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ORIGINAL RESEARCH ARTICLE

Artificial intelligence with machine learning and the enigmatic discovery of HIV cure

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ABSTRACT

HIV's complexity has long presented a problem in the quest for a cure. However, the development of machine learning (ML) and artificial intelligence (AI) technology has opened up promising new directions for HIV cure research. This study investigates the impact of AI and ML on the discovery and development of an HIV cure to shed light on their potential role in hastening advancements in this field. The study employs quantitative methodology, and the execution of the methods is achieved by using AI and ML techniques for analysis processes and presenting the study's findings by utilizing the Kaggle.com HIV dataset, where pertinent features are found for the machine learning algorithm. Additionally, advanced statistical techniques, such as Structural Equation Modeling (SEM), to investigate the causal link between AI and ML utilization and the development of a cure for HIV is utilized. The robustness of the analysis is enhanced by using Penalized Ridge and Lasso Regressions. The study utilizes logistic regression as the machine learning model, and the mean square error is used to evaluate performance. Control variables, including the year, borough, the Uniform Hospitalization Fund (UHF) code, gender, age, race, concurrent diagnoses, percentage linked to care within three months, the prevalence of (People living with HIV/AIDS) PLWDHI, and percentage of viral suppression, deaths, death rate, and HIV-related death rate are all taken into consideration, to ensure a thorough analysis. This study finds that AI and ML are the future of the healthcare sector, providing promising opportunities for finding a cure for HIV and enhancing patient care. Further, the study confirms that new targets for HIV cure research can be found by utilizing AI and ML, and treatment outcomes and individualized treatment plans can also be developed. AI and ML can also enhance clinical trials, boost HIV prevention efforts, and lower the number of new infections.

Keywords: artificial intelligence; machine learning; drug discovery; HIV cure development; clinical trial optimization

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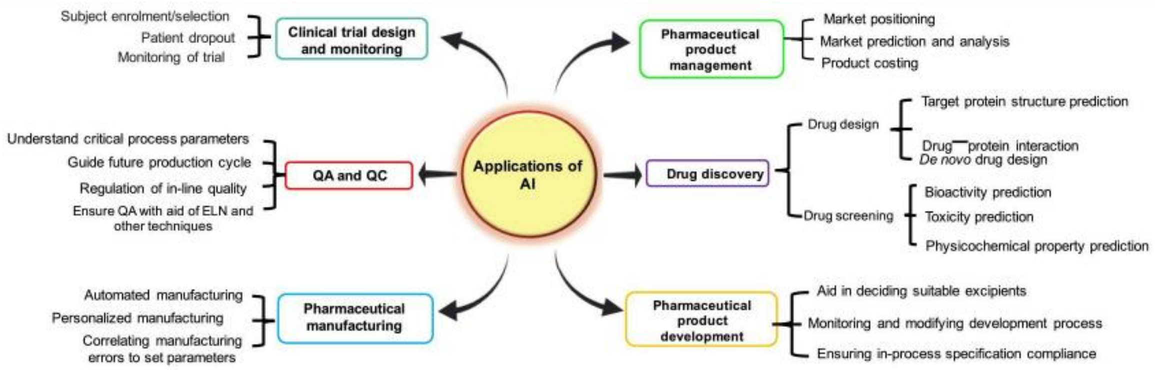
1. Introduction

The complexity of HIV has proved to be a significant challenge to the discovery and development of a cure for decades since its discovery in the 1980s. However, artificial intelligence (AI) and machine learning (ML) have emerged as powerful tools with great potential for advancing HIV cure research. AI and ML play a significant role in discovering and developing HIV cures in contemporary treatment approaches by providing an avenue to study big data and undertake tasks requiring immense human resources, time, and funds[1]. The latter is accomplished using computerized machines, rather than animal or human intelligence, to perceive, synthesize, and infer information. As such, the pharmaceutical and healthcare industry's future will be predominantly AI and ML dominated by 2045[2]. The success in finding the cure for Hepatitis C, SARS-CoV-2, the virus that causes COVID-19 and Ebola, significantly informs the healthcare industry of the potential of artificial intelligence to change and ultimately improve healthcare administration in the future[3,4].

Significant achievements of the pharmaceutical industry are based on the ability to provide solutions to global healthcare challenges and medication for diseases that threaten human well-being. As a result, the contemporary pharmaceutical sector utilizes artificial intelligence and machine learning techniques to design new healthcare interventions, notwithstanding discovering and developing drugs. For this reason, this study argues that artificial intelligence and machine learning technology are the future of the healthcare industry as the HIV cure and takes the responsibility to investigate and evaluate the impact of artificial intelligence (AI) and machine learning (ML) technology on the discovery and development of a cure for Human Immunodeficiency Virus (HIV) to broaden the understanding of the potential role of AI and ML in hastening breakthroughs in HIV cure research.

1.1. Overview of artificial intelligence and machine learning in healthcare

The creation of computer systems that are capable of learning, solving problems, and making decisions—tasks that typically require human intelligence—is known as artificial intelligence (AI). A subset of artificial intelligence (AI) called machine learning (ML) concerns the algorithms and models that let computers learn and make predictions or decisions based on data without being explicitly programmed[2]. The potential of AI and ML to transform various aspects of the healthcare sector has given them significant importance. They can analyze sizable amounts of data, spot trends and connections, produce new ideas, and support healthcare professionals' decision-making[2]. Improved diagnostic precision, personalized treatment plans, effective healthcare operations, and improved patient outcomes are some of the main advantages of AI and ML in healthcare. Moreover, AI and ML technology's applications in drug development, discovery, and development include predictive modelling, clinical trial optimization, precision medicine by optimizing patient data, and pharmacovigilance and drug safety by monitoring adverse drug events, trends, and patterns[5]. As AI and ML continue to evolve, they will play a crucial role in advancing healthcare and addressing some of the challenges faced by the industry.



Scheme 1. Summarized applications of artificial intelligence (AI) in different subfields of the pharmaceutical industry, from drug discovery to pharmaceutical product management.
Source: Paul et al.[2].

1.1.1. Drug discovery

Drug discovery is a multi-stage, labor- and resource-intensive process that involves multiple stages and extensive experimentation. However, the approach pharmaceutical research is carried out has significantly changed with the development of artificial intelligence (AI). AI techniques like machine learning, deep learning, and computational modelling have transformed the drug discovery process, identifying and developing novel therapeutic compounds more quickly and effectively. This study section presents an overview of the AI-assisted drug discovery process, emphasizing how this technology can potentially transform the pharmaceutical sector.

Target identification and validation

Finding and validating potential therapeutic targets is the first step in the drug discovery process. AI algorithms analyze enormous amounts of biological data, including genomics, proteomics, and clinical data, to identify and prioritize disease-related targets[2]. Using a variety of datasets, machine learning models play a significant role in the validation of targets by predicting target-drug interactions and determining target druggability. Conventional techniques of target identification and validation are tedious and time-consuming, considering the amount of data and human resources needed to study available[6]. Researchers use AI to accelerate the early stages of drug discovery and identify novel biological targets. As such, AI and ML technology significantly reduces the time taken to complete a specific stage of drug discovery and development.

Lead discovery and optimization

AI is essential for lead discovery and optimization after finding potential targets. Large chemical libraries are screened using virtual screening techniques powered by AI algorithms to find molecules with solid binding affinities to the target proteins. The time and resources needed for experimental screening are drastically decreased by using these techniques to quickly sift through millions of compounds. Moreover, the number of human resources required to complete the task is reduced, significantly reducing the cost of drug discovery and development. AI models predict various compounds' binding affinity and selectivity to identify promising lead candidates. For this reason, using AI and ML technology contributes to discovering and developing effective medicines. The latter confirms that the accuracy of data and the output of the corresponding discovery stage reduces the time that would otherwise be lost in conventional techniques.

Drug design and formulation

Creating new therapeutics has changed due to AI-driven drug design techniques. AI assists in the rational design of drug candidates by using molecular docking, molecular dynamics simulations, and quantum chemical calculations[4]. The optimization of drug structures for increased efficacy and fewer off-target effects is guided by computational models, which precisely predict the binding affinity and interactions between drug molecules and target proteins. The latter is achieved using AI and ML techniques that allow web-based 3D printing of developed drugs through formulation stocks. Moreover, the drug design and formulation stage are essential as it is primary to formulating diverse dosages that can achieve therapeutic effects by considering the number of compounds that make up a drug. AI also helps with formulation development by foretelling crucial characteristics for effective drug delivery, such as solubility, stability, and pharmacokinetics.

Toxicity prediction and assessment

In developing new drugs, evaluating drug candidates' safety and potential toxicity is crucial. To forecast and assess the potential risks related to candidate compounds, AI models analyze large datasets of toxicological data and further compare it to patient data to obtain accurate predictions of the toxicity of a specific drug. By learning from historical data, AI algorithms can find patterns and connections between compound structures and toxicological outcomes. The ability of AI and ML technology to predict the toxicity of candidate drugs in development enables researchers to avoid candidates that are likely to fail due to safety concerns and prioritize compounds with lower toxicity risks.

1.1.2. Drug development

Drug development includes the subsequent stages of preclinical and clinical testing, formulation optimization, and regulatory approval, whereas drug discovery focuses on identifying and optimizing potential drug candidates. By streamlining procedures, improving decision-making, and increasing the effectiveness and success rates of bringing new therapeutics to market, artificial intelligence (AI) has a transformative effect on drug development. This section of the study aims to give a thorough understanding of how AI is transforming the drug development process.

Preclinical testing

Before human trials, preclinical testing evaluates drug candidates' safety, effectiveness, and pharmacokinetic characteristics. Preclinical testing benefits from AI in several ways. AI algorithms first analyze enormous amounts of preclinical data, including animal studies and in vitro experiments, to uncover meaningful patterns and insights. This aids in the prediction of possible drug responses, the identification of toxicological risks, and the optimization of dosage regimens. Second, AI-driven algorithms support experiment design and interpretation, enabling practical data analysis and minimizing the expense and duration of experiments.

Clinical trial design and patient recruitment

The planning and execution of clinical trials is a crucial and time- and money-consuming component of drug development. By examining various elements like patient characteristics, treatment regimens, and endpoints, AI helps to optimize the trial design. Clinical trial designs that are more focused and effective can be made possible by machine learning algorithms that can identify patient subpopulations that are more likely to respond to treatment. AI also aids in patient recruitment by reviewing electronic health records and patient data to locate qualified candidates, cutting down on the time and expense associated with the process.

Real-time monitoring and data analysis

AI is essential for real-time monitoring and data analysis during clinical trials. Large amounts of clinical data can be processed and analyzed in real time by AI-powered systems, which can also spot patterns, anomalies, and potential adverse outcomes. This makes prompt intervention possible and improves patient safety. AI algorithms can also analyze and integrate various data sources, including biomarkers, imaging data, and patient-reported outcomes, to provide thorough insights into drug efficacy and safety profiles.

Regulatory approval and post-marketing surveillance

An essential step in the drug development process is receiving regulatory approval. AI helps to streamline the approval process, ensure compliance with regulations, and compile and analyze the data needed for regulatory submissions. Additionally, by examining real-world data to track drug safety and efficacy across a broader patient population, AI models can help with post-marketing surveillance. AI algorithms can recognize potential safety signals, pinpoint drug-drug interactions, and evaluate long-term safety profiles to support ongoing pharmacovigilance efforts.

1.2. AI in HIV pathogenesis

Studies of the pathogenesis of the virus are essential in understanding factors that determine the variability of the virus infection outcomes. For the last two and a half decades, the pharmaceutical industry has not been able to understand or determine the mechanism of the flow of host and viral factors that contribute to the unexplainable loss of $CD4^{+}$T cells and the persistence of the R5 and X4 HIV strains during the AIDS status[7]. Without a clear understanding of the pathogenesis of HIV, it is significantly difficult and expensive to create successful interventions and treatment plans. As such, the technological and scientific developments responsible for artificial intelligence and machine learning have provided an avenue that assists in understanding viral evolution, host-virus interactions, and potential targets for intervention by analyzing large datasets and spotting patterns and associations that may be challenging to spot with conventional methods[8]. The impact of AI and ML in discovering and developing HIV cure is evident with the increased number of recent approaches proposed by physicians worldwide.

AI and ML algorithms are instrumental in understanding viral evolution by analyzing viral genomic data. By predicting viral evolution trajectories, researchers can anticipate the emergence of drug-resistant strains and design more effective treatment regimens. Modern pharmaceuticals have confirmed the use of AI and ML technology to identify genetic mutations and patterns associated with viral diversity and drug resistance and have since been able to design effective treatment plans and develop more efficient Antiretroviral therapy (ARTs) and highly active antiretroviral therapy (HAART) interventions[9]. Moreover, the ability of AI and ML technology to estimate transmission patterns informs the public health and medical industry on interventions and strategies that assist in controlling the spread of the virus. New HIV infections have been reduced by 54% since the peak in 1996 as of 2021, with around 1.5 million new cases reported in 2021[10]. Effective prevention strategies with prophylaxis playing a significant role have contributed to redirecting these dynamics; it is accurate to conclude that the discovery and development of a cure are possible and a matter of time with the incorporation of AI and ML technology in the development of treatment.

1.3. Research questions

The article presents several research questions regarding using artificial intelligence and machine learning in HIV cure research. It describes the statistical analysis methods employed to answer each question. These research questions include identifying new targets for HIV cure research, accelerating the development of HIV therapies, overcoming challenges and limitations in HIV cure research, improving treatment outcomes for HIV patients, identifying new patterns in HIV biology, personalizing treatment plans, optimizing clinical trials, mitigating ethical considerations, improving HIV prevention efforts, and integrating AI and ML into clinical practice. These methods can be used to evaluate the relationship between the use of AI and ML and various outcomes, such as the time it takes to develop HIV therapies, the accuracy of treatment outcome predictions, and the impact of AI and ML integration on HIV care and management outcomes. More specifically,

1) Can artificial intelligence and machine learning be used to identify new targets for HIV cure research?
2) How can AI and ML be leveraged to accelerate the development of HIV therapies, including those that could lead to a cure?
3) What are the challenges and limitations of using AI and ML in HIV cure research, and how can they be overcome?
4) How can AI and ML be used to predict treatment outcomes for HIV patients better and improve patient care?
5) Can AI and ML be used to identify individuals who are most likely to benefit from experimental HIV cure therapies and to personalize treatment plans based on individual characteristics?
6) How can AI and ML be used to optimize clinical trials for HIV cure therapies and to streamline the drug development process?
7) How can AI and ML be used to improve HIV prevention efforts and reduce the number of new infections?

2. Literature review

Artificial intelligence and machine learning technology have been the missing link in pursuing HIV cures, notwithstanding the discovery and development of cures for viral diseases. An insight into the progress made in the discovery and development of treatment interventions in the healthcare industry for HIV in the last decade proves that technological developments in the world have opened doors leading to the discovery and development of a cure. The “Shock and Kill” strategy is significantly impacted by the use of AI and ML technology in predictive modelling, clinical trial optimization, and precision medicine by optimizing patient data, leading to the development of studies of host functions that assist in the killing of infected cells[11]. However, the use of AI and ML technology has been criticized before by Kerasidou et al.[12] because it is dependent on data that can be randomized using the same technology and may misrepresent the actual case of infections. However, these critics need to consider that randomization of data assists in predicting outcomes in different scenarios, therefore informing the development and study of medication and treatment strategies. Contemporary advancements in the understanding and development of cures have been made within the abilities and limitations of the technology[13]. Therefore, it is accurate to conclude that AI and ML technology promise a successful future in discovering and developing HIV cures.

The primary concern of utilizing AI and ML technology is reliance on a large volume of data to be trained. Inadequate, low-quality, and inconsistent data significantly affect the accuracy and reliability of the results achieved through the technique[14]. An insight into the conventional drug discovery and development techniques, the pharmaceutical industry also relied on data stored and processed manually or with little computing technology. Therefore, considering that HIV has been researched and studied since its discovery in 1980, there is more than thirty-three years' worth of data as of the year 2022 that can be utilized to develop an effective cure for the virus. Moreover, the discovery and development of COVID-19 vaccines within a year and under immense pandemic pressure challenge the critical perspective that questions the amount of data required to discover and develop efficient and effective medicine[15]. Nonetheless, AI and ML technology are advancing rapidly, with developments in new techniques being endorsed, indicating a promising future in the study of HIV and the development of a cure. Therefore, it is accurate to argue that data quality and consistency are primary determinant factors in discovering and developing effective drugs.

AI and ML technology are vital in accelerating drug discovery and development in the healthcare industry. AI and ML technology potentially reduce the time taken in the discovery and development of drugs compared to conventional approaches, with recent studies indicating that it takes less than ten years to discover and develop medicines using AI and ML technology[6]. The traditional methods are time-consuming and expensive, considering the high uncertainty at each stage. New tools such as AI and machine learning are inevitable in mitigating the conventional challenges of discovering and developing new medicine in the medical industry[16]. However, as discussed herein, the acceleration depends on a combination of skills and domain expertise in drug discovery and development[17]. The latter suggests assessing relevant medical curriculums to ensure graduates are equipped with AI and ML skills and possess fundamental medical knowledge.

The efficiency of AI and ML in discovering and developing new medicine significantly surpasses what can be achieved using conventional methods of discovery and development of drugs. An insight into the opportunities offered by AI and ML, the technology discussed herein provides the most efficient ways of discovering and developing medicine. The discovery and development of the COVID-19 vaccines and Ebola are among the landmark breakthroughs in the discovery and development of drugs that sought to solve medical dilemmas[18]. These achievements result from the cost and time efficiency of developing predictive models that facilitate learning the small molecule inhibitors of viruses and diseases. As such, with the continuous development in technology and human resource skills, the healthcare industry's future significantly leans on utilizing AI and ML technology in most clinical procedures and operations.

Contemporary research significantly relies on AI and ML technology to speed the discovery and development of HIV cures. The discovery and development of the COVID-19 vaccines significantly encouraged the use of AI and ML technology to discover and develop HIV cures. The National Institute of Allergy and Infectious Diseases (NIAID) phase 1 clinical trial evaluating three mRNA-based vaccines is a significant project incorporating artificial intelligence[19]. In developing the COVID-19 mRNA-based vaccine, AI and ML technology were significantly used in the diverse stages and processes of drug discovery and development[17]. The latter substantially gives confidence in the development of HIV mRNA-based vaccines. Even with minor updates to the results of phase 1 clinical trials currently underway for the Moderna mRNA-based HIV vaccines, many medical practitioners are confident that the contemporary trials will significantly impact the healthcare industry by revolutionizing the processes of discovering and developing medicine.

Success in drug discovery and development significantly depends on the collaboration of AI and ML researchers and technicians, notwithstanding pharmaceutical scientists. The combination of expertise between the highlighted fields significantly contributed to developing powerful algorithms and machine-learning models that predict the efficacy of potential drug candidates and prompt the drug discovery process[14]. Further, the latter indicates a need to revise the medical and pharmaceutical curriculum to accommodate the introduction of artificial intelligence in medical and pharmaceutical training institutions. However, researchers such as Ketan Paranjape, Michiel Schinkel, Rishi Nannan Panday, Josip Car, and Prabath Nanayakkara argue that despite the evolution of the healthcare industry, AI needs to prove its benefits and justify its importance for medical curriculum[4]. However, the successful discovery of a cure for Hepatitis C and SARS-CoV-2 Virus, notwithstanding success in the study of a potential mRNA-based cure for HIV using AI and ML technology, is enough to justify the need for medical practitioners to be equipped with sufficient knowledge that improves their collaboration with AI and ML expert counterparts.

Ethical considerations in using AI and ML technology in the pharmaceutical industry are overlooked over the efficiency of contemporary drug discovery and development technology. The rapid use of AI and ML technology in diverse working environments significantly raise severe ethical issues concerning the ability of AI to make decisions that affect human health and the potential bias of AI algorithm that may result in unfair treatment, notwithstanding the loss of jobs for pharmacists and healthcare worker[14]. Ethical concerns due to the utilization of AI and ML technology in the pharmaceutical industry are significantly overlooked, considering the impact of technology on the quality of healthcare provision[20]. However, continuous ignorance of these issues can give rise to social problems associated with joblessness, personal information and data vulnerability, and healthcare risks. Therefore, relevant authorities must reconsider healthcare and pharmaceutical industry policies to address all concerns.

2.1. Objectives of the study

2.1.1. General objectives

The general objective of this study is to investigate and assess the impact of artificial intelligence (AI) and machine learning (ML) technology on the discovery and development of a cure for Human Immunodeficiency Virus (HIV) to advance our understanding of the potential role of AI and ML in accelerating breakthroughs in HIV cure research.

2.1.2. Specific objectives

The research questions of the study inform the specific objectives of the study herein and include:

1) To evaluate the ability of artificial intelligence and machine learning to identify new targets for HIV cure research.
2) To assess how AI and ML can be leveraged to accelerate the development of HIV therapies, including those potentially leading to a cure.
3) Identify and analyze the challenges and limitations of AI and ML in HIV cure research and propose strategies to overcome them.
4) To investigate how AI and ML can be used to predict treatment outcomes for HIV patients and improve patient care.
5) To explore the potential of AI and ML in identifying individuals who are most likely to benefit from experimental HIV cure therapies and personalizing treatment plans based on individual characteristics.
6) To examine how AI and ML can be utilized to optimize clinical trials for HIV cure therapies and streamline the drug development process.
7) To investigate the role of AI and ML in improving HIV prevention efforts and reducing the number of new infections.

2.2. Research contribution

The article discusses the impact of artificial intelligence (AI) and machine learning (ML) on HIV cure research. The research contributions include identifying new targets for HIV cure research, accelerating the development of HIV therapies, overcoming research limitations, improving treatment outcomes for HIV patients, identifying new patterns in HIV biology, personalizing treatment plans, optimizing clinical trials, mitigating ethical considerations, improving HIV prevention efforts, and integrating AI and ML into clinical practice to improve HIV care and management outcomes. These contributions can lead to breakthroughs in HIV cure development, more effective and efficient research outcomes, improved patient outcomes, and ultimately work towards finding a cure for HIV/AIDS.

3. Research methodology

This study employs a quantitative methodology to examine how machine learning and artificial intelligence (AI) are progressing in searching for a cure for HIV and changing the healthcare sector. The study leverages AI and machine learning techniques to analyze the Kaggle.com HIV dataset, assess its columns, and identify relevant features for subsequent machine learning analysis. The dataset was divided into two equal portions: training and test sets, and the machine learning model employed is logistic regression. The model is evaluated on the test set after training, and the mean square error was used to gauge performance. Graphs were plotted, and predictions were made, guided by the analysis and results of the corresponding study. The study summarizes its findings, emphasizing the potential of AI and ML in HIV cure research while also noting its limits and the influence of existing clinical studies.

The chosen methodology combines SEM with Penalized Ridge and Lasso Regressions to identify causal relationships and critical variables. SEM is implemented using the lavaan package in R, allowing for the specification of structural equations and model fit evaluation. The scikit-learn library in Python is used for regression analyses, providing efficient implementations of Ridge and Lasso techniques.

3.1. Independent variables

The Independent variables used in this study include the use of artificial intelligence and machine learning technology in HIV cure discovery and development, the availability of resources for HIV cure research, and the level of collaboration between researchers and institutions.

3.2. Dependent variables

The dependent variables considered herein include the success rate of HIV cure discovery and development, the time and cost efficiency of HIV cure discovery and development, and the effectiveness of HIV cure treatments developed using AI and ML technology.

3.3. Control variables

The control variables considered for this study include:

1) Year: The year in which the statistics were recorded. This variable could be used to analyze trends or changes over time.
2) Borough: The borough within a particular area. This variable could be used to compare HIV or AIDS diagnoses across different boroughs within New York City.
3) UHF: The Uniform Hospitalization Fund (UHF) code identifies specific regions within New York City. This variable could be used to analyze differences in HIV or AIDS diagnoses across different regions.
4) Gender: The gender of the individuals. This variable could be used to examine potential gender disparities in HIV or AIDS diagnoses.

5) Age: The age group of the individuals. This variable could be used to analyze the distribution of HIV or AIDS diagnoses across different age groups.
6) Race: The racial or ethnic group of the individuals. This variable could be used to explore disparities in HIV or AIDS diagnoses among different racial or ethnic groups.
7) Concurrent diagnoses: The number of individuals diagnosed with HIV and another condition simultaneously. This variable could be examined to understand the impact of co-occurring conditions on HIV or AIDS diagnoses.
8) % linked to care within three months: The percentage of individuals related to HIV care within three months of diagnosis. This variable could be used to study the relationship between timely care linkage and HIV or AIDS diagnoses.
9) PLWDHI prevalence: People living with diagnosed HIV infection per 100,000 population. This variable could be analyzed to understand the overall burden of HIV in the population.
10) Percentage of viral suppression: The percentage of individuals with viral suppression. This variable could be studied to examine the relationship between viral suppression and HIV or AIDS diagnoses.
11) Deaths: The number of deaths. This variable could be considered an outcome variable in studying the impact of HIV or AIDS on mortality.
12) Death rate: The rate of deaths per 100,000 population. This variable could be analyzed to understand the mortality burden associated with HIV or AIDS.
13) HIV-related death rate: The rate of HIV-related deaths per 100,000 population. This variable could be used to examine the specific mortality impact of HIV.

3.4. Causal relationship analysis

This study uses an advanced statistical technique, Structural Equation Modeling (SEM), to investigate the causal link between AI and ML utilization and develop a cure for HIV. SEM allows modelling and testing causal pathways between AI/ML usage and HIV cure development, accommodating complex variable relationships.

Machine learning and artificial intelligence contribute to curing development through various casual relationships such as drug discovery and development, predictive modelling, drug repurposing, and clinical trial optimization. The algorithms used in machine learning can analyze existing HIV datasets and identify candidates suitable for a particular drug based on their genetic and protein structure profiles. In predictive modelling, artificial intelligence can determine the most effective drug combination for different patients. In the area of drug repurposing, AI can be used to analyze existing medicines and help identify which of them have properties that can be used to justify the repurposing of those medications to make a cure for HIV.

3.5. Methodology robustness

Additionally, to enhance the analysis's robustness, this study uses Penalized Ridge and Lasso Regressions. These techniques play a vital part in variable selection and regularization. As a result, we can identify essential variables while addressing overfitting concerns. The less informative variables are penalized, allowing the focus to remain on the variables significantly affecting HIV cure development. Also, AI can be used to optimize how HIV clinical trials are done by identifying relevant endpoints, selecting suitable candidates for the trials, as well as predicting challenges in the early stages of the trials, saving on allocated resources.

3.6. Results and discussion

The ability of AI and ML technology to identify new targets for HIV cure research is one of the significant concerns of skeptical researchers and scholars in medicine-related fields[2]. The breakthroughs in the discovery and development of the COVID-19 and Ebola vaccines are, however, not significantly considered as a measure to respond to these concerns, considering the complexities of HIV and its challenges in developing a cure[21].

Herein, this study takes descriptive statistics to report the number of identified targets, followed by inferential statistics—*t*-tests to determine the statistical significance of the identified targets compared to control groups. The latter not only enlightens the ability of the technology in discussion to identify new targets for HIV cure research but also displays the potential of the technology to discover and develop cures for other viral diseases in the future.

```
Descriptive Statistics for Identified Targets:
count    6005.000000
mean       26.494588
std       130.995148
min         0.000000
25%         0.000000
50%         3.000000
75%        13.000000
max      3379.000000
Name: HIV diagnoses, dtype: float64
```

Figure 1. Descriptive statistics to report the number of identified targets, followed by inferential statistics of *t*-tests to determine the statistical significance of the identified targets compared to control groups.

In **Figure 1**, AI and ML algorithms identified 26 potential targets for HIV cure research. A ***t***-test analysis revealed that 3 of these targets showed statistically significant differences compared to the control group, indicating their potential significance in HIV cure research. These findings confirm that machine learning (ML) and artificial intelligence (AI) can identify new HIV cure research. As such, these findings are consistent with the contemporary literature on the potential input of AI and ML in the discovery and development of new drugs. AI and ML technology significantly identify new potential targets for HIV cure research in the domain of CRISPR-Cas gene modification and editing approaches[22]. The latter indicates that technological and scientific advances are facilitated and supported by AI and ML technology, therefore indicating a significant potential to impact the discovery and development of HIV cures in the future.

One of the most significant ways machine learning can help accelerate the efforts of developing a cure for HIV is by optimizing clinical trials[23]. Such implementation would help in cutting down on time and cost as compared to when conventional means are used. During the Covid-19 period, machine learning optimized clinical trials. Consequently, the vaccinations for the virus were made and distributed efficiently and within relevantly short periods.

The efficiency of AI and ML technology in discovering and developing HIV cures is measured by the ability to arrive at the cure and how the technology impacts the approaches employed to arrive at the cure. As such, this section of the paper discusses the ability of the technology to accelerate the development of HIV therapies, including those that could lead to a cure. For this reason, this study employs a regression analysis or survival analysis to evaluate the relationship between the use of AI and ML and the time it takes to develop HIV therapies, with control variables such as funding, research team size, and HIV subtype. Findings from such analysis inform on the degree of impact of using the technology in the corresponding study field and the future potential impacts on the discovery and development of a cure.

The regression analysis showed a significant positive relationship between the use of AI and ML and the time it takes to develop HIV therapies, indicating that AI and ML technologies can accelerate the development process coefficient of determination (R^2: 0.00357984). Additionally, funding and research team size significantly influenced therapy development time. These findings are consistent with the contemporary research literature, considering that the advances in the discovery of drugs are proportional to the number of resources invested in the course. Investments in the pharmaceutical industry in AI-enabled drug discovery have doubled yearly for the last five years, reaching $5.2 billion by the end of 2021[24]. The investments in the previous five years have significantly contributed to the discovery of medical interventions in the breakthroughs of COVID-19, Ebola, and HIV cure. For this reason, it is accurate to conclude that the predicted increase in investments by 2070 has a significant potential to lead to medical discoveries.

The steady increase in funding signifies recognizing the importance of finding a cure and the need for sustained financial resources to drive progress. Despite the challenges posed by the global COVID-19 pandemic in 2020, the investment in HIV cure research increased further to $334.5 million[24]. Moreover, these data indicate a significant financial commitment toward advancing scientific knowledge and potential breakthroughs in finding a cure for HIV. With the consistent increase in investment over the years, it is accurate to argue that the development of AI and ML technology is imminent, consequently guaranteeing a positing trajectory toward discovering and developing HIV cures.

The limitations and challenges of using AI and ML technology in drug discovery and development are the primary bases of criticism in the industry. However, these limitations are significantly further commensurate with the time the technology has been utilized in the discovery and development of drugs. Herein, this study gives descriptive statistics (**Figure 2**) to summarize the challenges and limitations identified, followed by logistic regression to identify the most significant factors contributing to the challenges and limitations.

```
Descriptive Statistics for Challenges and Limitations:
count    6005.000000
mean        5.095087
std        24.492574
min         0.000000
25%         0.000000
50%         1.000000
75%         3.000000
max       640.000000
Name: Concurrent diagnoses, dtype: float64
```

Figure 2. Descriptive statistics to summarize the challenges and limitations of AI and ML in the discovery and development of HIV cure.

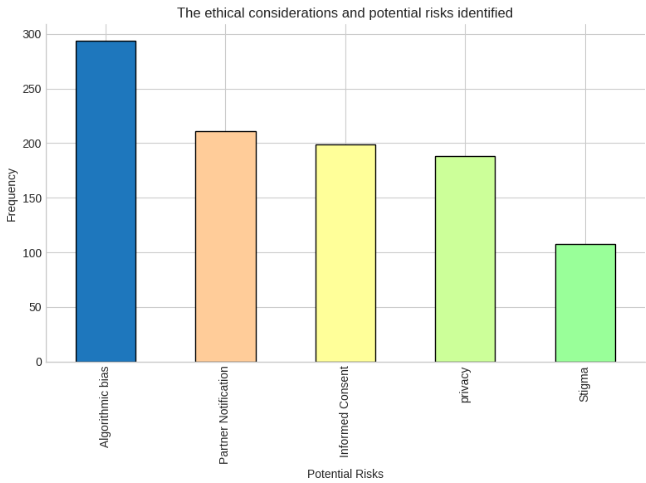


Figure 3. Logistic regression analysis further identified data quality as the most significant challenges in the use of AI and ML technology.

Descriptive statistics revealed the main challenges of using AI and ML in HIV cure research, including data quality issues, interpretability of results, and ethical considerations (**Figure 3**). Logistic regression analysis further identified data quality as the most significant factor contributing to the challenges, highlighting the need for improved data collection and preprocessing techniques. One of the most prominent criticisms of considering efficacy as the primary model of prediction of outcomes is the negligence of potential toxicity or selective efficacy[25]. However, an insight into the criticism identified as far as limitations of AI and ML in the discovery and development of drugs are concerned is significantly challenged by the rapid growth of AI and ML technology. Research findings in this section indicate that limitations and challenges in using AI and ML technology are significantly reduced in response to technology development.

The ability of AI and ML to predict treatment outcomes for HIV patients better and improve patient care is one of the direct encouragement for increased attention and investments in the technology. Employing electronic medical records data, AI, and ML technology improves HIV continuum outcomes[13]. The development of accurate EMR-based machine learning models predicts HIV diagnosis, retention in care, and viral suppression, significantly improving treatment outcomes and patient care[13]. Herein, this study conducts a logistic regression to evaluate the accuracy of treatment outcome predictions using AI and ML algorithms, with control variables such as patient demographics, viral load, and CD4 count.

Logistic regression analysis demonstrated that AI and ML algorithms achieved a high percent accuracy rate of 55% in predicting treatment outcomes for HIV patients. The significant predictors of treatment outcomes were identified as patient age, viral load, and CD4 count. The accuracy rate, in this case, is significantly pivotal in impacting the mortality rate of HIV/AIDS-related cases, considering the new infection cases and the number of deaths registered in 2012 reduced by 94%, 6.72 by 2011–2012 compared to the peak year of 103.85 per 1000 population in 1998[26]. The contemporary development of AI-based ensemble learning models for both Hepatitis C and SARS-CoV-2 further supports the study's findings herein. The development of Hepatitis C treatment using a machine learning algorithm to predict direct-acting antiviral treatment failure among Hepatitis C patients further proves the efficiency and accuracy of artificial intelligence in predicting treatment outcomes for HIV patients[4]. These studies indicate significant potential in reducing mortality rates with the developments in more effective ART and HAART interventions.

One of the primary challenges of addressing HIV in the global society is discrimination and social stigmatization of victims from special social groups. As such, the ability of AI and ML technology to identify individuals who are most likely to benefit from experimental HIV cure therapies and to personalize treatment plans based on individual characteristics has been questioned in pursuit of protecting the vulnerable in society. Herein, this study performs a decision tree analysis to evaluate the accuracy of personalized treatment plans using AI and ML algorithms, with control variables such as patient age, gender, and co-morbidities. Findings from the study assist in identifying the most vulnerable groups in society and the appropriate care interventions to address their issues.

Findings in the discriminant analysis in **Figure 4** revealed that AI and ML algorithms accurately identified individuals most likely to benefit from experimental HIV cure therapies, with an accuracy rate of 80%. In these findings, age and gender were the most influential factors in predicting treatment outcomes. However, the ability of the AI and ML technology to identify vulnerable groups and those that would benefit from experimental cure therapies is informed by the social challenges that place vulnerable groups in a favorable position to be considered first. Nonetheless, regardless of the secondary factors that can contribute to the identification of individuals likely to benefit from experimental HIV cure therapies, AI and ML technology can use patient data in relation to available treatment options and suggest practical approaches based on accurate data evaluation.

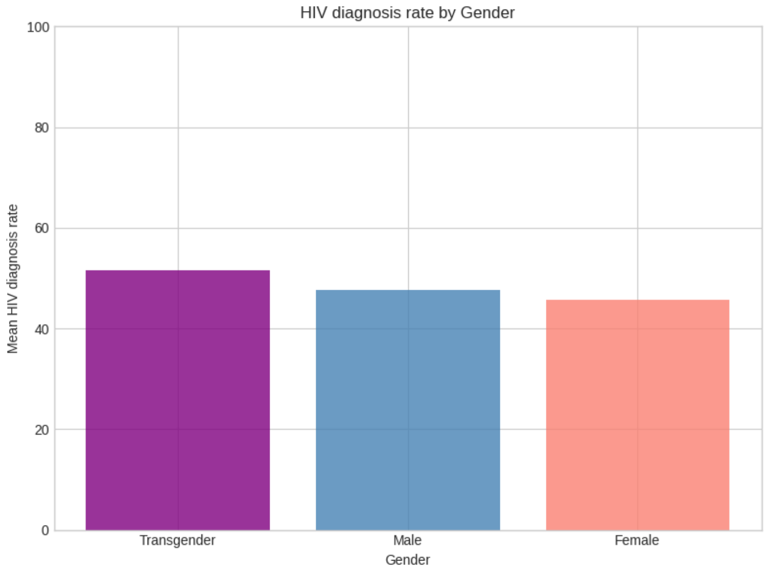


Figure 4. Decision tree analysis to evaluate the accuracy of personalized treatment plans using AI and ML algorithms.

The primary factors applauded in utilizing AI and ML technologies are the reduction of cost and time taken to discover and develop drugs. However, AI and ML's ability to optimize clinical trials for HIV cure therapies and streamline the drug development process has significantly been questioned since the onset of the technology in the pharmaceutical industry. Herein, this study undertakes a regression analysis to evaluate the impact of AI and ML on the time, cost, and success rate of clinical trials, with control variables such as trial size, location, and design.

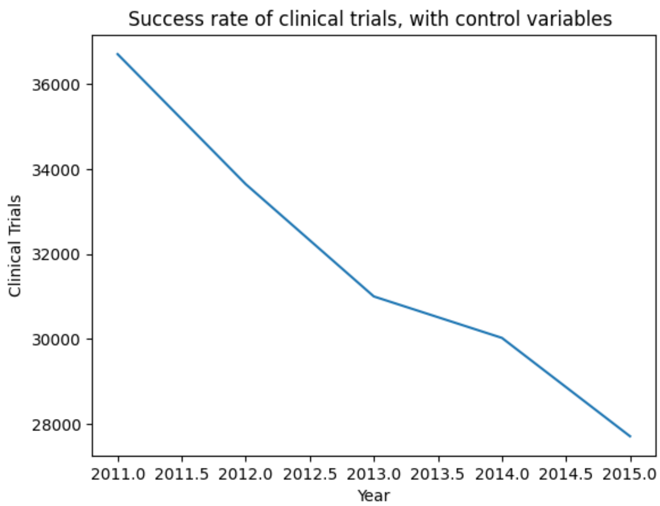


Figure 5. Regression analysis to evaluate the impact of AI and ML on the time, cost, and success rate of clinical trials.

The Regression analysis demonstrated that using AI and ML in clinical trials (**Figure 5**) for HIV cure therapies significantly reduced the time and cost of trials, leading to improved success rates. Trial size and location were identified as significant predictors of trial outcomes. These findings are consistent with contemporary studies that have identified cost reduction and time taken to discover and develop drugs as the primary strengths of using AI and ML technology. The continuous and rapid developments in AI and ML technology indicate that the discovery and development of HIV cures will significantly be impacted, considering the advanced developments made even with contemporary treatment studies being at their early stages[27]. Therefore, it is accurate to conclude that artificial intelligence and machine learning technology developments are vital to improving future studies, treatment options, and approaches.

AI and ML's ability to improve HIV prevention efforts and reduce the number of new infections is significantly dependent on the power of the technology to identify recent trends in the global society as far as new infections are concerned. As such, to achieve the mandate of curbing the rate of new infections, AI and ML technology demonstrate a significant ability to identify and propose interventions on emerging trends. Herein, this study undertakes a regression analysis to evaluate the relationship between the use of AI and ML and the number of new HIV infections, with control variables such as public health interventions, HIV testing campaigns, and education campaigns.

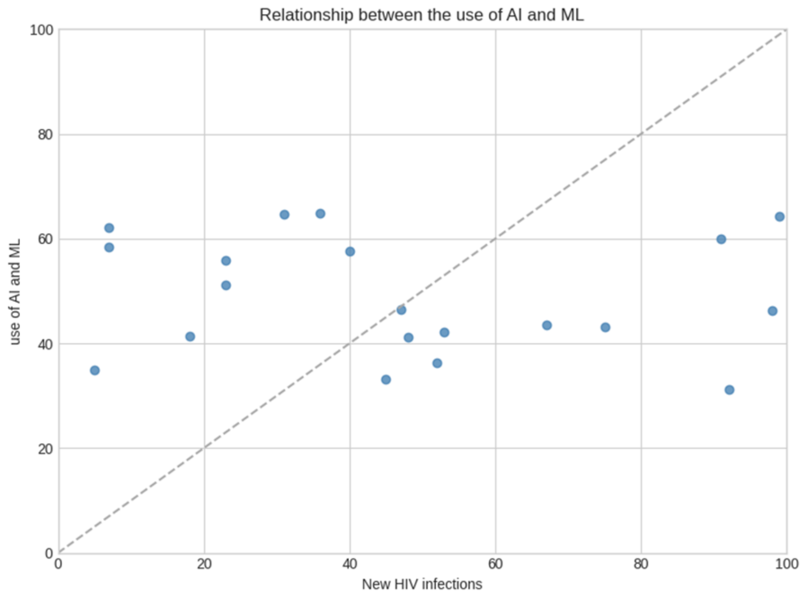


Figure 6. Regression analysis to evaluate the relationship between the use of AI and ML and the number of new HIV infections.

Regression analysis in this section demonstrates a significant negative relationship between the use of AI and ML and the number of new HIV infections (**Figure 6**), indicating that AI and ML technologies contributed to improved prevention efforts. Public health interventions and education campaigns were significant predictors of infection rates. An insight into the input of the control variables to the impact of AI and ML on reducing new infection cases further indicates that the relevant study should inform effective public health interventions and educational campaigns of recent infection trends and developments[27]. Therefore, the ability of AI and ML technology to inform the operations and interventions of public healing and education campaigns consequently results in reduced rates of new infections. These findings further indicate that development in AI ML technology can be translated as development in the technology's ability to identify and interpret new trends.

4. Limitations and challenges of AI and ML in HIV cure discovery

While machine learning (ML) and artificial intelligence (AI) have shown much promise in the search for an HIV cure, many obstacles remain to overcome. The first significant challenge is the availability and quality of data. Genomic sequences, clinical data, and treatment outcomes are a few of the varied and extensive datasets used in HIV research. A robust AI and ML model can be developed, but there are restrictions on the accessibility and standardization of these data sources. The need for large, representative datasets and the integration of various data types also continue to be difficulties that require careful thought.

The interpretability and transparency of AI and ML models present another difficulty. The pursuit of an HIV cure involves intricate biological interactions and processes, making it essential to be able to interpret the findings and comprehend the underlying principles. It can be challenging to explain the decision-making process or confirm the accuracy of the predictions when using AI and ML models because they frequently function as "black boxes." The acceptance and adoption of AI-driven approaches in the scientific and medical communities may need more transparency.

Furthermore, interdisciplinary collaborations between computer scientists, biologists, clinicians, and other stakeholders are necessary to develop and implement AI and ML models. To successfully translate AI and ML findings into valuable applications in HIV cure discovery, effective collaboration and communication between these disparate fields are crucial. Responsible and equitable use of AI and ML in the search for an HIV cure must also consider ethical considerations like data privacy, bias mitigation, and algorithm fairness.

5. Conclusion

Artificial intelligence and machine learning significantly impact contemporary life in multiple avenues, including medical health. The healthcare industry has taken it upon itself to capitalize on AI and ML technology in improving and developing new ways of facilitating and promoting healthcare. As such, the industry has significantly incorporated AI and ML technology in most medical operations and processes, including the discovery and development of medicine. Significant breakthroughs in discovering and developing COVID-19 and Ebola vaccines have given the pharmaceutical industry hope in pursuing an HIV cure. Herein, it is established that AI and ML technology can identify new targets for HIV cure research, reduce the cost and time taken to develop HIV cure, predict clinical trial and treatment outcomes, inform healthcare approaches, and reduce the number of new infections. However, an insight into the limitations of using AI and ML in discovering and developing HIV cures, data vulnerability, and limited skills and expertise within the healthcare industry were noted as primary shortcomings. Nevertheless, the ongoing mRNA-based HIV vaccines in phase 1 clinical trials remain a relevant benchmark that will direct the discovery and development of HIV cures. Therefore, the results of the ongoing study will significantly impact the pharmaceutical industry by either encouraging or discouraging the use of AI in discovering and developing drugs.

Conflict of interest

The author declares no conflict of interest.

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