DIGITAL TWIN FOR PREDICTIVE DRUG CONSUMPTION AND GENERATIVE AI FOR PERSONALIZED TREATMENT PLANS.

Abstract

In recent years, the prevalence of substance abuse has emerged as a pressing public health concern, particularly among vulnerable populations. This study seeks to utilize digital twin technology and machine learning techniques to predict drug consumption patterns and generate personalized treatment plans for individuals. By creating a digital twin profile based on demographic and personality data, we aim to understand the interactions between various factors influencing drug use. The dataset utilized comprises responses from 1,885 individuals, including demographic information, personality assessments, and self-reported drug usage across 18 substances. Our exploratory data analysis (EDA) revealed significant correlations between personality traits and drug consumption patterns. Employing Random Forest and Support Vector Machine (SVM) models, we achieved promising preliminary results, demonstrating the potential of predictive models to identify individuals at risk of substance abuse. This innovative approach aims to enhance early detection and facilitate targeted interventions in the realm of public health.

Keywords: Digital Twin, Predictive Medicine, Drug Consumption, Patient profile, Generative AI.

Introduction and Background

Substance abuse remains a pervasive global issue, imposing significant social and economic burdens, including increased healthcare costs and a rising number of drug-related fatalities. Addressing this crisis requires innovative approaches capable of accounting for the complex interplay of factors influencing drug consumption, such as demographic variables, psychological traits, and social environments. Traditional methods often fail to capture these dynamics, necessitating the adoption of advanced computational tools. Digital twin technology, which creates virtual representations of patients, offers a promising framework for simulating and predicting substance abuse behaviors in real-time. Digital twins provide a dynamic and personalized perspective on individual risk factors by incorporating physiological responses, behavioral tendencies, and adherence patterns.

Simulation, particularly through agent-based modeling, enhances this framework by modeling the progression of drug consumption behaviors across distinct states, such as "Never Used," "Experimental," and "Addicted." Agents in the simulation represent patients, with their behaviors governed by key variables like neuroticism, impulsivity, and education level. Transitions between states are driven by a probabilistic risk score derived from these parameters, capturing. Unlike static models, these simulations dynamically adjust to changes in input data, ensuring real-time adaptability and precision.

Integrating generative AI further strengthens this approach by enabling the creation of evolving treatment plans tailored to individual needs. These plans optimize medication schedules and therapies, considering patient-specific data while dynamically adapting to health status and adherence patterns. Simulation tools also facilitate early detection of high-risk behaviors and enable targeted interventions, addressing the limitations of traditional strategies. Together, digital twin technology and simulation provide a robust, multidimensional approach to understanding and combating substance abuse, paving the way for more effective prevention, treatment, and relapse management strategies.

Literature Review

Simulation and digital twin technologies have gained traction in addressing the complexities of drug abuse prediction and management. Researchers have employed various modeling approaches to optimize treatment and improve patient outcomes, each with distinct contributions and limitations.

Simulation tools have been pivotal in studying substance use patterns. For instance, logistic regression and Random Forest models were applied to predict substance use among teenagers, focusing on alcohol and cannabis consumption [1]. While effective in leveraging demographic and behavioral data, the study lacked consideration of psychological traits, limiting the depth of its predictions for addiction tendencies.

Neural networks have also been explored for predicting opioid usage. By integrating demographic data with medical history, these models achieved high prediction accuracy [2]. However, their lack of interpretability poses challenges in clinical settings where transparency is crucial, suggesting a need for explainable AI (XAI) integration to improve usability.

Digital twin frameworks have been utilized for chronic disease management, including diabetes, offering real-time simulations of patient conditions [3]. While effective in predicting outcomes and optimizing treatment, these models often exclude psychological and behavioral traits, a critical aspect in the context of drug addiction.

Generative adversarial networks (GANs) have been applied in cancer treatment to create personalized intervention plans, significantly improving survival rates [4]. However, their applications in substance abuse remain underexplored, highlighting an opportunity to expand generative AI into this domain.

A study on digital twin technology for mental health monitoring demonstrated its potential in predicting depression relapses through real-time patient data [5]. While innovative, it failed to leverage generative AI for proactive treatment planning, leaving a gap in comprehensive care for mental health and addiction.

Explainable AI has been emphasized in healthcare to enhance model transparency. For example, Shapley Additive Explanations (SHAP) were used to explain predictions in diabetes management [6]. Despite its relevance, few studies have applied XAI to drug consumption prediction, an area requiring further exploration due to its high-stakes nature.

Integrated approaches combining machine learning, digital twins, and XAI have shown promise in predicting patient readmission rates [7]. While achieving high accuracy, these models have primarily focused on chronic diseases, leaving substance abuse applications unexplored. Generative AI's integration into such frameworks remains a potential avenue for improvement.

Drug consumption monitoring studies using Random Forest models have demonstrated accuracy in predicting substance use based on demographic factors [8]. However, the omission of psychological and social dimensions reduces the effectiveness of these models in real-world applications, underscoring the need for more holistic approaches.

Digital twins have also been used for demand forecasting in healthcare, particularly during periods of high patient inflow [9]. While adaptable, these models often rely on historical trends, limiting their utility in addressing rapidly changing drug abuse scenarios.

Another study focused on using neural networks to model drug abuse intervention strategies, incorporating socio-economic data for predictions [10]. Despite its strong predictive performance, the lack of real-time adaptability restricted its practical implementation in dynamic healthcare settings.

Gaps in Existing Literature

The existing literature on predictive drug consumption and personalized treatment reveals several gaps. There is limited application of digital twin technology for real-time, personalized monitoring of drug use. Most models fail to integrate psychological traits like impulsivity and sensation-seeking, reducing prediction accuracy. Explainable AI (XAI) remains underutilized in drug consumption models, hindering transparency. Current solutions also lack scalability across a wide range of drugs. Lastly, the use of generative AI for dynamic, personalized treatment plans in substance abuse remains underexplored, presenting an opportunity for innovation in adaptive, data-driven healthcare solutions.

Computational Problem

The computational problem addressed in this research is predicting drug consumption and developing personalized treatment plans using dynamic simulation models. The primary challenge lies in the multidimensional complexity of patient-specific data, including physiological responses, behavioral tendencies, and adherence patterns, which are highly interconnected and require modeling of non-linear dynamics and high-dimensional relationships. Furthermore, treatment plans must dynamically adapt to continuous changes in a patient's health, behavior, and lifestyle, making static models inadequate. Another layer of complexity arises from the need to optimize multiple factors of efficacy, safety, simplicity, and adherence while considering individual patient contexts and behaviors. Additionally, data variability and class imbalance in datasets, such as the underrepresentation of certain drug use cases, necessitate advanced preprocessing to ensure predictive accuracy across all patient subgroups.

Proposed Solution.

To address this problem, our proposed solution integrates digital twin technology with generative AI to enable both predictive modeling of drug consumption and the generation of personalized treatment plans. By creating a digital twin for each patient, we can simulate their physiological responses, behavioral tendencies, and adherence patterns under various scenarios. The model will use advanced machine learning techniques to predict future drug consumption behavior based on various data. This predictive capability will allow healthcare professionals to foresee potential non-adherence and intervene before it negatively impacts patient outcomes.

In addition to predictive modeling, the generative AI component will develop personalized treatment plans that evolve with the patient's health data. These AI-generated plans will recommend medication schedules, dosages, and alternative therapies, optimizing treatment based on the patient's unique status, and predicted adherence behavior. As new data from the digital twin is continuously integrated, the treatment plan will be dynamically adjusted to ensure it remains aligned with the patient's needs and maximizes adherence.

To ensure that these AI-driven predictions and recommendations are transparent and interpretable, explainable AI (XAI) techniques, such as SHAP (SHapley Additive exPlanations) values, will be employed. This will provide healthcare professionals with clear insights into the factors driving the predictions and the reasoning behind specific treatment recommendations. By integrating predictive modeling, digital twin technology, and generative AI, this solution offers a novel approach to tackling the challenges of drug consumption prediction and personalized treatment planning, ultimately improving patient outcomes and advancing the application of AI in healthcare.

Methodology

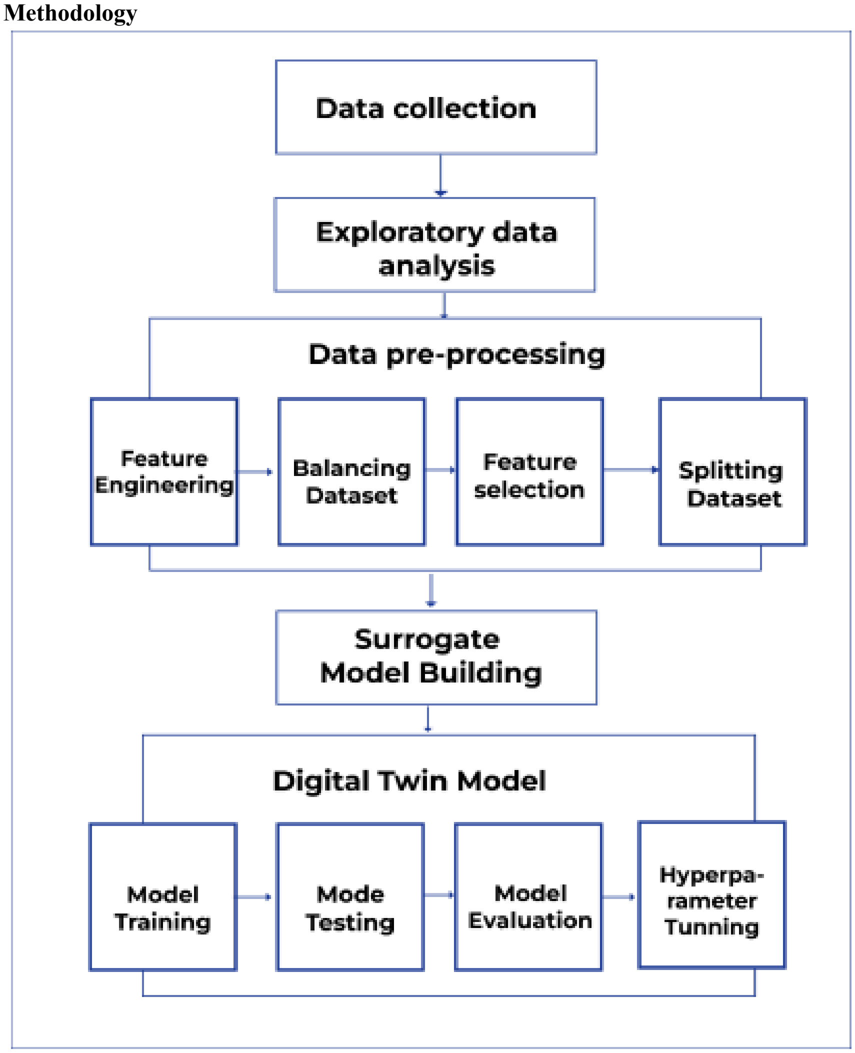

Figure 1: An overview of the methodology for creating the digital twin**.**

Dataset Description

The dataset was obtained from the UCI machine learning data repository and it contains records for 1885 respondents. Features include personality measurements which include NEO-FFI-R (neuroticism, extraversion, openness to experience, agreeableness, and conscientiousness), BIS-11 (impulsivity), ImpSS (sensation seeking), level of education, age, gender, country of residence, and ethnicity.

In addition, the dataset contains 18 legal and illegal drugs (alcohol, amphetamines, amyl nitrite, benzodiazepine, cannabis, chocolate, cocaine, caffeine, crack, ecstasy, heroin, ketamine, legal highs, LSD, methadone, mushrooms, nicotine, and volatile substance abuse and one fictitious drug (Semeron)
The shape of the dataset is: (1884, 32) with no missing values.

Exploratory Data Analysis and Initial Findings:

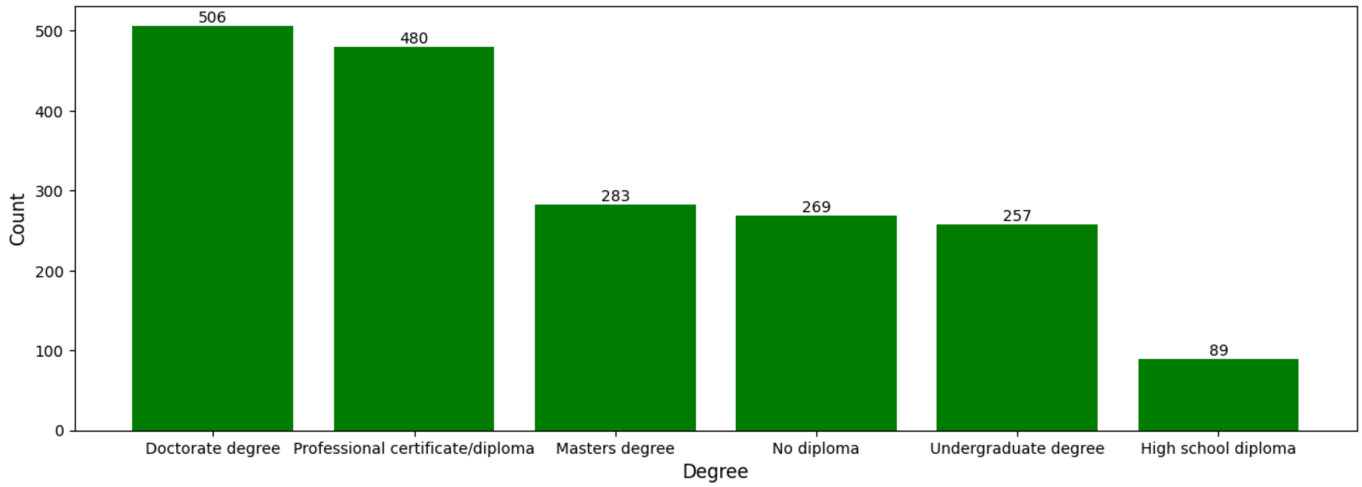

Figure 2: A graph showing the distribution of education in the dataset.

From the dataset, most of the individuals have an upper-level degree like a master's or doctoral, or a professional certificate. There are more higher-educated individuals compared to those with no high school or lower-level diplomas.

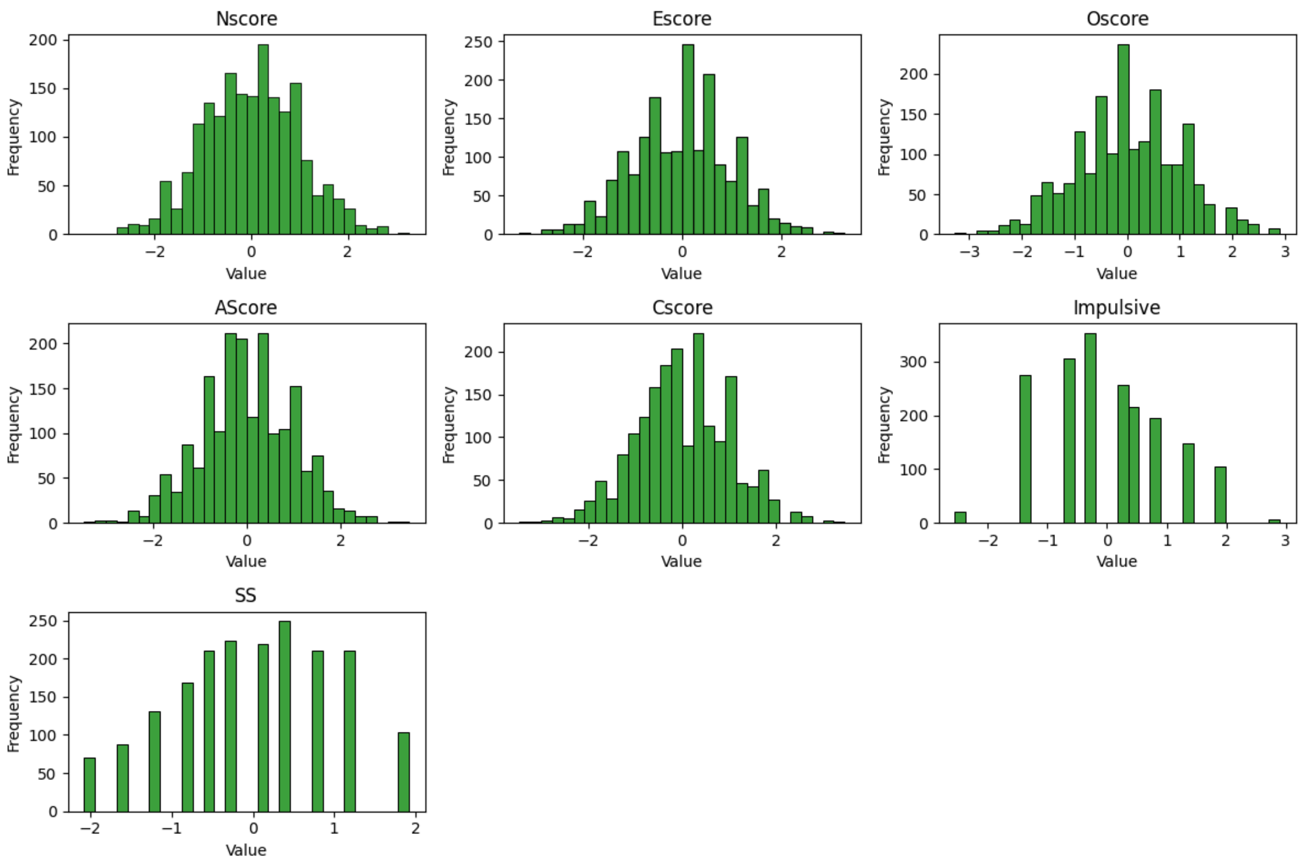

Figure 3: A compilation of graphs showing the distribution of different features like Ncore, Escore, Ocore, Score, Cscore, Impulsive, and SS

From the graphs, we can conclude that most of these features are normally distributed with the scores centered around the mean.

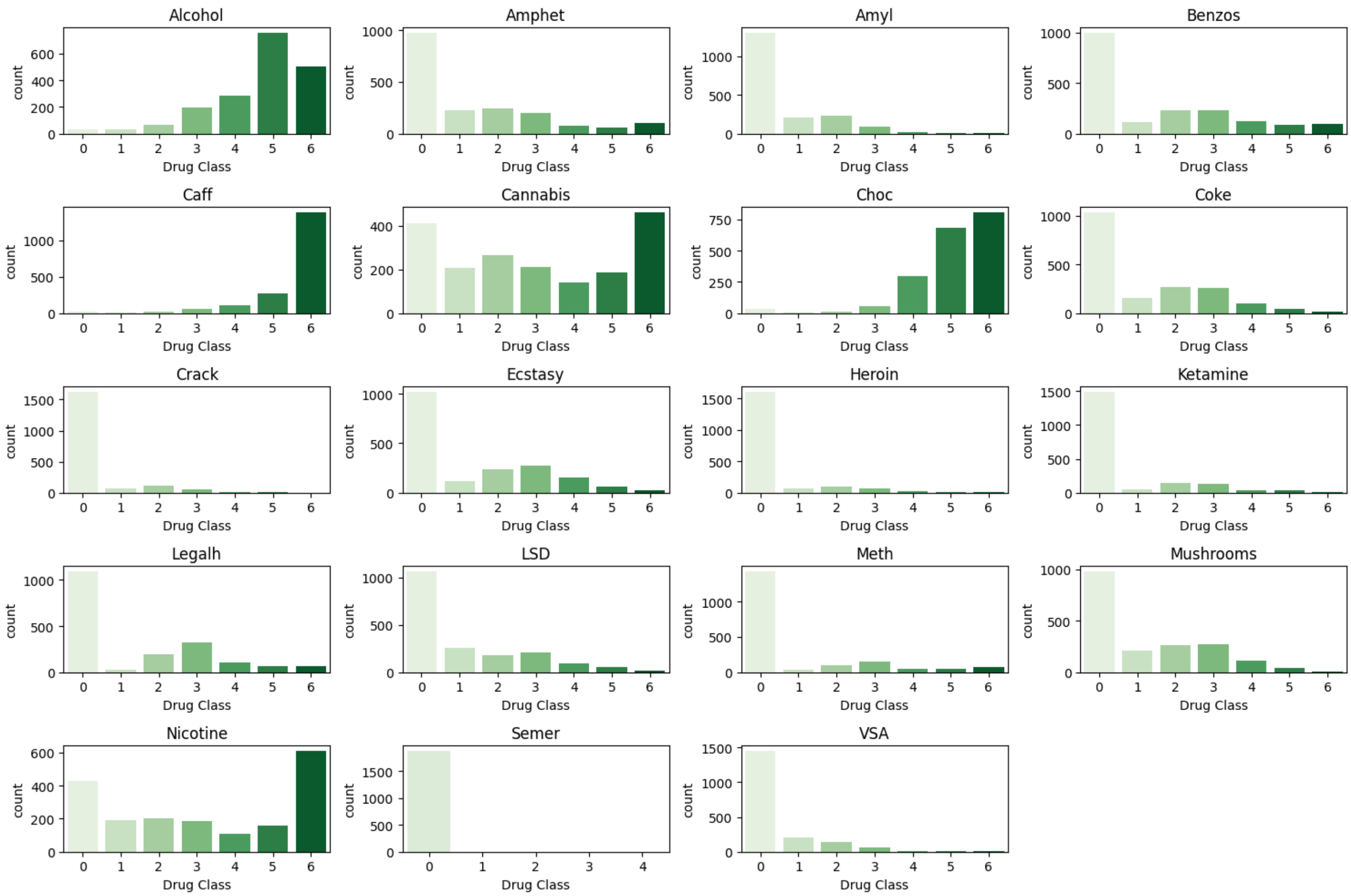

Figure 4: A collection of graphs showing the distribution of drug usage in our dataset for each drug.

From the graphs, we discovered that our dataset is imbalanced as there are several users or non-users compared to other categories for each drug. We also learned that drugs like alcohol, caffeine, cannabis, chocolate, and nicotine are the most frequent users.

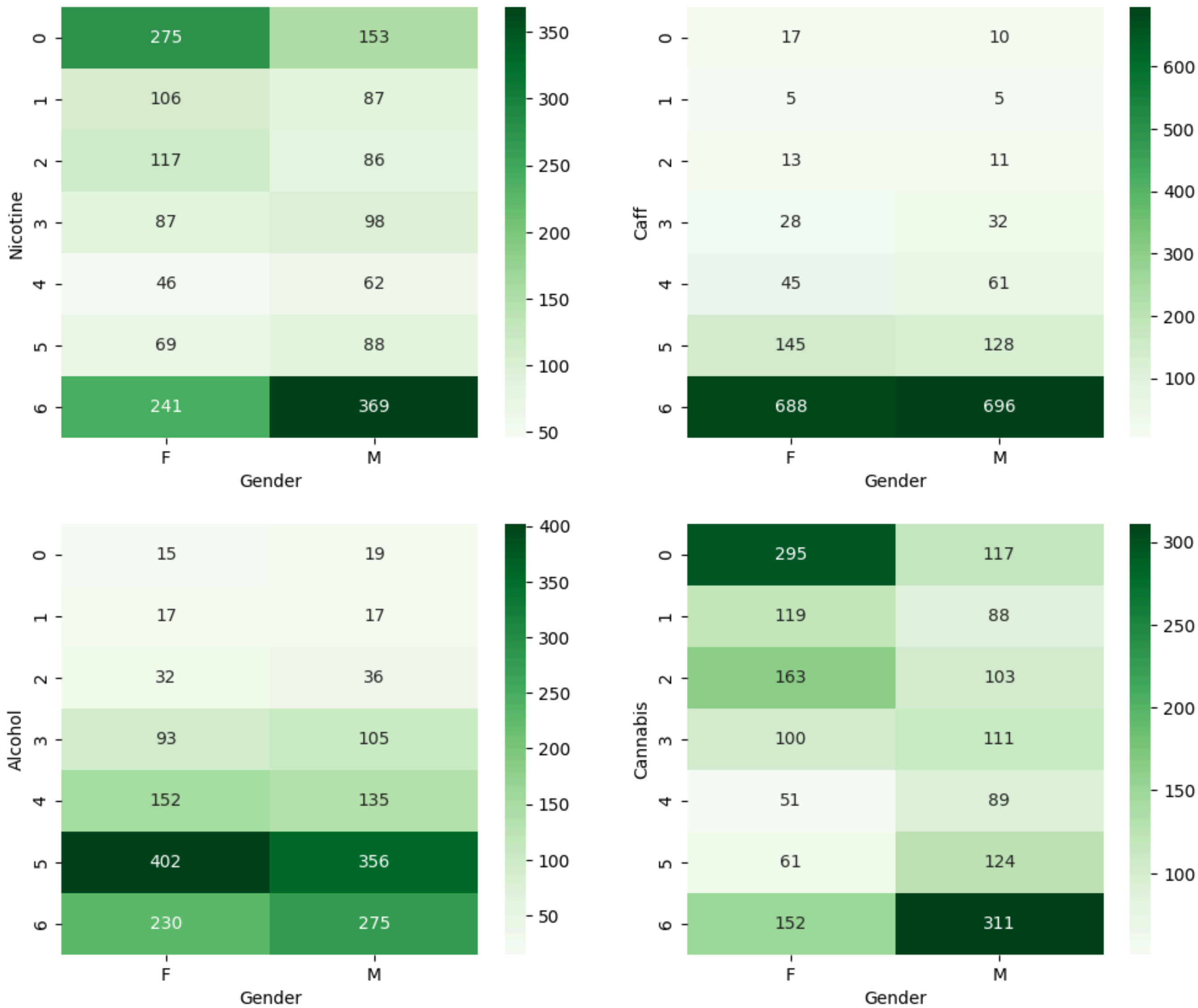

Figure 5: A graph showing the gender distribution against frequency of drug usage.

There are more women than men who have never tried nicotine or cannabis, but there are no major differences between the consumption of men compared to women otherwise.

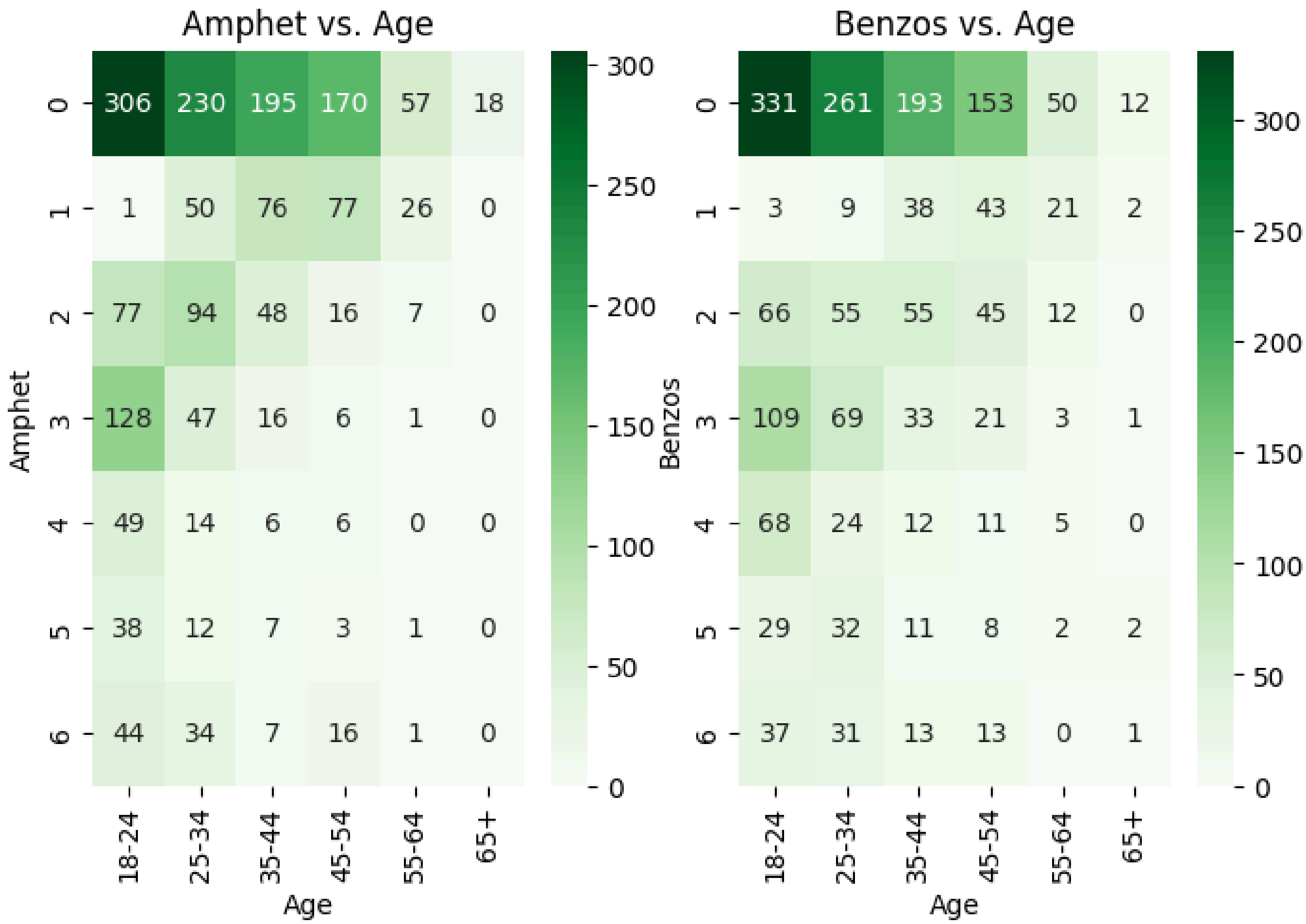

Figure 6: A graph showing age distribution against drug usage frequency.

The older the individual there are less observations of those who have never tried these drugs. We also notice that there are younger individuals who take these drugs more frequently than older individuals.

We addressed class imbalance for drug prediction using SMOTE, balancing the training data. Feature selection was performed using Recursive Feature Elimination (RFE) with a Random Forest classifier, identifying the top 10 relevant features.

The data was then standardized to improve model performance. Key insights revealed strong correlations between personality traits like neuroticism and impulsivity and drug consumption, laying the foundation for predictive modeling and highlighting the psychological factors influencing heroin usage.

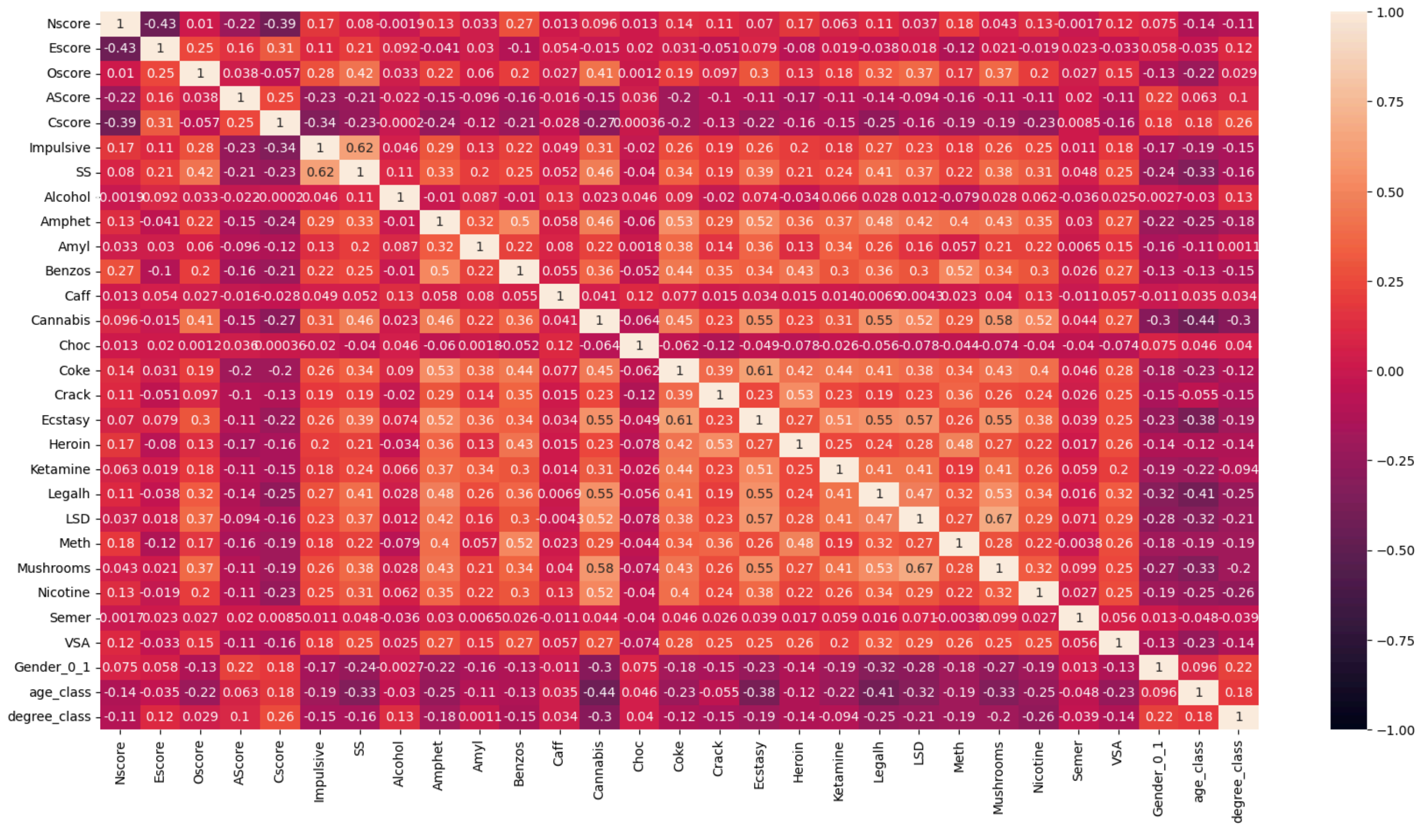

Figure 7: The heatmap shows correlations between demographic factors and drug use, indicating significant co-occurrence patterns.

Modeling and XAI Results

In the modeling phase, we implemented binary classification and multi-label classification approaches to predict drug usage across multiple substances, including heroin and others. We utilized various machine learning algorithms, such as Logistic Regression, Ridge Classifier, Support Vector Machine (SVM), and Random Forest, to analyze the features derived from the dataset. Each model was trained on a balanced dataset using SMOTE to address class imbalance and hyperparameter tuning was conducted through GridSearchCV to optimize performance. Metrics such as accuracy, precision, recall, and ROC-AUC were employed to evaluate model effectiveness, allowing for comprehensive insights into drug consumption patterns and enabling tailored intervention strategies.

BINARY CLASSIFICATION

HEROIN		**AMPHETAMINE**	
Logistic regression	**0.49**	**Logistic Regression**	**0.58**
Ridge classifier	**0.48**	**Ridge Classifier**	**0.37**
SVM	**0.98**	**SVM**	**0.90**
Random Forest	**0.98**	**Random Forest**	**0.88**

Table 2: Model results for four models predicting amphetamine addiction.

MULTI-LABEL CLASSIFICATION

MODEL ACCURACY	
Logistic regression	0.5242654683719322
XGBoost	0.8816425870534454
Extra Tree Classifier	0.649152886731757
CAT Boost	0.6562664371578532

Table 3: Results from four models under multi-label classification.

With Binary classification, Support vector machine models averagely produced the best results followed by Random forest and Logistic regression, which competed with the Ridge classifier for the third and fourth position. During multi-label classification XGBoost model performed best while CAT Boost performed second, Extra Tree Classifier came third and finally, Logistic regression performed worst.

Explainability

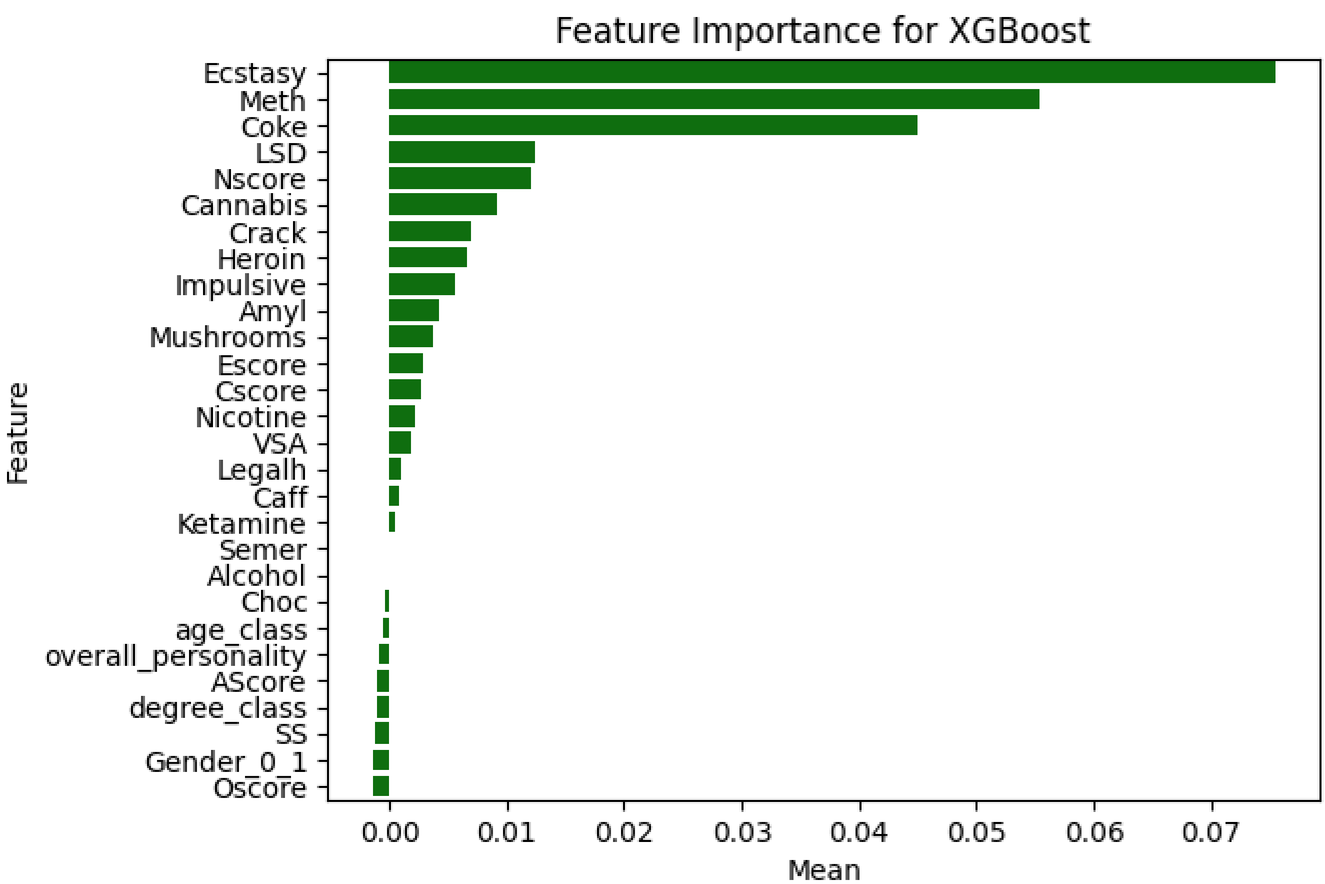

Figure 8: A graph showing the feature importance for the XGBoost model

The plot gives insight into which factors the XGBoost model considers most important when predicting drug addiction or drug usage. Ecstasy, Meth, and Coke stand out as the most influential factors, while personality traits like Nscore and Impulsive also contribute, albeit to a lesser degree. Less relevant features like gender and agreeableness have minimal impact on the predictions.

For deeper insights into feature importance and model decision-making, we employed SHAP (SHapley Additive exPlanations) values. SHAP provides a unified measure of feature impact, allowing us to understand the contribution of each feature to the model's predictions. The summary plot generated from SHAP values illustrated how specific demographic factors influenced the likelihood of drug use. Features like age, impulsivity, and certain drug use patterns demonstrated significant contributions, aiding stakeholders in comprehending the predictive mechanisms behind our model. By integrating these XAI techniques, we not only enhance transparency in our modeling process but also ensure that our findings can be effectively communicated to stakeholders, fostering trust in the model's predictions.

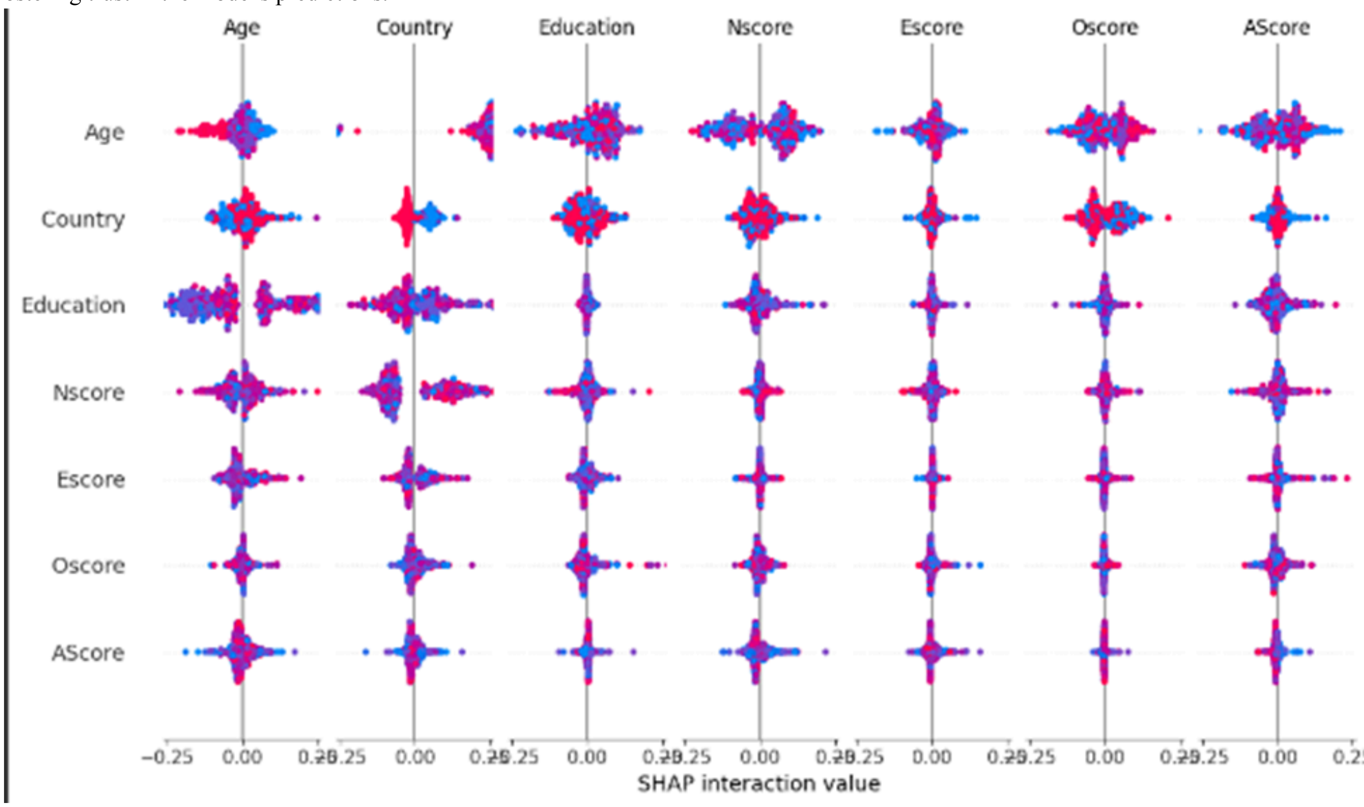

Figure 9. SHAP interaction values to offer explainability for the model.

Figure (9) visualises how demographic factors (age, country, education) affect drug use predictions, indicating the relationships between these variables and the likelihood of drug consumption, as determined by the model. The distribution reveals insights into how certain features positively or negatively influence the model's predictions for various drug classes.

DIGITAL TWIN RESULTS

We developed our digital twin in python by creating a surrogate logistic regression model and an error correction XGBoost model which we later merged to create a single digital twin model that performs predictions on data, we later tested our model on data from our test split data and our model was evaluated on some metrics including accuracy and area under a curve.

Our digital twin model yielded an **accuracy of 88%** after several tests.

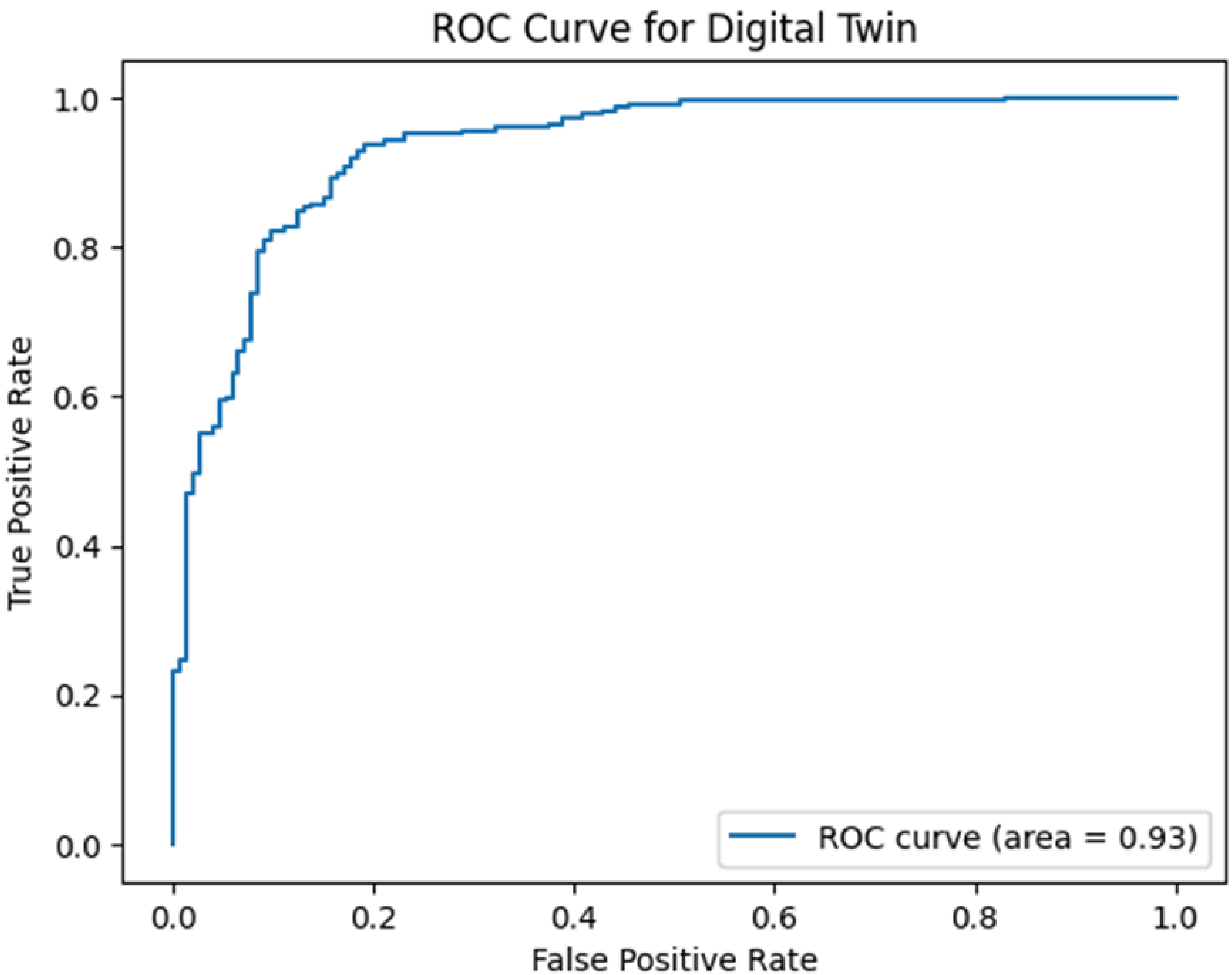

Figure 10: A graph showing the area under a curve results for the digital twin model.

The **area under the curve (AUC)** is shown to be **0.93**, which is a strong indicator of the model's performance. An AUC of 1.0 represents a perfect model, while an AUC of 0.5 means the model performs no better than random chance. In this case, an AUC of 0.93 indicates that the digital twin model has high accuracy in distinguishing between drug users and non-drug users.

DIGITAL TWIN MODEL EXPLAINABILITY.

The shap plot gives insight into which factors the digital twin model considers most important when predicting drug addiction or drug usage. Ecstasy, Meth, and Coke stand out as the most influential factors, while personality traits like **Nscore** and **Impulsive** also contribute, albeit to a lesser degree. Less relevant features like gender and agreeableness have minimal impact on the predictions.

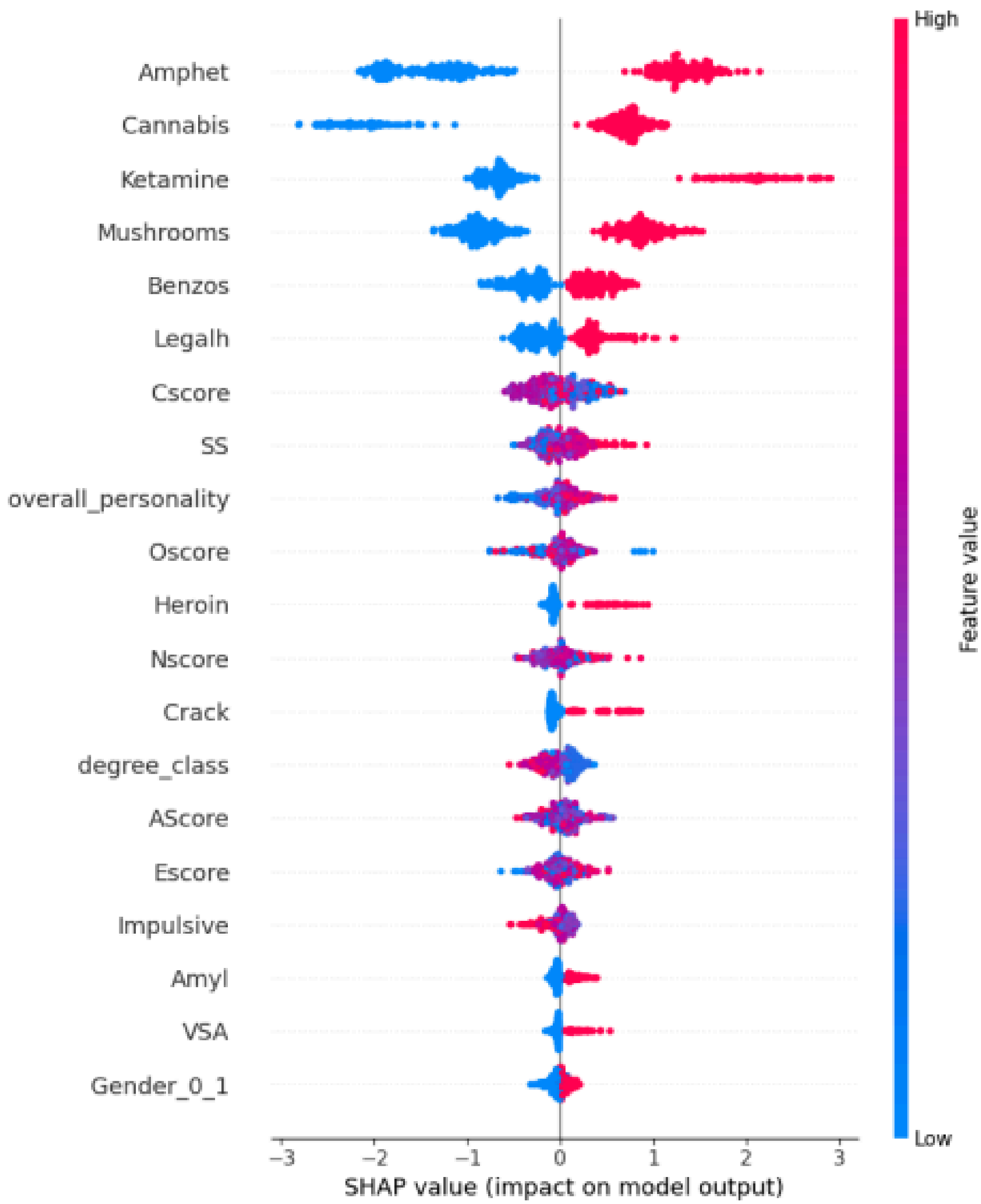

Figure 11: SHAP explainability graph for the digital twin model.

SIMULATION

The simulation aspect of this research utilizes an agent-based modeling approach to replicate and analyze the dynamics of drug consumption behaviors across a simulated population. This methodology leverages the parameters derived from the dataset to create a digital twin for each patient, enabling personalized and adaptive modeling. Agent-based simulation (ABS) was chosen due to its ability to model complex systems where individual behaviors, interactions, and environmental factors influence overall outcomes. Each agent in the simulation represents an individual with unique characteristics derived from the dataset, such as age, education, personality traits, and psychological scores, excluding the direct drug consumption data. These characteristics serve as input parameters that govern the agent's progression through predefined states of drug consumption.

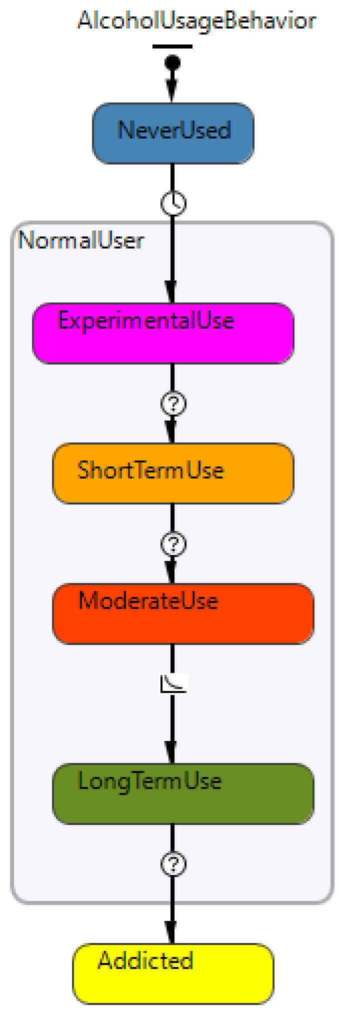

Figure 12: A flow diagram of the different states that an agent goes through to addiction. They included "Never Used," "Experimental," "Short-Term Use," "Moderate Use," "Long-Term Use," and "Addicted."

Each agent transitions between these states based on a dynamically calculated risk score which score is a probabilistic variable determined by the weighted contributions of the agent's attributes, such as neuroticism, impulsivity, sensation-seeking tendencies, and demographic factors like age and education.

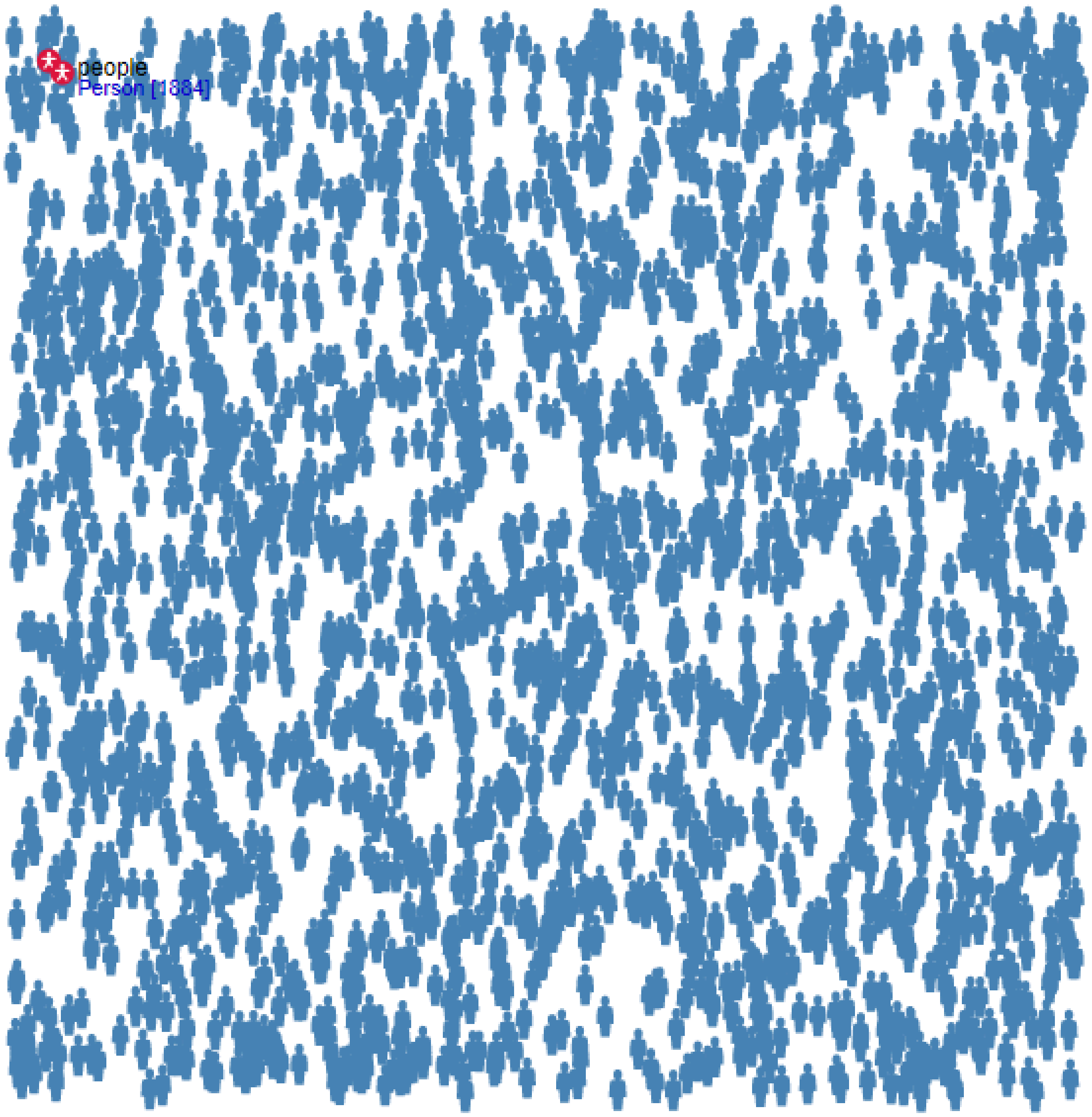

Figure 14: The image above shows a visual representation of the 1880 agents that were used in the simulation. The agents all have a single color (Blue) at the moment because they are still in their initial state.

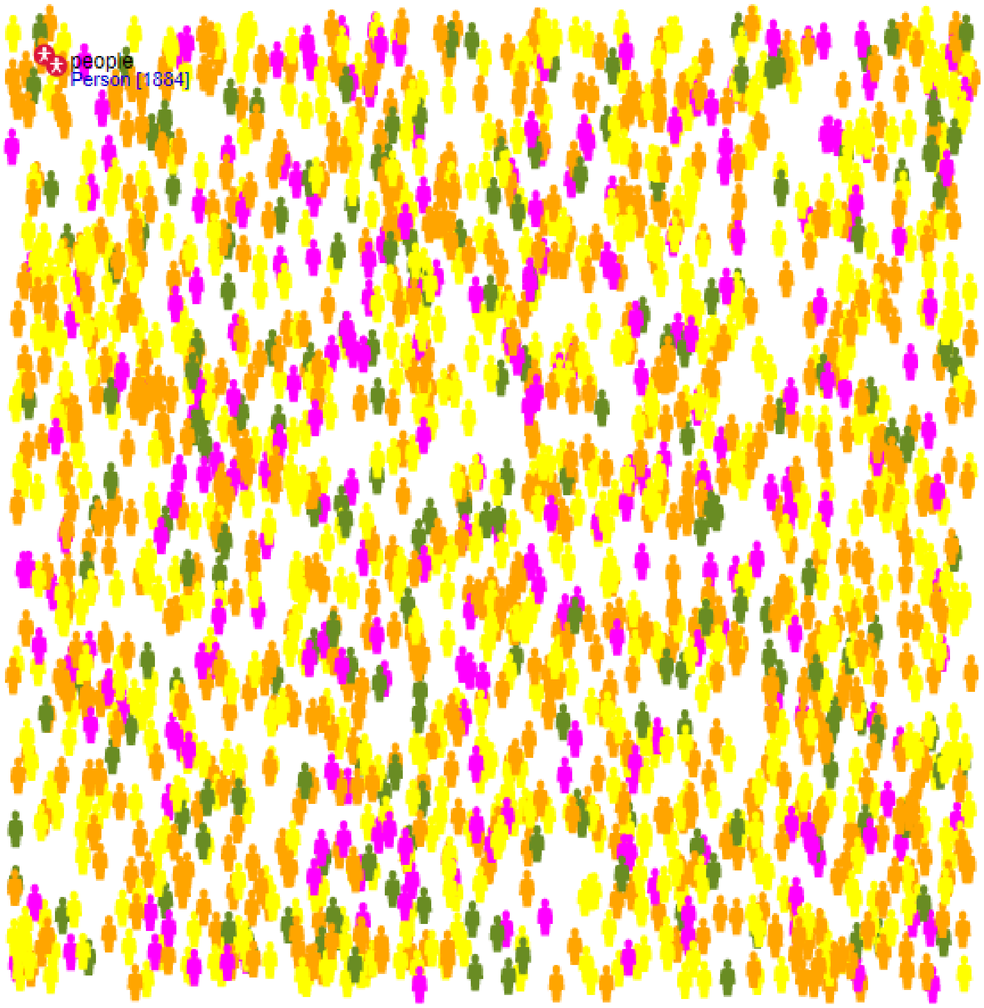

Figure 14: The image above shows a visual representation of the 1880 agents that were used, the different colors of the agents represent the different states in which and agent can be at a different time as shown in Figure eight.

The simulation outcomes provide valuable insights into the progression of drug consumption behaviors and the underlying risk factors. By analyzing the transitions of agents through the states, the model identifies high-risk populations and potential early indicators of addiction. These results align closely with real-world trends, where certain demographics and psychological traits correlate strongly with higher addiction risks. Additionally, the simulation facilitates targeted intervention strategies by identifying individuals at risk of progressing to more severe states. This makes the model not only a predictive tool but also a foundation for designing personalized treatment plans.

PERSONALISED TREATMENT PLANS GENERATION.

Drug addiction is a multifaceted medical condition that requires customized treatment plans tailored to the unique risk factors of each patient. In our project, we integrate a digital twin model with a GPT-3.5-based generative model to develop a comprehensive pipeline for generating personalized treatment plans. By leveraging data-driven predictions from the digital twin model and the natural language generation capabilities of GPT, the system aims to enhance treatment outcomes by delivering precise and personalized recommendations for each individual.

The digital twin processes patient data and provides predictions on drug consumption risks, which are subsequently classified into binary categories. These predictions, along with patient-specific features, are passed to the GPT model to create tailored treatment plans.
The generative component uses augmented prompts to incorporate critical information, including individual demographics, predicted risk probabilities, and model accuracy.

A caching mechanism was implemented to store GPT responses, enabling efficient reuse and faster performance for recurring queries. The retrieval-augmented component simulated a document retrieval system to provide relevant medical guidelines or treatment protocols. These guidelines were included in the GPT prompts to ensure the recommendations were aligned with current best practices and evidence-based standards.

The GPT-3.5 model successfully generated personalized treatment plans for each patient based on their predicted risk, demographics, and additional contextual information. These plans were comprehensive, including suggested therapies such as counseling, medication-assisted treatments, lifestyle interventions, and recommendations for follow-up care. The inclusion of contextual information retrieved from external guidelines ensured the treatment recommendations were grounded in best practices.

Case studies.

We tested our generative on several subjects from our test dataset and results from the digital twin model. And the results from the generative model are as follows with the generative model explaining the medical condition 0 representing no addiction, 1 representing addiction, as well as explaining the key factors and probabilities of the results.

Patient 1 Treatment Plan:

Based on the patient's Nscore predicting a condition of 0, it is recommended to focus on ways to prevent drug addiction rather than implementing a treatment plan. Here are some ways to avoid addiction to drugs:

1. Avoid peer pressure: Surround yourself with positive influences who support your decision to stay drug-free.

2. Stay busy: Get involved in hobbies, sports, or other activities that keep your mind occupied and away from drugs.

3. Seek support: Talk to a counselor, therapist, or support group if you are struggling with temptation or addiction.

4. Practice self-care: Take care of your physical and mental health through exercise, healthy eating, and stress management techniques.

5. Educate yourself: Learn about the effects of drugs on the body and mind to understand the risks involved in their use.

Remember, prevention is key to avoiding the harmful effects of drug addiction. It's important to prioritize your well-being and make choices that align with your values and goals. If you ever feel overwhelmed or in need of assistance, don't hesitate to reach out for help.

Patient 3 Treatment Plan:

Based on the predicted condition of 1 for drug addiction, the personalized treatment plan for the patient may include the following components:

1. Medical Detoxification: The patient may require medical detoxification to safely and effectively rid their body of the substance(s) they are addicted to. This process should be supervised by healthcare professionals to manage withdrawal symptoms and ensure the patient's safety.

2. Cognitive Behavioral Therapy (CBT): CBT is a commonly used therapeutic approach for treating drug addiction. It helps individuals identify and change harmful thoughts and behaviors related to substance abuse. This can help the patient develop healthier coping mechanisms and reduce cravings.

3. Support Groups: Encourage the patient to participate in support groups such as Narcotics Anonymous or SMART Recovery. These groups provide peer support, guidance, and encouragement from others who have similar experiences with addiction.

4. Medication-Assisted Treatment (MAT): Depending on the specific substance(s) the patient is addicted to, MAT may be beneficial. Medications such as methadone or buprenorphine can help reduce cravings and withdrawal symptoms for opioids, while medications like

disulfiram or acamprosate can be used for alcohol addiction.

5. Lifestyle Changes: Encourage the patient to make healthy lifestyle changes, such as incorporating regular exercise, practicing mindfulness and stress-reduction techniques, and prioritizing self-care activities.

If the patient's condition is 0 and no treatment plan is needed, it is still important to provide education on ways to prevent addiction to drugs. This may include promoting healthy coping mechanisms, and mindfulness practices, and educating the patient on the risks and consequences of drug abuse. Additionally, promoting a supportive environment and addressing any underlying mental health issues can also be beneficial in preventing addiction.

Patient 4 Treatment Plan:

Based on the predicted condition of 1 and the high prediction probability of 1.98, it is likely that the patient is experiencing some form of agreeableness-related issue. With a model accuracy of 0.88, we can be fairly confident in the accuracy of this prediction.

To create a personalized treatment plan for the patient, we will take into account their age, gender, education level, country of origin, and other relevant features such as their level of agreeableness, neuroticism, extraversion, openness to experience, and conscientiousness.

It is important to involve the patient in decision-making and consider their preferences when developing the treatment plan. This can include discussing their alcohol, drug, and substance consumption habits, as well as any other relevant lifestyle factors.

Based on the predicted condition of agreeableness related issue, treatment options may include therapy or counseling to address any interpersonal difficulties the patient may be facing. It may also be beneficial to explore stress management techniques or coping strategies to help the patient navigate challenging social situations.

Additionally, addressing any potential substance abuse issues, such as alcohol, drug, or substance consumption, is crucial for overall wellness and mental health. This could involve referral to a specialized treatment program or support group for further assistance.

Regular follow-up appointments and monitoring of the patient's progress will be important to ensure the effectiveness of the treatment plan and make any necessary adjustments. Collaboration with other healthcare professionals, such as therapists, psychologists, or addiction specialists, may also be beneficial in providing comprehensive care for the patient.

Overall, the personalized treatment plan should prioritize the patient's well-being, address the identified agreeableness-related issue, and consider their individual needs and preferences to promote long-term health and happiness.

Patient 7 Treatment Plan:

Based on the patient data provided, with a predicted condition of 0 and a prediction probability of 0.03, it appears that the patient may not be significantly at risk for severe health issues. However, it is important to note that the model accuracy is 0.88, indicating that there is still some level of uncertainty in the prediction.

Given the patient's Sensation Seeking score, it may be beneficial to focus on addressing any potential risk-taking behaviors. It is important to consider the patient's Age, Gender, and other relevant factors such as Education level, Country of origin, and Ethnicity when creating a personalized treatment plan.

In terms of treatment recommendations, it may be helpful to explore interventions that promote healthy decision-making and risk reduction strategies. Behavioral therapy or counseling could be beneficial in addressing any impulsive tendencies or risky behaviors related to substance use. Additionally, promoting healthy lifestyle choices and stress management techniques may also be important in supporting overall well-being.

It is essential to work closely with the patient to understand their individual preferences and goals for treatment. Open communication and a collaborative approach will be key in developing a personalized plan that is effective and aligned with the patient's needs.

Continued monitoring and follow-up care will be important to assess progress and make any necessary adjustments to the treatment plan. It is also recommended to involve other healthcare professionals as needed to provide comprehensive care and support for the patient.

Challenges and Limitations

Despite its effectiveness, the system has certain limitations. The accuracy of the digital twin model, though robust, may require further fine-tuning to handle specific patient subgroups or rare conditions. GPT-3.5 relies heavily on the quality of the prompts and contextual information provided, which can introduce variability in the treatment recommendations. Ethical considerations also play a significant role, as AI-generated plans must always be reviewed by qualified medical professionals to ensure patient safety. Furthermore, handling sensitive patient data necessitates stringent security measures to maintain privacy and compliance with legal regulations.

Future Improvements

Several enhancements can be made to improve the system's effectiveness and reliability. Implementing a more robust document retrieval system would allow for dynamic sourcing of medical guidelines and real-time updates. Incorporating real-time patient monitoring data could enable adaptive treatment plans that respond to changes in patient conditions. Adding explainable AI (XAI) capabilities would provide justifications for predictions and recommendations, fostering trust among clinicians and patients. Finally, deploying the system in clinical trials would provide valuable feedback, helping to refine its capabilities and measure its real-world impact on treatment outcomes.

Conclusion

In conclusion, digital twin technology has shown the ability to revolutionize the existing methods of diagnosing and predicting substance abuse based on individual personalities and demographic data to create personalized treatment plans with generative AI. In the future, we would want to update our digital twin with real-world data as it changes to perform better predictions. We would also want to design a graphical interface for our digital twin to make the technology more visually appealing. We would want to perform advanced hyperparameter tuning on our digital twin models to provide better predictions.

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