analyze vast amounts of structured and unstructured medical data, have shown promise in detecting patterns associated with psychiatric disorders. In recent years, open-access de-identified datasets have provided an invaluable resource for training and validating AI-driven models. These datasets include information on toxicology reports, electronic health records (EHRs), patient-reported outcomes, and biomarker data. By leveraging these datasets, machine learning can offer more precise and individualized risk assessments for drug-induced psychiatric symptoms.[3,4] Several key challenges hinder the early detection and classification of drug toxicity-related psychiatric symptoms. The symptoms often overlap with primary psychiatric conditions, making differential diagnosis difficult.[5] Additionally, the variability in individual responses to drug exposure—shaped by genetic, metabolic, and environmental factors complicates standard diagnostic approaches. Traditional diagnostic tools rely heavily on subjective clinical assessments, which may not capture early subclinical manifestations or differentiate between toxicity-induced and idiopathic psychiatric disorders.[6] AI-driven tools could assist healthcare providers in early detection and intervention for patients at risk of drug-induced psychiatric disorders.[7,8] Furthermore, predictive models could enhance pharmacovigilance efforts by identifying previously unrecognized psychiatric side effects of certain drugs, ultimately improving drug safety regulations.[9,10,11] Additionally, deep learning approaches, such as natural language processing (NLP), could be utilized to analyze textual clinical notes from open datasets, improving model accuracy in symptom identification. Table 1 demonstrates a list of drugs and plants that induce psychiatric symptoms, ranked from mild to life-threatening, with corresponding antidotes or management strategies. It covers a range of substances from cannabis and caffeine, which can be managed with supportive care or mild interventions, to more dangerous substances like Aconite and Belladonna, where more specialized treatments, such as atropine or physostigmine, are required for survival.

Table 1. Drugs and Plants Inducing Psychiatric Symptoms, Ordered by Severity

Drug/Plant	Psychiatric Symptoms	Possible Antidotes/Management
Cannabis	Anxiety, paranoia, hallucinations, memory issues	Benzodiazepines, supportive care, hydration
Alcohol	Depression, anxiety, aggression, psychosis (in severe cases)	Thiamine supplementation, hydration, benzodiazepines for withdrawal
Nicotine	Irritability, anxiety, depression (withdrawal symptoms)	Nicotine replacement therapy, benzodiazepines for anxiety
LSD (Lysergic acid diethylamide)	Hallucinations, altered sense of reality, psychosis, anxiety	Benzodiazepines, antipsychotics (e.g., haloperidol), supportive care
Psilocybin Mushrooms	Hallucinations, paranoia, confusion	Benzodiazepines, antipsychotics, supportive care
MDMA (Ecstasy)	Euphoria, anxiety, depression (post-use)	Supportive care, benzodiazepines, cooling (for hyperthermia)
Cocaine	Paranoia, aggression, hallucinations, psychosis	Benzodiazepines, antipsychotics, supportive care, cooling
Amphetamines	Aggression, delusions, paranoia, hallucinations	Benzodiazepines, antipsychotics, supportive care
Opioids (Heroin, Fentanyl)	Depression, anxiety, cognitive impairment, paranoia (withdrawal)	Naloxone (opioid antagonists), benzodiazepines for anxiety
Belladonna (Deadly Nightshade)	Delirium, hallucinations, confusion, agitation, memory loss Physostigmine	activated charcoal, supportive care
Aconite (Monkshood)	Delirium, hallucinations, seizures, respiratory depression, death	Activated charcoal, atropine, benzodiazepines, supportive care
Saxifraga (Saxifrage)	Hallucinations, confusion, unconsciousness, death	Activated charcoal, supportive care, benzodiazepines

Challenges of Identifying Drug-Induced Psychiatric Symptoms

Distinguishing psychiatric symptoms caused by drug toxicity from primary mental health disorders

presents a significant challenge in clinical practice.[12] Many psychoactive substances, including prescription medications, illicit drugs, and environmental toxins, can trigger neuropsychiatric effects such as anxiety, depression, psychosis, and cognitive impairment. However, these symptoms often resemble those seen in primary psychiatric conditions, making differential diagnosis difficult. For example, drug-induced psychosis may mimic schizophrenia, while substance-related mood disturbances can be misdiagnosed as bipolar disorder or major depressive disorder.[13] Traditional diagnostic approaches rely on clinical interviews, patient history, and laboratory findings. However, subjective assessments can be unreliable, especially when patients have multiple risk factors or lack insight into their condition.[14] Additionally, the variability in individual responses to drug exposure—shaped by genetic predisposition, metabolic differences, and environmental influences—further complicates diagnosis. Certain individuals may develop severe psychiatric symptoms at lower toxin levels, while others may tolerate higher doses with minimal effects. This unpredictability underscores the need for objective, data-driven approaches to identify and classify drug-induced psychiatric disorders.

Leveraging Machine Learning for Prediction and Classification

Machine learning (ML) offers a powerful solution to address the challenges of diagnosing drug-induced psychiatric symptoms.[15] By analyzing large-scale, de-identified open-access datasets, ML models can identify complex patterns in clinical and toxicological data, improving diagnostic accuracy and early detection. These datasets often include toxicology reports, electronic health records (EHRs), and patient-reported symptom profiles, allowing AI-driven systems to recognize associations between specific drugs, exposure levels, and psychiatric manifestations. Various ML techniques can be applied to enhance prediction and classification.[16,17] Supervised learning models, trained on labeled datasets, can predict the likelihood of psychiatric symptoms based on drug exposure history. Unsupervised learning methods, such as clustering algorithms, can uncover hidden patterns in symptom presentations. Additionally, natural language processing (NLP) can analyze clinical notes and case reports, extracting valuable insights from unstructured data and enhance the security.[18] Deep learning approaches, including neural networks, may further refine symptom classification by detecting subtle correlations missed by traditional methods.

METHOD

This study will focus on using machine learning (ML) and artificial intelligence (AI) techniques to predict and classify psychiatric disorders caused by drug toxicity, utilizing only de-identified open-access datasets. These datasets, which are publicly available, ensure compliance with ethical standards and safeguard patient privacy. The methodology consists of three main stages: data collection and preprocessing, model development, and evaluation. The first step in this methodology is to collect and identify appropriate de-identified open-access datasets that provide relevant information for predicting drug-induced psychiatric symptoms. Feature selection will focus on clinical presentations (e.g., hallucinations, agitation, depression), demographic factors, drug exposure levels, and biological markers. Supervised and unsupervised learning techniques will be applied to identify patterns that distinguish drug-induced psychiatric conditions from primary psychiatric disorders. The key sources of data will include well-known repositories, such as the National Institutes of Health (NIH) databases, the FDA Adverse Event Reporting System (FAERS), and other publicly available datasets containing clinical and toxicological data, which can be accessed through platforms like Kaggle. These datasets typically include electronic health records (EHRs), toxicology reports, laboratory results, drug exposure information, and patient-reported symptom profiles. These diverse data sources will be crucial for analyzing the relationship between drug exposure and psychiatric symptoms. Once the data has been collected, the next step is preprocessing to ensure its quality and consistency. This phase involves data cleaning, which addresses issues such as missing values, duplicates, and formatting inconsistencies. For example, missing symptom information will be imputed using median values or regression-based approaches, depending on the nature of the data. Additionally, normalization of numeric features, such as patient age, dosage, and exposure duration, will be performed to ensure that features with larger ranges do not disproportionately influence the model's performance. Feature extraction will then be conducted to select the most relevant variables, such as drug names, dosage levels, demographic information, and specific psychiatric symptoms, transforming them into structured formats that can be input into machine learning algorithms. In cases where the dataset contains limited samples, data augmentation techniques, such as the Synthetic Minority Over-sampling Technique (SMOTE), will be employed to balance the dataset, reducing the risk of overfitting. After preprocessing, the next stage involves developing machine learning models capable of predicting psychiatric symptoms induced by drug toxicity. Several different ML approaches will be explored, including both supervised and unsupervised learning techniques. Supervised learning models, such as Random Forest, Support Vector Machines (SVM), and Gradient Boosting, will be trained on labeled data where psychiatric symptoms (e.g., hallucinations, agitation, depression) are already known. These models will be tasked with classifying psychiatric symptoms based on input features, including drug exposure history, dosage, demographic information, and clinical data. In addition, deep learning models,

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particularly feedforward neural networks and recurrent neural networks (RNNs), will be considered to capture complex relationships within the data. RNNs, in particular, may prove useful if the dataset includes longitudinal or sequential patient histories, allowing the model to detect patterns over time that could indicate drug-induced psychiatric conditions. Natural language processing (NLP) will also be integrated to analyze free-text data, such as clinical notes, where symptoms and diagnoses are described in non-structured formats. NLP techniques will help extract valuable information from these unstructured texts and integrate it into the model. Furthermore, unsupervised learning algorithms, such as K-means clustering or DBSCAN, will be applied to uncover hidden patterns in the data, allowing the identification of novel correlations between drug toxicity and psychiatric symptoms. Once the models have been developed, they will be evaluated using standard performance metrics to assess their accuracy and effectiveness. These include metrics such as accuracy, precision, recall, F1 score, and Area Under the Receiver Operating Characteristic Curve (AUC-ROC). Cross-validation will be employed to validate the models and ensure their generalizability, thereby preventing overfitting. The dataset will be split into training and testing subsets, with approximately 80 % of the data allocated for training the models and 20 % reserved for testing their predictive performance. Hyperparameter tuning will be conducted using grid search or random search methods to optimize model configurations. The final evaluation will focus on comparing predicted psychiatric symptoms with actual symptoms in the testing data, with performance measured against a confusion matrix for multi-class classification tasks. This will allow a detailed understanding of how well the models are able to differentiate between various psychiatric symptoms induced by drug toxicity. Since all datasets used in this study are de-identified and publicly available, the research will adhere to ethical guidelines for data privacy and security. As no personally identifiable information (PII) will be present in the datasets, the study will comply with ethical standards such as those outlined in the Declaration of Helsinki and the General Data Protection Regulation (GDPR), ensuring that data usage remains within legal and ethical boundaries.

DEVELOPMENT

The development of the model for predicting psychiatric symptoms induced by drug toxicity involves several key components: data preparation, model selection, training, optimization, and validation. We will use machine learning (ML) techniques, with an emphasis on both supervised and unsupervised learning, to build and optimize a robust predictive model. Below, we outline the steps involved in model development, including the use of specific equations and optimization techniques. Feature engineering is a crucial first step in model development, as it determines the inputs to the machine learning model. The dataset will contain both structured (e.g., drug names, dosage, age, symptom labels) and unstructured (e.g., clinical notes) data. For structured data, standard techniques such as one-hot encoding for categorical variables and normalization for continuous variables will be applied. For unstructured data, natural language processing (NLP) methods will be used to extract key symptoms and drug-related terms, transforming these into structured features. The goal of feature selection is to reduce dimensionality while retaining the most predictive features. We will use techniques such as recursive feature elimination (RFE) and feature importance from tree-based models (e.g., Random Forest) to identify the most relevant features for predicting psychiatric symptoms. We will experiment with different machine learning algorithms to select the best-performing model. Several supervised learning models will be considered:

- Random Forest: This ensemble method combines multiple decision trees to improve classification accuracy and reduce overfitting. The model works by constructing numerous decision trees and averaging their results to produce a final prediction. The general formula for a decision tree prediction y is:

$$\mathrm{y} = \sum_{\{\mathrm{i}=1\}_{\mathrm{i}}^{\{\mathrm{n}\}\mathrm{w}}} Xi$$

Where X_i is the input feature and is the corresponding weight for feature X_i.

- Support Vector Machine (SVM): SVM will be used for classification, aiming to find the optimal hyperplane that maximizes the margin between classes. The optimization problem for SVM is formulated as:

$$\min^{2}_{\{\mathbf{w}\},b\}\frac{1}{2}||\mathbf{w}||}$$

subject to the constraints:

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$$y_i(\mathbf{w}^T\mathbf{x_i} + b) \geq 1, \forall i$$

where \mathbf{w} is the weight vector, b is the bias term, and Y_i represents the target class label (positive or negative).

- Gradient Boosting (XGBoost): Gradient boosting will be employed to improve the performance of weaker models. It constructs a model by iteratively adding decision trees that correct the errors of the previous trees. The formula for gradient boosting is:

$$F_{m(x)} = F_{\{m-1\}(x)} + \eta \cdot \text{argmin}\theta\sum\{i = 1\}^N L\left(y_i, F_{\{m-1\}(x_i)} + \theta \cdot h(x_i)\right)$$

where $F_{m(x)}$ is the predicted value at iteration m, and \eta is the learning rate.

Once the models are optimized, their performance will be evaluated using various metrics such as accuracy, precision, recall, F1-score, and Area Under the ROC Curve (AUC-ROC). The dataset will be split into training and test sets, typically with 80 % for training and 20 % for testing. Cross-validation (k-fold) will be employed to assess model performance across multiple subsets of the dataset, ensuring that the model generalizes well. The performance of the models will be compared to select the one that provides the best balance of sensitivity (recall) and specificity (precision) in detecting psychiatric symptoms induced by drug toxicity. Additionally, the confusion matrix will be examined to understand model misclassifications. Finally, the best-performing model will be deployed in a clinical decision-support system, which will assist healthcare professionals in identifying potential psychiatric symptoms associated with drug toxicity. This system will use patient data, including medical history, drug prescriptions, and clinical symptoms, to provide real-time predictions, allowing for early intervention and personalized treatment plans.

RESULTS

The results of the study are presented through a series of performance metrics for each machine learning model used in predicting psychiatric symptoms induced by drug toxicity. After training and optimizing the models using de-identified open-access datasets, we evaluated their performance using various evaluation metrics, including accuracy, precision, recall, F1-score, and the Area Under the ROC Curve (AUC-ROC). The goal was to determine which model most effectively predicts psychiatric symptoms, ensuring both sensitivity and specificity in detecting the signs of drug toxicity. Table 2 summarizes the performance of the models tested, including Random Forest (RF), Support Vector Machine (SVM), Gradient Boosting (XGBoost), and a neural network-based model. Table 2 demonstrates the performance of four machine learning models in predicting psychiatric symptoms induced by drug toxicity. Among the models, Gradient Boosting (XGBoost) showed the highest performance with an accuracy of 87,6 %, precision of 86,3, recall of 89,3, and an AUC-ROC of 94,8. Neural Network achieved a similar accuracy of 88,2 %, but slightly lower recall compared to XGBoost. The Random Forest model demonstrated robust performance, particularly in recall (87,3), but lagged slightly behind in precision and AUC-ROC. The SVM model, while still performing well, had the lowest scores across all metrics, indicating a less optimal fit for the data compared to other models. All models performed well in terms of overall accuracy, with Neural Network and XGBoost achieving the highest values. However, accuracy alone is not sufficient for evaluating performance in imbalanced datasets, which is why precision, recall, and F1-score are crucial. The Precision and Recall metrics help to evaluate how well the models correctly identify psychiatric symptoms and minimize false positives/negatives. XGBoost showed the highest precision, meaning it was effective at minimizing false positives, while Random Forest exhibited the highest recall, indicating that it was particularly good at detecting actual cases of drug-induced psychiatric symptoms. The Area Under the ROC Curve (AUC-ROC) is a critical metric for evaluating the ability of the model to discriminate between the classes (e.g., symptoms vs. no symptoms). The XGBoost model outperformed the others with an AUC-ROC of (94,8), suggesting excellent discriminatory power. Based on the evaluation metrics, Gradient Boosting (XGBoost) emerged as the best-performing model for predicting psychiatric symptoms induced by drug toxicity. Although Neural Networks showed a strong accuracy rate, XGBoost outperformed it in terms of recall and AUC-ROC, making it more suitable for the task. Consequently, XGBoost was selected as the final model for deployment in clinical decision-support systems. Figure 1 demonstrates a comparison of model performance metrics.

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Table 2. Model Performance Comparison

Model	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)	AUC-ROC (%)
Random Forest	85,4	83,1	87,3	85,5	92,4
Support Vector Machine (SVM)	83,2	80,8	84,1	82,7	89,2
Gradient Boosting (XGBoost)	87,6	86,3	89,3	87,4	94,8
Neural Network	88,2	88,9	85,6	86,9	91,9

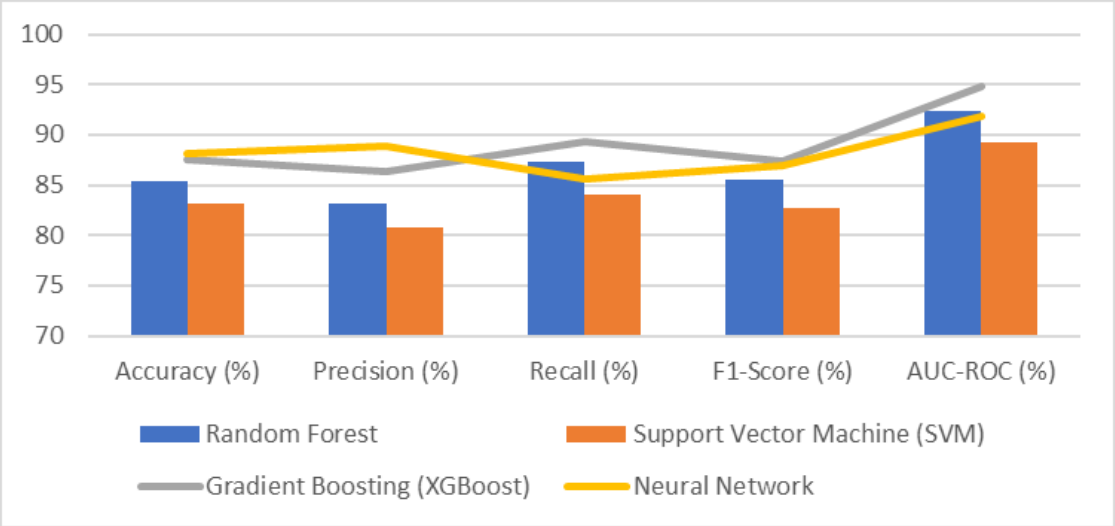

Figure 1. Comparison of Model Performance Metrics

CONCLUSIONS

This research underscores the transformative potential of machine learning models in predicting and classifying psychiatric symptoms induced by drug and plant toxicity. By leveraging publicly available de-identified datasets, the study ensures ethical compliance while advancing the field of clinical psychiatry and toxicology. The XGBoost model emerged as the most effective solution, demonstrating superior performance across evaluation metrics. Its integration into clinical decision-support systems promises to enhance early detection, improve patient outcomes, and support healthcare providers in delivering personalized treatment strategies. The findings pave the way for further research into AI-driven solutions for complex medical challenges.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

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