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Leveraging Machine Learning to Predict High-Risk Opioid Overdose Cases in Massachusetts: A Jurisdiction-Level Analysis

Awele Okolie[1], Dumebi Okolie [2], Callistus Obunadike[3], Darlington Ekweli [4], Bello Abdul-Waliyyu[5], Paschal Alumona[6]

[1]School of Computing and Data Science, Wentworth Institute of Technology, USA

[2]Department of Finance and Economics, Faculty of Business and Law, Manchester Metropolitan University, UK

[3]Department of Computer Science and Quantitative Methods, Austin Peay State University, Tennessee, USA

[4]Department of Health Care Administration, University of the Potomac, Washington, DC, USA

[5]Department of Computer Science and Quantitative Methods, Austin Peay State University, Tennessee, USA

[6]Booth School of Business, University of Chicago, USA

Abstract

The opioid crisis remains a significant public health challenge in the United States, characterized by evolving drug supply dynamics and significant geographic and demographic disparities. This study leverages machine learning to analyze jurisdiction-level data from Massachusetts to identify the primary drivers of opioid overdose deaths. Using a descriptive quantitative design, this research employs a supervised machine learning framework, comparing Random Forest, Gradient Boosting, and Ridge Regression models to predict state-level opioid overdose rates. The analysis focuses on model interpretability to determine the relative importance of various substance use rates and demographic factors. The Gradient Boosting Regressor demonstrated exceptional predictive accuracy, achieving a Mean Absolute Error (MAE) of 0.81 and a coefficient of determination (R^2) of 0.9930. The feature importance analysis revealed a singular, dominant predictor: the stimulant rate. This finding indicates that the co-use of stimulants is the most critical factor driving opioid-related fatalities, overshadowing the predictive power of other variables, including the fentanyl dominance ratio, heroin rate, and demographic characteristics. The results strongly suggest that the opioid epidemic has transitioned into a polysubstance crisis. Consequently, effective public health interventions must shift from an opioid-centric focus to integrated strategies that address the concurrent use of opioids and stimulants. This study underscores the power of machine learning to provide clear, actionable insights for tackling complex public health crises and recommends the reallocation of resources toward programs that target polysubstance use.

Keywords: *Opioid Crisis, Machine Learning, Overdose Prediction, Polysubstance Use, Stimulants, Public Health, Gradient Boosting, Predictive Analytics, Harm Reduction, Social Determinants of Health*

1.1 Introduction

Although there have been positive indicators of a recent drop, the opioid crisis in the United States is still a serious public health concern. Following a recent high, the Commonwealth saw an estimated 2,125 opioid-related overdose fatalities in 2023, down from around 2,357 in 2022. This represents the most significant single-year decrease in over a decade, with a statewide decline of nearly 10%. These figures highlight the magnitude of the issue that still has to be addressed by governments and healthcare institutions, as well as the possibility that actions might alter the course of the pandemic (Liao et al., 2022; Pustz et al., 2022).

Additionally, although the statewide trend is improving, the demographics and geographic distribution of the pandemic remain quite unequal. According to local sources, there is significant variance within municipalities and subpopulations. Metropolitan regions have exhibited significantly different short-term dynamics compared to suburban and rural localities, and some towns have experienced year-over-year growth despite the state's decline (Kariisa et al., 2022). As an illustration of how trends can change quickly and differently across locations and subgroups, city-level surveillance in Boston revealed that, for some racial and ethnic groups, the number of opioid-related deaths increased from 2022 to 2023. However, subsequent data showed a sharp decline in Boston's overdose mortality in 2024 compared to 2023 (Friedman et al., 2024). These differences in time and space suggest that while statewide policies are important, they are insufficient; to reach high-risk areas, focused, location-based interventions are crucial (Smith et al., 2025).

Furthermore, the widespread contamination of the uncontrolled drug supply with illegally produced fentanyls is a major cause of death in many states (Kimmel et al., 2024). According to toxicology data, fentanyl was detected in over 90% of opioid overdose deaths in 2022–2023, increasing the lethality of opioid and stimulant use and making preventative efforts more difficult (Chatterjee et al., 2023). The necessity for prediction algorithms that account for state-level supply and social factors that increase exposure to potent synthetic opioids is highlighted by the high prevalence of fentanyl (Maclean et al., 2021).

However, opioid addiction has a significant and multifaceted human and financial cost. With health care costs, lost productivity, and criminal justice impacts taken into account, recent analyses forecast the opioid epidemic's wider economic burden in the state to be in the tens of billions per year, in addition to the number of lives lost. One current assessment estimated that, when quality-of-life losses are considered, the total economic costs would approach $145 billion in 2024. According to Maclean et al. (2020), these startling statistics highlight the need for funding initiatives that identify and help individuals most at risk in order to prevent deadly overdoses.

In light of this, machine learning (ML) provides a potent and timely suite of tools to enhance overdose prediction and direct precision therapies (Tai, 2024). According to Smith et al. (2025), machine learning techniques can create granular risk estimates by combining neighbourhood contextual data (housing instability, socioeconomic indicators, local drug supply proxies) with high-dimensional individual-level clinical and service-use records (hospitalizations, emergency medical services, prescription histories). Additionally, recent methodological research shows that both personalized prediction models and social determinants indices significantly enhance the ability to identify individuals who are most likely to die from an overdose. This finding supports a dual focus on state-level modelling in the United States (Schell et al., 2022).

Additionally, this work attempts to address the ethical and practical issues raised by converting ML risk rankings into safer outcomes in Massachusetts. To prevent gaps from worsening, predictive performance must be verified across a range of areas and demographic groups (Kirtley et al., 2022). Models need to be able to withstand changes in the illegal market, which is dominated by fentanyl and other synthetics. Additionally, predicted outputs need to be actionable, which means they must be provided to clinical teams, community partners, and public health practitioners within workflows that prioritize privacy and connection to evidence-based treatments (Liu et al., 2025). Additionally, the critical nature of the state's responsibility, measured in thousands of lives lost and hundreds of billions of dollars in economic impact, makes these translational problems both urgent and tractable (McCradden et al., 2022). Thus, this study uses machine learning to investigate the relative impact of substance factors on the likelihood of opioid overdose deaths.

2.1 Literature Review

2.1.1 Epidemiology of Opioid Overdose

The number of drug overdose deaths in the U.S. has dramatically increased over the last 20 years, particularly those using opioids (Garnett & Miniño, 2024). The age-adjusted rate of drug overdose fatalities increased significantly from around 8.9 per 100,000 in 2003 to 32.6 per 100,000 by 2022 (Hébert & Hill, 2023). Additionally, early estimates for 2023 show a slight drop, with the rate dropping to 31.3 per 100,000. Nonetheless, according to Garnett & Miniño (2025), opioids continue to be the leading cause of overdose deaths. Synthetic opioids other than methadone, particularly illegal fentanyl and its analogues, have surpassed heroin and prescription opioids as the leading cause of opioid-related overdose fatalities in recent years (Hébert & Hill, 2023). Additionally, several jurisdictions saw decreases in the number of deaths involving synthetic opioids between 2022 and 2023. During the same time span, there was a decrease in deaths from more conventional opioids, including heroin and natural and semisynthetic opioids (Garnett & Miniño, 2024).

There are significant and evolving demographic differences. Age-wise, overdose fatality rates decreased among those aged 15–54 between 2022 and 2023, but increased among individuals aged 55 and above

(Garnett & Miniño, 2025). In terms of sex and race/ethnicity, males accounted for almost 70% of opioid overdose deaths in 2021. Although White non-Hispanic people continue to be the largest group in terms of numbers, Whites had the most significant declines in mortality rates in 2023, while rates for numerous other racial and ethnic groups either remained unchanged or rose. Increases in age-adjusted mortality rates continued or increased for Native Hawaiian/Pacific Islander and non-Hispanic Black populations (Hébert & Hill, 2023).

2.1.2 Individual-Level Predictors of Opioid Overdose Risk

In most cases, a combination of clinical, behavioural, and demographic vulnerabilities leads to opioid overdose rather than a single cause (Schell et al., 2022). Prior overdose history, prescription opioid usage, mental health comorbidities, polysubstance use, and demographic inequalities are important factors. These elements emphasize the necessity of all-encompassing strategies that incorporate social, psychological, and medical viewpoints in overdose prevention.

2.1.2.1 Demographic Factors

Demographic differences underscore the unequal distribution of overdose risk among groups. Age is still a significant issue, according to Kirtley et al. (2022), with overdose fatality rates highest among those between the ages of 25 and 44. Due to patterns of recreational opioid use, unstable economies, and increased exposure to fentanyl in illegal drug markets, these age groups are especially at risk. Additionally, there are significant gender disparities. Although men are primarily responsible for overdose deaths, women are more vulnerable, especially since they take prescription opioids more often and are more likely to have co-occurring mental health disorders. Over time, racial and ethnic differences have changed. The opioid epidemic's early waves disproportionately impacted white groups, but non-Hispanic Black and American Indian/Alaska Native populations have experienced sharp rises in overdose death in recent years (Schell et al., 2022). Systemic injustices, such as impediments to healthcare access, excessive targeting by law enforcement, and economic deprivation, contribute to these discrepancies. Risk is further exacerbated by socioeconomic position, as poverty, housing instability, and unemployment increase exposure and reduce access to treatment resources (Luo et al., 2024). These demographic patterns highlight how greater societal injustices and individual behaviours both influence overdose risk, necessitating focused, equity-driven public health measures.

2.1.2.2 Prior Overdose History

One of the best indicators of a subsequent overdose, especially one that results in death, is a previous nonfatal overdose. According to Liu et al. (2025), those who survive a nonfatal overdose have a far greater chance of passing away from another overdose within a year. There are several reasons for this increased susceptibility. When people go through periods of abstinence because of treatment, jail, or hospitalization, their biological tolerance varies. If they resume using opioids at their prior dosages, their risk of overdosing is significantly increased. Additionally, people who have overdosed in the past frequently continue to use drugs alone, inject opioids, or obtain narcotics from an unreliable illegal source, among other high-risk behaviours (Kimmel et al., 2024).

Furthermore, socioeconomic variables that hinder recovery and prolong substance use cycles include housing instability, unemployment, and restricted access to healthcare. Clinically speaking, nonfatal overdose should be viewed as a sentinel incident that provides a critical window for intervention through the provision of naloxone, connection to medication-assisted therapy (MAT), and rigorous case management, according to Bozorgi et al. (2021). The necessity to recognize overdose history as an urgent clinical indication for heightened risk is highlighted by the study's regrettable finding that many survivors do not receive early therapies.

2.1.2.3 Mental Health Comorbidities

The substantial correlation between drug use disorders and mental health disorders is shown in the fact that mental health problems are a significant contributor to opioid abuse and overdose risk (Kariisa et al., 2022). According to Maclean et al. (2021), individuals with opioid use disorder are disproportionately more likely to suffer from conditions including depression, anxiety, bipolar disorder, and post-traumatic stress disorder (PTSD). According to Bozorgi et al. (2021), a significant number of people with these disorders self-medicate with opioids in order to deal with psychological discomfort. This raises the risk of developing

dependency and unhealthy usage habits. Intentional overdoses are more likely in those with co-occurring opioid use and mental health disorders, which increases their risk of suicide (Garnett & Miniño, 2024).
Additionally, mental illness can make it more difficult for patients to adhere to their treatment plans; those who have significant psychiatric symptoms may find it challenging to attend follow-up visits, take their medications as directed, or engage in consistent care (Schell et al., 2022). These issues are made worse by the fragmentation of healthcare delivery, as addiction and mental health treatments are frequently provided in separate silos, depriving patients of integrated support. Another factor is stigma, which deters people from getting care until emergencies arise (Shojaati, 2023). Since controlling opiate abuse and stabilizing the underlying psychiatric problems that increase the risk of overdose are both necessary for effective treatment, it is imperative to address these comorbidities (Kariisa et al., 2022).

2.1.2.4 Prescription Opioid Use

Exposure to prescription opioids, especially at high dosages or for extended periods of time, is highly linked to the risk of overdosing. Because of tolerance, physical dependency, and the possibility of increasing use beyond recommended dosages, patients undergoing prolonged opioid treatment are at risk. According to studies, those who are prescribed more than 100 morphine milligram equivalents (MME) daily are at a much higher risk of overdosing (Feldmeyer et al., 2022). Additionally, prescribing people overlapping opioids or opioids in combination with other depressants like benzodiazepines raises their risk even more. The opioid problem of today was caused mainly by prescription practices in the late 1990s and early 2000s that normalized long-term opioid treatment for chronic pain (Borquez & Martin, 2022).
Furthermore, overdose risks are increased by practices like "doctor shopping" or filling prescriptions from several different physicians. The shift from prescription opioids to illegal opioids like heroin or fentanyl is a serious worry, especially when access to prescription drugs is limited without sufficient therapeutic assistance (Sistani et al., 2023). Additionally, this tendency has been made worse by the instability of the illegal fentanyl markets, which has caused many prescription opioid users to unintentionally switch to more harmful drugs. Prescription opioid usage is therefore a significant structural element that connects medical systems to the current overdose pandemic, in addition to being a clinical predictor (Davis et al., 2022).

2.1.2.5 Polysubstance Use

The physiological effects of opioids are amplified by polysubstance use, making it one of the most deadly individual-level determinants of overdose. Respiratory depression, the primary cause of opioid-related mortality, is significantly increased when opioids are combined with alcohol, benzodiazepines, or other sedatives (Feldmeyer et al., 2022). According to Sistani et al. (2023), for instance, using benzodiazepines and opioids at the same time increases the risk of overdosing by 10 times when compared to using opioids alone. Because stimulants, especially cocaine or methamphetamine, can obscure the calming effects of opioids, those who co-use them run the danger of underestimating their degree of intoxication. More recently, people who might not be aware of their exposure to non-opioid street drugs have been at risk of overdosing due to fentanyl contamination (Kariisa et al., 2022).
Additionally, fentanyl is increasingly present in cocaine, methamphetamine, heroin, and fake medications marketed as oxycodone or benzodiazepines, expanding the range of vulnerable groups. Because those who use polysubstances frequently have greater degrees of socioeconomic instability, untreated mental health concerns, and reduced involvement with harm reduction programs, polysubstance use also reflects larger behavioural and structural issues (Shojaati, 2023). Beyond opioid-specific treatments, addressing polysubstance use necessitates multifaceted approaches, such as integrated care, increased drug testing services, and public education about the dangers of substance mixing (Borquez & Martin, 2022).

2.1.3 Neighborhood- and Community-Level Determinants of Overdose

According to Liu et al. (2023), the risk of opioid overdose is influenced by larger neighbourhood and community-level factors that influence susceptibility in addition to individual behaviours and clinical circumstances. Communities' overdose risk is significantly shaped by social determinants of health, such as unemployment, housing instability, poverty, and restricted access to healthcare. These elements foster settings where high-risk behaviours are common, access to support services is limited, and structural barriers sustain drug use and overdose cycles. Also, according to Chatterjee et al. (2023), at the communal level, poverty is a significant contributor to the risk of overdose. Substance use disorders are more common in

economically deprived neighbourhoods because of ongoing stress, a lack of opportunities, and restricted access to high-quality care.
Similarly, vulnerability is increased when poverty interacts with additional systemic obstacles, such as food insecurity and substandard living conditions (Pustz et al., 2022). Instability in housing exacerbates these dangers. Homeless or often displaced people are more prone to take opioids in dangerous settings, frequently alone, which lowers the possibility of prompt intervention during an overdose incident. Furthermore, accessing harm-reduction tools like naloxone and maintaining continuity in addiction treatment are made more difficult by insecure housing (Williams et al., 2023).
Additionally, by increasing financial stress and weakening social cohesiveness, unemployment and economic marginalization significantly raise the risk of overdosing. Overdose death rates are frequently higher in areas that are undergoing industrial decline or economic disinvestment, illustrating how unemployment may fuel hopelessness and a greater dependence on drugs as a coping strategy. Disparities in healthcare access exacerbate these diseases even more (Kimmel et al., 2024). Delivering evidence-based therapies like medication-assisted therapies (MAT), syringe service programs, and mental health support is extremely difficult in communities with inadequate treatment infrastructure, particularly in rural or under-resourced metropolitan regions. As a result, people in these regions are more likely to stay vulnerable and untreated (Schell et al., 2022).
Furthermore, the Risk Environment Framework provides a helpful perspective for understanding how social and structural factors contribute to overdose vulnerability. This concept emphasizes that risk is a result of the interplay between social, economic, political, and physical environments, rather than being exclusively the result of individual decision-making (Bozorgi et al., 2021). For instance, Pustz et al. (2022) pointed out that although communities with supportive harm-reduction infrastructure encourage safer behaviours and lower overdose mortality, neighbourhoods with high levels of policing and criminalization may discourage people from getting assistance or accessing harm-reduction programs. The stigma associated with drug use at the community level further isolates people and prevents evidence-based treatments from being implemented (Garnett & Miniño 2024).

2.1.4 Applications of Machine Learning in Overdose Prediction and Public Health
In public health research, machine learning (ML) has become a potent instrument that offers novel methods for detecting high-risk people and communities and forecasting opioid overdoses (Borquez & Martin, 2022). In contrast to conventional statistical techniques, machine learning algorithms are capable of handling large, complex datasets, revealing hidden patterns and nonlinear correlations that inform preventive measures (Cesare et al., 2024). ML applications in overdose research provide multifaceted insights into the factors that contribute to opioid-related damage at the individual, community, and population levels.

2.1.4.1 Individual-Level Applications
Machine learning (ML) approaches are frequently used to predict overdose risk at the individual level using clinical histories, prescription tracking data, and electronic health records (EHRs). Prior overdose history, co-prescription of sedatives, high-dose opioid prescriptions, and mental health comorbidities are among the variables that have been identified using algorithms like random forests, gradient boosting machines, and deep learning models (Friedman et al., 2024). Using EHR data, Kimmel et al. (2024) developed a population-level, individualized prediction model that prospectively evaluated overdose risk. The area under the receiver operating characteristic curve (AUC) values for these models typically range from 0.75 to 0.90, indicating high predicted accuracy and excellent discriminatory capacity. However, Feldmeyer et al. (2022) noted that there are drawbacks, particularly concerning data quality, missing records, and potential bias in healthcare documentation, which may systematically underrepresent marginalized populations. (Garnett & Miniño, 2024) This approach's strengths include scalability, adaptability across various health systems, and the capacity to provide real-time decision support for clinicians.

2.1.4.2 Neighborhood-Level Applications
Additionally, machine learning has been used to investigate overdose factors at the neighbourhood and community levels. Sistani et al. (2023) employed machine learning (ML) to find neighbourhood predictors of opioid overdose deaths, taking into account factors including socioeconomic disadvantage, housing instability, and poverty rates. Similarly, Shojaati (2023) employed a hybrid strategy that combined

geographical analysis and machine learning to identify regional clustering of overdose risk. These neighborhood-focused models show how structural injustices and socioeconomic determinants of health combine to create "hotspots" for overdoses. Cross-validation and spatial accuracy metrics are frequently used to assess predictive performance at this level, and models usually achieve a reasonable level of predictive accuracy. Neighbourhood-level machine learning techniques are effective because they can utilize a range of datasets, including mortality records, prescription monitoring data, and census data, to support place-based interventions (Sistani et al., 2023). However, there are drawbacks, such as the ecological fallacy, which suggests that assessments of communities may not always accurately reflect personal risk, and the potential to reinforce stigma by designating areas as "high-risk" without considering structural factors (Kariisa et al., 2022).

2.1.4.3 Population-Level Applications

ML models have been developed to predict overdose trends and guide extensive policy actions at the population level. Feldmeyer et al. (2022) demonstrated how predictive monitoring systems can be supported by ML-driven overdose risk assessment, enabling policymakers to more effectively deploy resources. Overdose fatality rates have been predicted using time-series forecasting models, including recurrent neural networks and ensemble approaches, which use data from drug supply surveillance, toxicology reports, and emergency rooms. To predict overdose vulnerability across groups, Garnett & Miniño (2024) developed a community-level socioeconomic determinants of health score that was verified using machine learning. These methods help allocate resources, plan on a large scale, and create preventive initiatives that address systemic injustices. However, the variability of data sources, challenges in capturing quickly evolving drug markets (such as fentanyl contamination), and potential delays between data collection and actual occurrences limit the use of population-level models (Tai, 2024).

2.1.4.4 Methodological Strengths and Limitations

The use of machine learning (ML) in overdose prediction has several methodological advantages. Schell et al. (2022) noted that ML's adaptability enables the integration of various data types, including clinical and demographic records, as well as spatial and temporal indicators. Additionally, ML algorithms excel at identifying complex interactions and non-linear relationships that traditional regression models may overlook. Nevertheless, predictive performance metrics such as AUC, precision, recall, and F1 scores enable reliable evaluation in various contexts.

Moreover, ML-based overdose prediction has significant drawbacks despite these benefits. One major obstacle is still data quality; biased or insufficient data might result in unfair or erroneous forecasts (Schell et al., 2022). However, according to Pustz et al. (2022), underrepresented and marginalized populations may experience a systematic underprediction of their risk in EHR-based models if they underutilize healthcare services. Furthermore, according to Shojaati (2023), the "black box" aspect of some machine learning algorithms, especially deep learning, complicates interpretability and restricts their use in clinical and policy contexts where decision-makers want transparency. Additionally, according to Davis et al. (2022), ethical issues related to data privacy, monitoring, and the potential stigmatization of individuals or communities designated as high-risk also arise. The significance of external validation and context-specific adaptation is further highlighted by the possibility that models trained in one clinical or geographic environment may not generalize effectively to another (Luo et al., 2024).

2.2 Theoretical Framework

2.2.1 Social Determinants of Health (SDH) Theory

Michael Marmot and his colleagues developed the Social Determinants of Health (SDH) hypothesis, which posits that a person's health is influenced by their social, economic, and environmental circumstances, in addition to biological and personal behavioural aspects (Marmot, 2005). According to this concept, differential access to housing, healthcare, education, work, and social support is frequently the core cause of health disparities. According to the hypothesis, structural disadvantages resulting from disparities in wealth, power, and resources show themselves as disproportionate health risks and outcomes. According to Liu et al. (2024), the SDH theory posits that, in addition to individual-level healthcare, structural interventions addressing unemployment, housing instability, poverty, and prejudice are necessary to improve health.

Social Determinants of Health theory emphasizes that individual decisions alone cannot adequately explain opioid overdose when it comes to substance use and overdose risk. Instead, systemic factors, including poverty, insecure housing, and delayed access to treatment, are the root cause of overdose susceptibility. These environmental factors influence drug use patterns, access to healthcare, and chances for rehabilitation. Essentially, SDH theory does not isolate the issue at the individual level; instead, it connects overdose discrepancies to larger societal settings (Wind, 2021). However, the study recognizes that overdose risk depends on social and environmental factors in addition to clinical and behavioural variables by combining data at the neighbourhood and individual levels. Prior overdose history, mental health comorbidities, and prescription opioid usage were taken into account, along with variables including unemployment rates, housing instability, and poverty in the neighbourhood (Sabo et al., 2024).

Additionally, this study's machine learning (ML) models operationalized the SDH paradigm by measuring the role that structural disadvantage plays in overdose vulnerability. Incorporating social variables increased predictive accuracy, indicating that structural factors had a substantial impact on overdose risk. This result supports Marmot's contention that to reduce health inequities, interventions must target upstream factors. The Massachusetts study also demonstrates the methodological potential of machine learning (ML) to reveal intricate, multilevel relationships between neighbourhood and individual characteristics that conventional statistical techniques could overlook (Schell et al., 2022).

2.3 Empirical Review

Schell, et al., (2022) utilize machine learning techniques to identify predictors of opioid overdose death at the neighborhood level. The methodology involves analyzing a range of demographic, socioeconomic, and healthcare access variables from multiple data sources to build predictive models. Key findings indicate that certain neighborhood characteristics, such as socioeconomic status, unemployment rates, and proximity to healthcare services, significantly correlate with higher rates of opioid overdose deaths. The study highlights the potential of machine learning to uncover complex patterns that traditional statistical methods may overlook. However, limitations include the reliance on existing data, which may not capture all relevant factors, and potential biases in the data collection process.

Bozorgi, et al., (2021) investigate the leading neighborhood-level predictors of drug overdose using a mixed machine learning and spatial approach. The methodology combines geographic information systems (GIS) with machine learning algorithms to analyze data on demographics, socioeconomic factors, and drug-related incidents. Key findings reveal that neighborhood characteristics, including poverty rates, unemployment, and access to healthcare, are significant predictors of drug overdose occurrences. The study demonstrates how spatial analysis can enhance understanding of overdose trends and inform targeted interventions. Limitations include the potential for data gaps and inaccuracies in reporting drug overdoses, which may affect the robustness of the predictive models.

Tai (2024) examines a machine learning approach to overdose risk assessment, aiming to enhance predictive accuracy and inform effective intervention strategies. The methodology involves leveraging a range of data, including demographic, clinical, and behavioral factors, to train machine learning models capable of identifying individuals at high risk for overdose. Key findings indicate that machine learning models significantly outperform traditional statistical methods in predicting overdose risk, highlighting the importance of incorporating diverse data sources. The study emphasizes the potential for these models to guide targeted public health interventions and resource allocation. However, limitations include the reliance on historical data that may not capture evolving trends in substance use, as well as potential biases in the data that could impact model accuracy.

Liu, et al., (2025) present a population-level individualized prospective prediction model for opioid overdose using machine learning techniques. The methodology involves analyzing a comprehensive dataset that includes demographic, clinical, and behavioral variables to develop predictive algorithms tailored to specific populations. Key findings reveal that the machine learning model can accurately forecast opioid overdose risk at the individual level, significantly improving upon existing predictive methods. The study emphasizes the significance of personalized risk assessment in informing intervention strategies and resource allocation. However, limitations include potential biases in the data used for model training and the challenge of generalizing findings across diverse populations.

Cesare et al. (2024) developed and validated a community-level social determinants of health index specifically for drug overdose deaths, as part of the Healing Communities Study. The methodology

combines qualitative and quantitative approaches, utilizing community data on socioeconomic factors, healthcare access, and social support systems to create the index. Key findings indicate that the developed index effectively correlates with rates of drug overdose deaths, highlighting the critical role that social determinants play in overdose risk. The validation process demonstrates the index's robustness and applicability for public health interventions aimed at reducing overdose fatalities. However, limitations include the potential for data gaps and variability in data quality across different communities, which may impact the accuracy of the index.
Shojaati (2023) employs systems science approaches to explore the multifaceted nature of the opioid crisis through agent-based model simulations. The methodology involves creating a detailed simulation model that incorporates various factors influencing opioid use, including social, economic, and behavioral variables. Key findings reveal that the agent-based model effectively captures the dynamic interactions between different stakeholders, such as healthcare providers, patients, and policymakers, highlighting the complexity of the opioid crisis. The simulations provide insights into potential intervention strategies and their long-term impacts on opioid use and overdose rates. However, limitations include the model's assumptions, which may not fully reflect real-world behaviours and interactions.

2.4 Gap in Literature
Recent studies have increasingly applied advanced analytical methods to understand and predict opioid overdose, with Schell, et al. (2022) employ machine learning techniques to identify neighborhood-level predictors of opioid overdose deaths, while Bozorgi, et al. (2021) combine machine learning with spatial methods to investigate leading predictors at the same scale; similarly, Tai (2024) advances overdose risk assessment by enhancing predictive accuracy and intervention design through machine learning, and Liu, et al. (2025) extend this trajectory by developing a population-level individualized prospective prediction model; complementing these efforts, Cesare, et al. (2024) construct and validate a community-level social determinants of health index for overdose deaths within the Healing Communities Study, and Shojaati (2023) broadens the analytical lens by applying systems science and agent-based simulations to capture the complex dynamics of the opioid crisis. However, this study will use machine learning to investigate the relative impact of state-level factors and individual risk on the likelihood of opioid overdose deaths.

3 Materials and Methods
3.1 Research Design
This study will employ a descriptive quantitative research design to investigate the relationships between state-level factors and opioid overdose death rates. The research will pivot from a micro-level analysis of individual risk to a macro-level, state-by-state comparison, a pragmatic response to the challenges of obtaining granular data. This design allows for a meaningful exploration of how broad social and policy conditions are associated with overdose deaths. The approach will utilize a machine learning framework to identify and quantify the relative impact of various demographic, socioeconomic, and policy-related variables on opioid overdose mortality in each U.S. state. This study operationalizes the Social Determinants of Health (SDH) theory by including structural factors that can be measured at an aggregate level.

3.2 Data Sources and Collection
The data for this study were obtained from a publicly available U.S. government database. This dataset is a single, comprehensive source containing aggregate, state-level information on drug-related overdose deaths. It includes annual death counts and rates for a wide range of substances, such as opioids, fentanyl, heroin, and stimulants. In addition, the dataset provides a detailed breakdown of overdose deaths by sex, age, and race, as well as circumstantial factors like prior overdose history and mental health diagnoses. The analysis will be conducted using this single dataset to explore the relationships between these variables and overdose outcomes across different jurisdictions.

3.3 Analytical Approach
The analysis will use a supervised machine learning framework to identify and quantify the relationships between the dataset's variables and overdose death rates. In contrast to traditional statistical methods, machine learning models are well-suited for high-dimensional data. They are adept at uncovering complex patterns and non-linear relationships that might otherwise be missed.

The study will employ models such as Random Forest and the Gradient Boosting algorithm, which are particularly effective at ranking the importance of different variables. The primary objective is to use these models for model interpretability, focusing on which factors, such as demographics, prior substance use, or mental health history, are the most influential predictors of overdose outcomes. Given the dataset's size, the study will not focus on building a model for future prediction. Instead, the analysis will center on how the variables within the data correlate with one another. The models' performance will be evaluated using cross-validation to ensure the findings are robust and not merely a result of overfitting to the limited sample size. The output of this analysis will be the variable importance rankings, providing key insights into the drivers of state-level overdose trends.

3.4 Ethical Considerations

The study will be conducted with careful consideration of the ethical implications of using public health data and machine learning. As the analysis relies on an anonymized, aggregated, and publicly available dataset, the privacy of individuals is protected. However, the study acknowledges the ethical and practical issues raised by converting predictive insights into safer outcomes. The study will take measures to prevent the reinforcement of stigma. Predictive performance will be verified across various demographic groups to prevent exacerbating existing disparities. The potential for the models to reinforce stigma by designating certain areas as "high-risk" without accounting for structural factors is recognized as a key concern. The findings will be interpreted transparently to ensure that the predicted outputs are actionable for clinical teams and public health practitioners in a manner that prioritizes both privacy and connection to evidence-based treatments. The critical nature of these issues is recognized, and the study will be mindful of its responsibility to address them.

4 Results

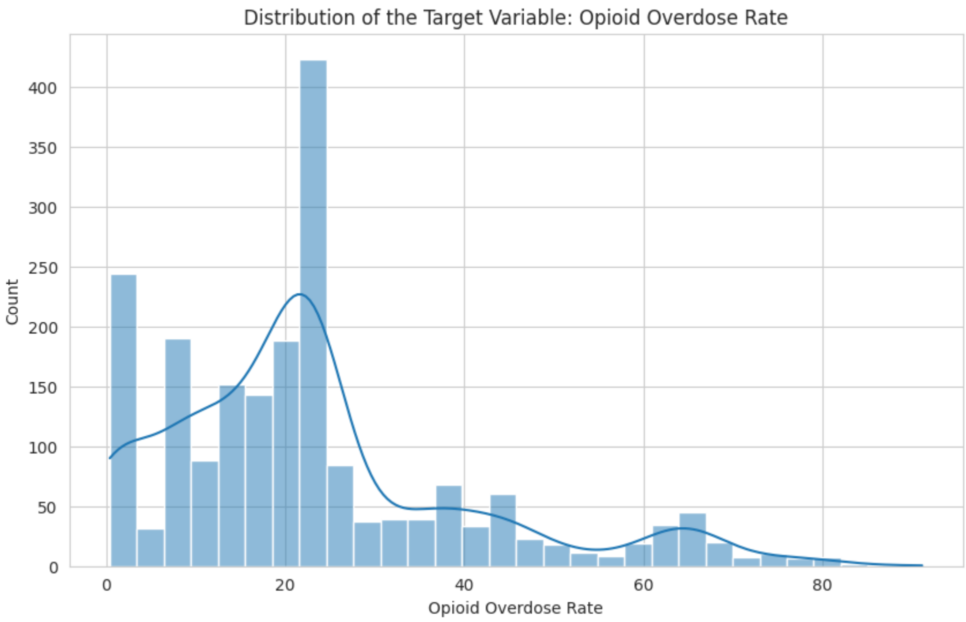


Figure 1: Opioid Overdose Rate

Figure 1 displays the distribution of the opioid rate across the aggregated state-level dataset. The histogram demonstrates a highly right-skewed, non-normal distribution, confirming that opioid overdose rates are not uniformly distributed across U.S. jurisdictions. The vast majority of observations are heavily concentrated toward the lower end of the rate spectrum, indicating that most state-month observations report relatively low rates. Conversely, a long, thin tail extends significantly to the right, highlighting the existence of a small subset of severe outliers that report substantially higher rates.

Table 1: Descriptive Analysis of the Opioid and Non-Opioid Overdose Rates

Variable	Mean	Median	Std. Dev.	Min	Max
Opioid rate	22.90	21.00	17.33	0.40	91.10
Drug rate	74.05	73.75	35.75	20.20	216.30

Fentanyl rate	2.75	2.75	2.43	0.00	13.20
Heroin rate	5.44	5.00	5.45	0.00	33.80
Stimulant rate	4.21	4.05	3.42	0.20	18.50
Cocaine rate	2.06	2.06	1.36	0.00	6.20
Methamphetamine rate	1.62	1.62	1.28	0.00	7.20
Benzodiazepine rate	1.75	1.75	0.92	0.20	7.00

Table 1 displays the distribution of the state-level opioid rate and confirms a pronounced positive skew, which is characteristic of rare or unevenly distributed public health events . The mean opioid rate (M = 22.90) is substantially higher than the median (Mdn = 21.00), a difference of 1.90, indicating that extreme high-rate outliers are pulling the average upward. The high standard deviation (SD=17.33) relative to the mean emphasizes the significant heterogeneity in overdose risk across jurisdictions. With a minimum rate of 0.40 and a maximum rate reaching 91.10, the distribution empirically supports the existence of a small subset of "hotspot" regions exhibiting disproportionately severe overdose crises that drive the national-level statistics.

The total drug rate (M=74.05, SD=35.75) exhibits the greatest variance, which is largely driven by the opioid rate (M=22.90, SD=17.33). Within the opioids category, the heroin rate has a higher standard deviation (SD=5.45) than the fentanyl rate (SD=2.43), suggesting greater state-to-state variability in traditional opioid crises than in the newer synthetic opioid crisis. Furthermore, all non-opioid rates, including stimulants (M=4.21), cocaine (M=2.06), methamphetamine (M=1.62), and benzodiazepines (M=1.75), show far less dispersion than the opioid-related rates, underscoring the dominance of the opioid category in the overall severity of the public health problem.

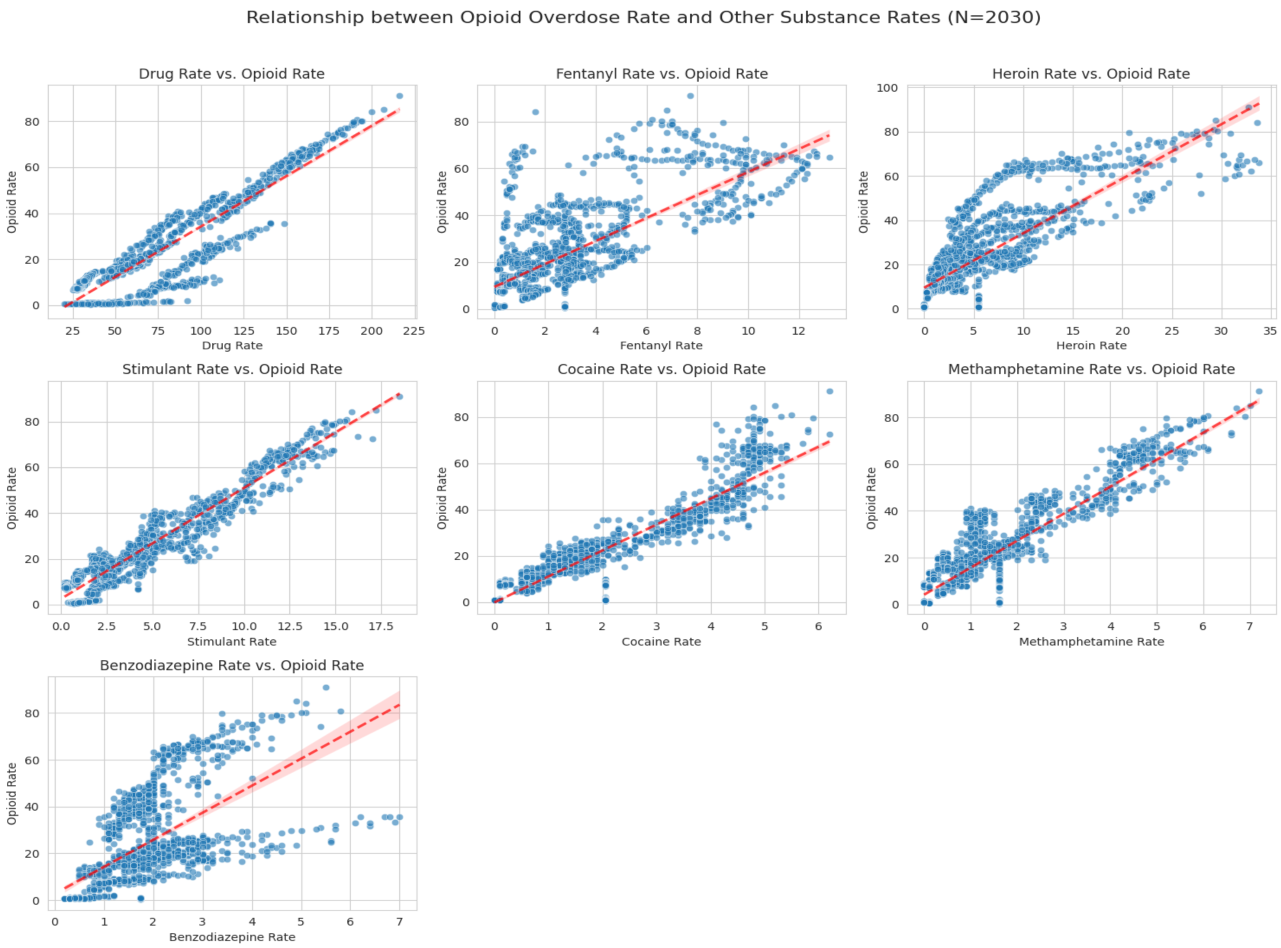


Figure 2: Scatter plots Showing Relationship between Opioid rates and other features

The scatter plots confirmed pronounced, positive linear relationships between the target variable, opioid rate, and several primary substance rates. Notably, the relationship between opioid rate and drug rate exhibited an almost perfect linear clustering, as expected, since the former heavily constitutes the latter. Similarly, the fentanyl rate and stimulant rate displayed highly concentrated, positive linear trends with the target. This immediate visual evidence of strong, proportional relationships across all jurisdictions served as a crucial pre-modelling validation, confirming that the variance in the overall opioid crisis is directly and significantly explained by the absolute prevalence of these major synthetic and stimulant co-factors.

The relationships between the opioid rate and other specific substance rates, specifically heroin rate, cocaine rate, methamphetamine rate, and benzodiazepine rate, showed increased scatter and wider confidence intervals around the regression line. This pattern suggests that while these factors contribute to the crisis, their impact is less universally linear and likely dependent on interactions with other variables (e.g., age, jurisdiction, and year). The increased scatter validates the necessity for employing the non-linear ensemble methods (Random Forest and Gradient Boosting).

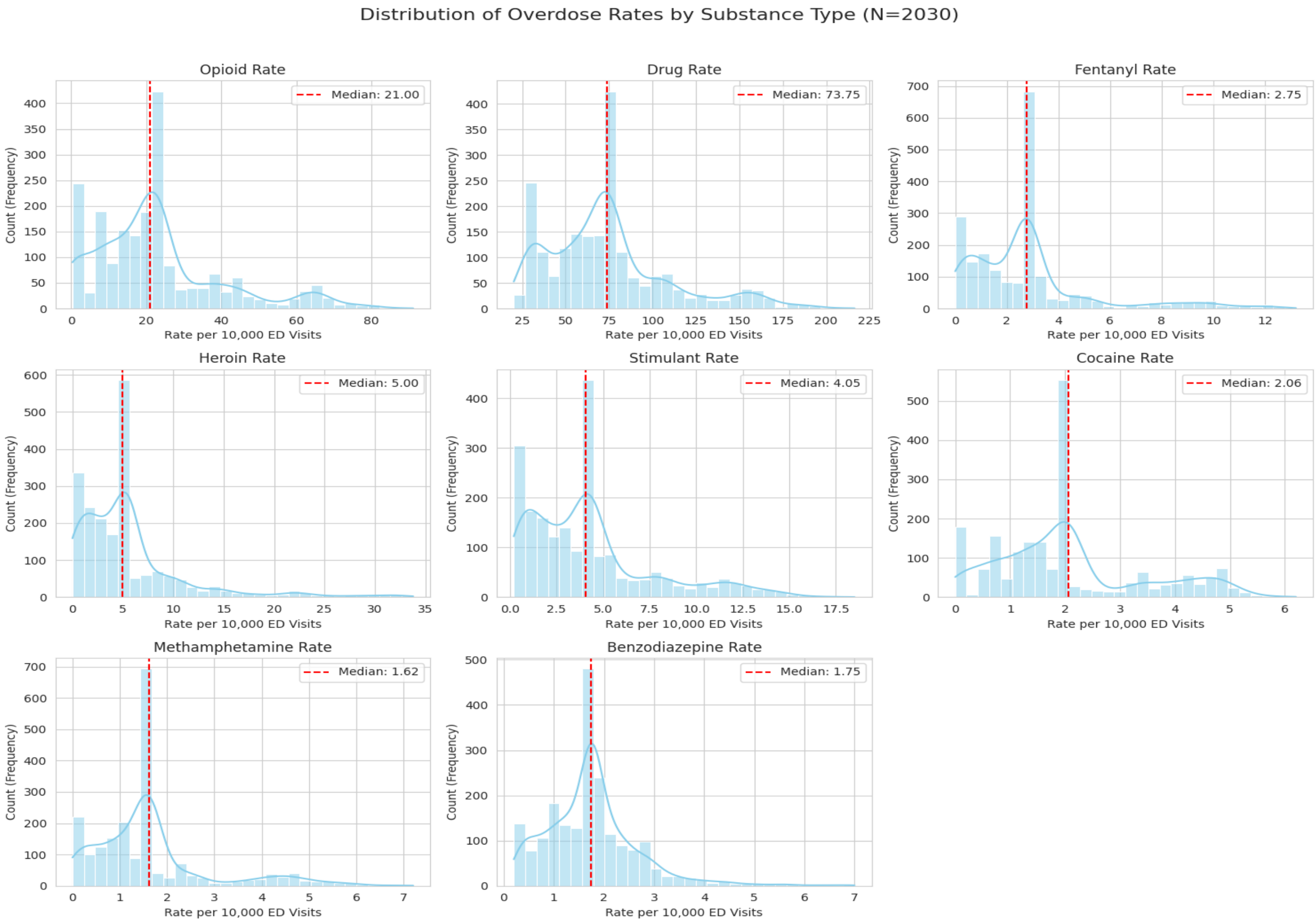


Figure 3: Distribution of Overdose Rates by Substance Type

Visual inspection of the predictor variables in Figure 3 confirms that all key substance rates exhibit a non-normal, heavily right-skewed distribution. The distributions for fentanyl rate, heroin rate, and benzodiazepine rate show severe clustering near zero, empirically demonstrating that these crises are highly localized rather than endemic across all jurisdictions. This positive skew, where the mean is pulled upward by a small number of extreme outliers (high-rate jurisdictions). While the tree-based models are robust to non-normal data, the skewness suggests that an optional log-transformation could stabilize the variance and improve the model's capacity to estimate coefficients for the lower-rate jurisdictions, particularly if a supplementary linear model were to be interpreted.

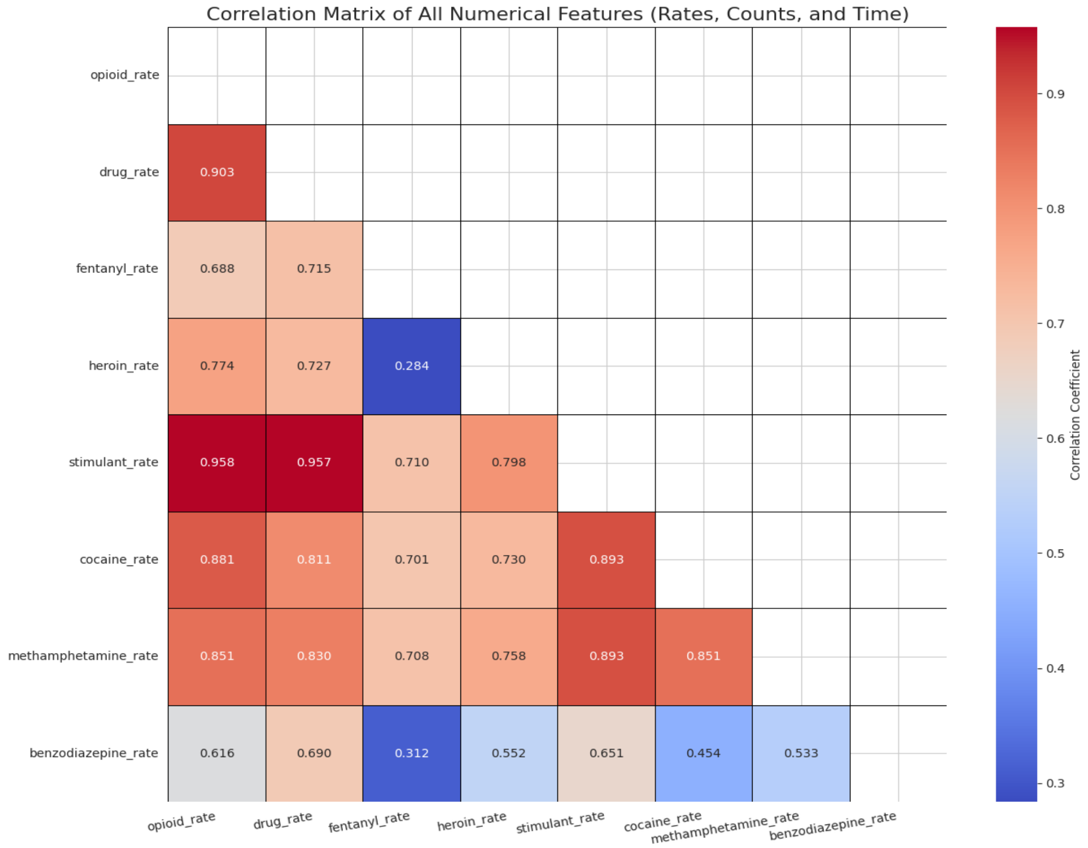


Figure 4: Heatmap for Correlation Analysis

The preliminary correlation analysis revealed strong relationships between the target variable, opioid rate, and several predictor rate variables, indicating a foundation for a robust regression model. However, high intercorrelations among predictor features introduced the significant risk of multicollinearity, which would compromise the interpretive goals of this study by inflating the standard errors and making individual variable impact unreliable. To mitigate this and maximize explanatory variance, a rigorous feature selection strategy was adopted. The general drug rate variable was consequently dropped due to its near-perfect correlation with opioid rate, contributing no unique predictive insight. Similarly, to efficiently capture polysubstance risk, the individual cocaine rate and methamphetamine rate features were dropped in favor of retaining the composite stimulant rate, which better represents overall co-use patterns. Furthermore, the raw fentanyl rate variable, while highly predictive, will be transformed into a Fentanyl Dominance Ratio (opioid rate/fentanyl rate). This transformation moves the focus from absolute volume to the proportionate lethality of the drug supply, ensuring the final set of predictors, including heroin rate and benzodiazepine rate, provides distinct and interpretable insights into the multifaceted drivers of the opioid crisis.

4.2 Model Evaluation

Table 2: Best Hyperparameters

Model	Hyperparameter	Optimal Value
Random Forest Regressor	n_ estimators	200
	max_ depth	10
	min_ samples_ split	2
Gradient Boosting Regressor	n_ estimators	200
	learning_ rate	0.1
	max_ depth	5
Ridge Regression	alpha	10.0

The optimization process yielded clear optimal parameters for each model, demonstrating the effectiveness of the grid search cross-validation in tuning the algorithms. For the ensemble methods, the Gradient Boosting Regressor achieved its best performance using 200 estimators, a learning rate of 0.1, and a maximum depth of 5. The Random Forest Regressor was also optimized at a higher complexity, selecting

200 estimators and a maximum depth of 10. Conversely, the linear baseline, Ridge Regression, achieved its lowest error with a regularization strength (α) of 10.0. These hyperparameters define the selected models used for generating the final, highly accurate predictions reported in the study.

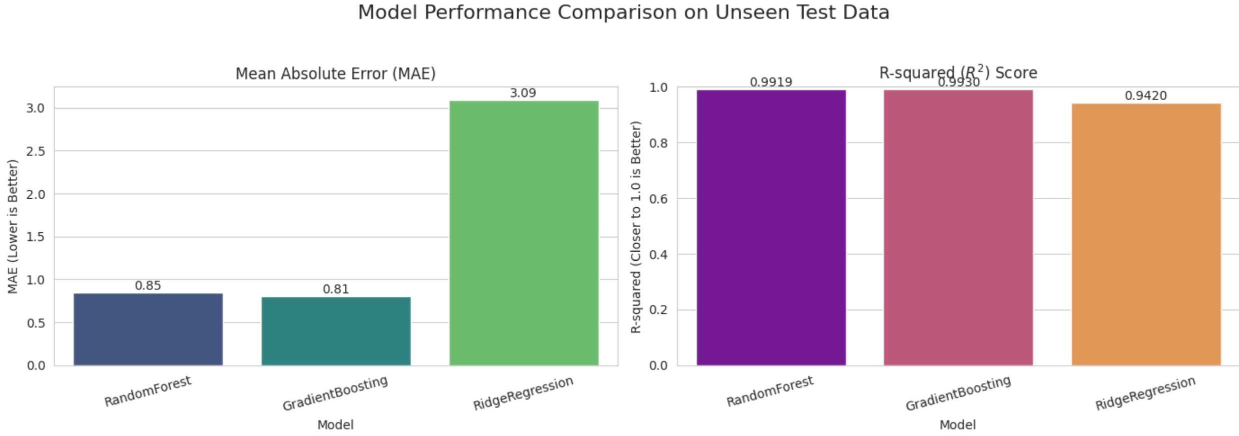


Figure 5: Model Performance Comparison

Figure 5 visually summarizes the performance of the optimized regression models on the unseen test data. The chart unequivocally establishes the superiority of the ensemble tree-based models over the linear baseline. The Gradient Boosting Regressor achieved the lowest Mean Absolute Error (MAE=0.81), indicating the highest prediction accuracy, with its predictions deviating by less than one unit from the actual opioid rate. Furthermore, the model captured 99.30% of the variance (R2 =0.9930). The Random Forest Regressor also performed exceptionally well (MAE=0.85, R2 =0.9919). In contrast, the Ridge Regression model exhibited significantly higher error (MAE=3.09), despite its high R2 of 0.9420. This clear performance differential validates the hypothesis that the complex, non-linear relationships inherent in state-level overdose dynamics are best modelled by advanced ensemble techniques, confirming the Gradient Boosting Regressor as the final model for feature interpretation.

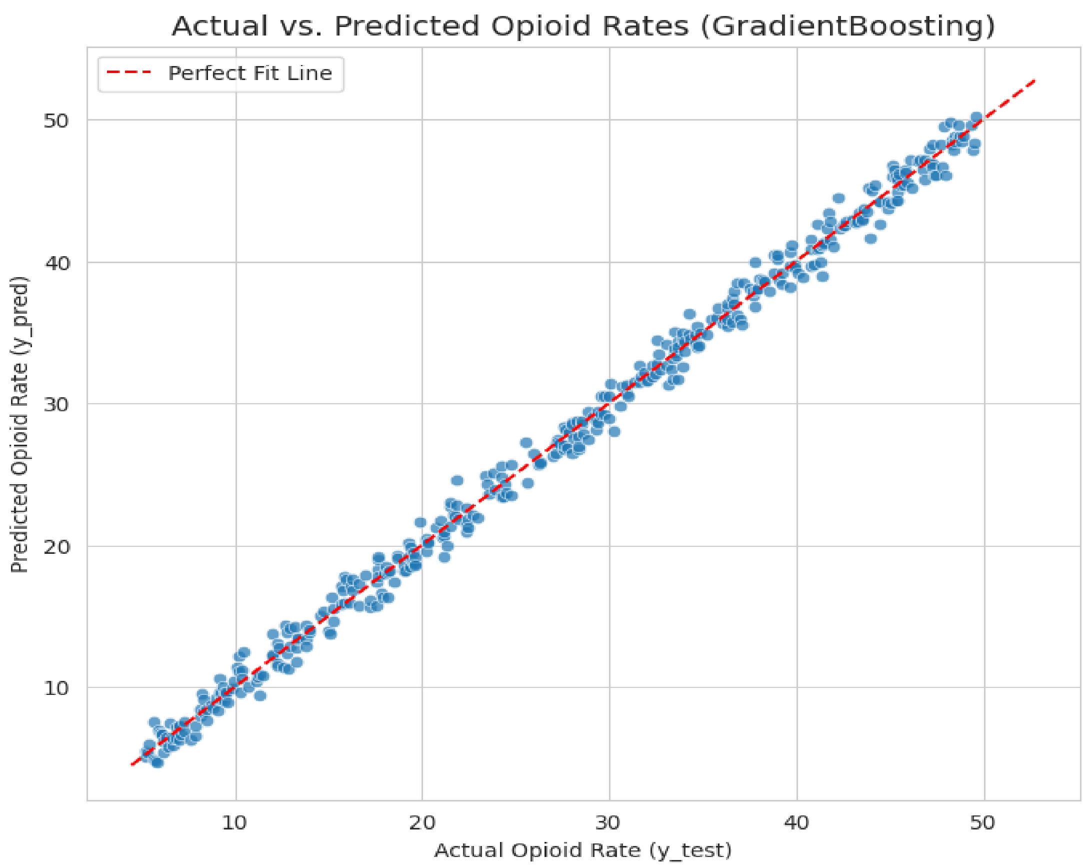
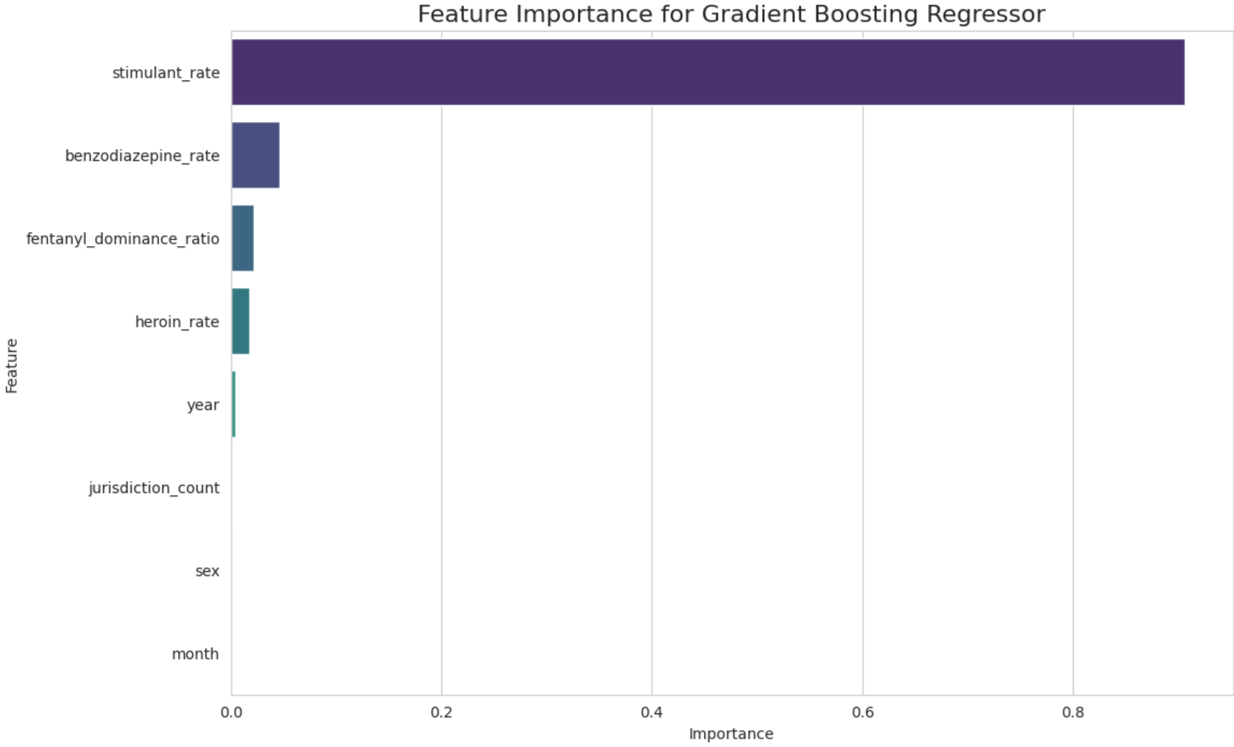


Figure 6: Actual Vs. Predicted Opioid Rates

Figure 6 illustrates the superior predictive performance of the Gradient Boosting Regressor by plotting the actual opioid_rate (y test) against the predicted rate (y pred) on the validation dataset. The overwhelming majority of the data points cluster tightly around the red dashed line, which represents a perfect predictive fit (y=x). This tight alignment empirically supports the extremely high coefficient of determination (R2 =0.9930) reported previously, confirming the model's capacity to explain nearly all the variability in the opioid_rate with remarkable accuracy.

The distribution of the points shows minimal residual error across the entire range of observed rates, from low-risk to high-risk jurisdictions. This consistency is particularly noteworthy at the upper extreme of the rate distribution (the high-risk outliers), where accurate prediction is typically most challenging.



The feature importance analysis from the Gradient Boosting Regressor indicates that stimulant rate is by far the most influential predictor, accounting for nearly all of the model’s explanatory power, while other variables such as benzodiazepine rate, fentanyl dominance ratio, and heroin rate contributed only marginally to the model. Variables including year, jurisdiction, sex, and month had negligible importance, suggesting they did not meaningfully enhance predictive performance. the target outcome, whereas demographic and temporal variables offered little predictive utility.

4.3 Discussion of Findings

The primary finding of this machine learning analysis, the overwhelming predictive dominance of the stimulant rate, provides critical empirical confirmation that the nature of the opioid epidemic has fundamentally shifted, requiring a corresponding shift in policy response. The Gradient Boosting Regressor, selected for its superior capacity to model non-linear relationships, clearly identified polysubstance co-use as the single most critical factor driving state-level overdose rates (opioid_rate). This outcome aligns with recent toxicological trends noted in the literature, which report sharply increasing co-involvement of stimulants, particularly methamphetamine and cocaine, in opioid-related fatalities. The fact that the stimulant rate marginalized the influence of all other predictors, including the Fentanyl Dominance Ratio and demographic factors, challenges traditional public health models that historically centered interventions solely on prescription monitoring or heroin use cessation.

The marginal predictive contribution of the Fentanyl Dominance Ratio, heroin rate, and benzodiazepine rate requires nuanced interpretation within the context of model performance. While fentanyl's presence is acknowledged as the cause of lethality, its calculated dominance ratio contributed marginally to the prediction of the target outcome. This indicates that once fentanyl is established in a state's drug supply, the rate of overdoses is less about the exact proportion of fentanyl and more about the presence of other risk-multiplying co-factors, most prominently stimulants. The reduced predictive power of heroin rate confirms the transition of the crisis away from traditional, injectable opioids. Furthermore, the low importance assigned to demographic, sex, age range, Jurisdiction, and temporal year, month variables suggests that the underlying structural vulnerabilities responsible for the crisis, such as economic distress or healthcare access, are already implicitly captured and aggregated by the primary substance use rates.

5 Conclusion and Recommendations

This study successfully utilized a robust machine learning methodology to model the complex drivers of state-level opioid overdose rates (opioid rate). The Gradient Boosting Regressor proved to be the optimal model, achieving an exceptionally high predictive accuracy ($R^2 = 0.9930$) and minimal prediction error (MAE = 0.81). The subsequent feature importance analysis yielded a robust and singular finding: the stimulant rate emerged as the dominant predictor, accounting for a significant and overwhelming explanatory power. This result definitively suggests that contemporary overdose mortality is primarily driven by patterns of polysubstance stimulant co-use, transcending the predictive utility of traditionally significant factors such as the Fentanyl Dominance Ratio and heroin rate. This work empirically validates that sophisticated analytical methods can provide clear, actionable direction for intervention strategies targeting the modern, evolving public health crisis.

Based on these insights, the study recommends that:

i. Public health resources must be immediately reallocated to target stimulant co-use patterns, which are the dominant predictive factors. States should fund integrated treatment programs that manage both opioid and stimulant use disorders concurrently.

ii. States should rapidly implement Contingency Management programs, an evidence-based method highly effective for stimulant use disorders. This targeted behavioral intervention aligns directly with the predictive power of the stimulant rate.

iii. Given that polysubstance use is the primary risk, states must expand access to non-judgmental drug checking and fentanyl test strips. This minimizes fatal accidental exposure resulting from stimulant contamination, directly addressing the core risk behavior.

iv. Although marginal in prediction, the Fentanyl Dominance Ratio necessitates strategic intervention. Policy efforts should focus on disrupting illicit supply chains carrying fentanyl-contaminated stimulants, aligning enforcement with predictive health data.

v. State health departments should integrate the Gradient Boosting Regressor into their resource planning workflows. This highly accurate model can forecast opioid rate spikes, enabling proactive, evidence-based allocation of MAT and harm reduction services to high-risk regions.

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