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Intelligent science: The way AI is transforming the field of pharmaceuticals – A Review

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Abstract

Artificial intelligence (AI) is a branch of computer science that deals with the creation and application of machines that can mimic human behaviour, especially when it comes to the intelligent analysis and interpretation of data. Natural language processing (NLP), machine learning (ML), deep learning (DL), and other methods are all part of artificial intelligence (AI), which uses specific algorithms to function. Consequently, artificial intelligence has found use in the fields of pharmaceutical chemistry and medicine. The AI models used cover a wide range of approaches, such as unsupervised clustering methods applied to patients or pharmaceuticals to identify suitable patient cohorts or possible therapeutic molecules. Furthermore, the effectiveness of therapeutic drug monitoring is improved by the use of supervised machine learning techniques. Additionally, AI-assisted prediction of clinical outcomes

Key Words: Artificial Intelligence, Transforming, Pharmaceuticals, Drugs, Medicine

Introduction

Artificial intelligence (AI), and more especially machine learning (ML), have found significant traction in the field of healthcare applications during the past few decades [1]. In the field of pharmacology, artificial intelligence and machine learning techniques are applied to analyse various data sources efficiently. These sources cover a broad range, from the detailed chemical makeup of a medicinal ingredient to the entirety of a patient's clinical characteristics [1]. Additionally, the analysis encompasses genomic data and illness features [1]. The quantitative and categorical characterization of pharmaceutical molecules can be achieved through the development of molecular fingerprints and other QSAR descriptors [2]. In recent decades, there has been notable advancement in computational algorithms, especially those related to artificial intelligence and parallel computing.

Artificial Intelligence surpasses human skills through complex mathematical computations, research, and data analysis [3]. As a subset of AI, machine learning (ML) employs sophisticated computer algorithms to assess enormous volumes of data without the need for human participation [3]. Machine learning (ML) generates predictions by employing algorithms to learn from collected data, recognize patterns, and then generate predictions. Therefore, ML can be of great assistance at several stages of drug discovery, including pharmacological research such as identifying lead compounds [4]. As a result, this study offers a summary of the most recent advancements in artificial intelligence (AI) technologies utilized in clinical trials, pharmacovigilance, drug discovery, and design. Knowledge of the most recent developments is essential for researchers from many domains who work with pharmaceutical specialists.

Drug discovery and design

AI can be used from the bench to the clinical stage in the creation of a novel medication or any pharmaceutical product. bedside because of its capacity for logical medication design planning. Because of the rapidly growing pharmaceutical business, the creation of new pharmaceuticals is becoming more difficult and time-consuming due to a lack of state-of-the-art equipment [5]. A newly developed pharmaceutical product is then introduced into the market after a labour-intensive and multifaceted process known as discovery, which includes the identification of potential therapeutic targets, the synthesis and assessment of novel chemical entities, and more [6]. Because AI can interpret large amounts of data, it can effectively oversee the drug development process at every level.

In order to assist in the discovery of possible therapeutic targets for a variety of disease categories, including cancer, cardiovascular disease, and neurodegenerative disorders, among others, AI algorithms may also be able to examine genomic and proteomic data [5]. The in-silico Medicine startup recently used artificial intelligence (AI) to find the medicine for idiopathic pulmonary fibrosis. According to https://clinicaltrials.gov/ct2/show/NCT05154240, the therapy's phase I trials have produced encouraging results. AI is used in a number of procedures that are involved in the design and discovery of new drugs [7].

Drug-drug interactions Target binding affinity and predictions

Drug-target interaction phenomena are the intricate, physiologically active interactions that take place between chemicals and drug targets in the body. It is essential to forecast the drug-target interaction in order to determine a medication's therapeutic efficacy [8]. Understanding the potential and efficacy of a pharmacological substance as a treatment depends critically on the prediction of its interaction with a receptor or protein [5,9]. The absence of contact between the drug molecules and the targeted proteins will hinder the therapeutic activity of the medicine [5]. While it is possible to ascertain the bioactivity through in vitro and in vivo tests, these methods are costly and time-consuming [7]. Toxicity may also arise from the drug molecule's interaction with an unwanted protein or receptor.

A variety of databases have been established and relevant information has been systematically compiled by a thorough study of relevant literature and the synthesis of collected experience [10]. Consequently, an initial screening of established interaction data obtained from many databases, including Drug Bank, UniProt, PubChem, KEGG, and others, is one of the novel methodologies documented for drug-protein interaction predictions [11]. The vast majority of the information stored in these databases is freely available to the general public [10]. With the application of ML techniques, difficulties in drug-target interaction prediction can be effectively addressed thanks to the availability of this data [12]. Databases may provide datasets to researchers including a range of information according to their particular needs.

ML-based methods evaluate the degree of similarity of medicines and protein molecules to determine DTBA, such as Kronecker-regularized least squares (KronRLS). Regression trees

are used by Sim Boost to predict DTBA, and the model considers both feature-based and similarity-based interactions [13]. The first drug-target binding affinity model to be developed was based on deep learning techniques, such as DeepDTA. Convolutional neural networks (CNNs) are used to model compound 1D representations and protein sequences. This approach outperformed KronRLS77 and SimBoost in terms of concordance index (CI) performance [14]. Additionally, a more recent DL-based prediction model called wideDTA was used using word sequence data related to biology and chemistry. The maximum common molecular weight, ligand SMILES, protein sequence, and protein domains and motifs are the four word- or text-based sources that it uses.

Prediction of drug toxicity

Toxicity refers to the potential harm chemicals can cause to internal organs or systems. Drug toxicity prediction is crucial in drug development for identifying safety issues and creating safer medications. Regulatory bodies like the FDA and EMA set safety standards for drugs. Common machine learning methods for toxicity prediction include random forests, decision trees, k-nearest neighbor, and support vector machines. Advanced deep learning techniques such as deep neural networks, recurrent neural networks, convolutional neural networks, and various graph-based neural networks are also used. DeepTox, an AI tool using a three-layered deep neural network, reportedly outperforms traditional methods in drug toxicity prediction. Its workflow involves data cleaning, chemical descriptor generation, model evaluation, and ensemble prediction [16, 17].

Clinical trials (CT) of drugs

Artificial Intelligence (AI) is becoming recognized more and more as a practical means of attaining optimal and sustainable medication development. As a result, there is continuous discussion and investigation on the practical uses of AI in clinical trials [18]. Software applications that use target information can be used to forecast a drug's potential for toxicity. It is possible that existing pre-clinical methods such in vitro and animal models may be replaced by effective toxicity forecasts [19].

Predicting the clinical trial success

AI can be utilized in the early stages of clinical trials to forecast the drug's bioactivity, protein target interaction, toxicity, etc. Multi-instance learning (MI) algorithms are able to analyze the entire trail success since they are able to anticipate the disease's prognosis [18]. Being able to predict clinical trial outcomes in advance could improve pharmaceutical R&D efficiency, open up new financing sources, and produce innovative financial tools to support biotechnology research [20].

AI programs like PrOCTOR can predict drug-induced CT failure by analyzing drug descriptors, interactions, and expression levels. Similarly, Clinico CTOP models forecast outcomes of Phase II studies based on a drug's efficacy and target selection. For instance, the first-in-class factor B inhibitor LNP023 demonstrated that Clinics could effectively treat paroxysmal

nocturnal haemoglobinuria, even without prior knowledge of the drug's clinical significance. [21]. Creating a "AI arm" to go along with the study and control arm is another way to include AI technology into randomized controlled trials (RCTs) so that the trial's potential can be verified regardless of its main goal [22].

Pharmacovigilance

The main goal of the approach known as pharmacovigilance (PV) is to restrict the introduction of drugs that have adverse side effects to broad populations. Concerning the safety of pharmaceuticals, including over-the-counter medicines, prescription drugs, and herbal supplements, it deals with the methodical collection, examination, and reporting of data. Adverse drug reactions (ADRs) were organized, regulated, and thoroughly examined after the thalidomide debacle [23]. The enormous volume, complexity, manual data processing, and regulatory requirements are the main disadvantages of traditional pharmacovigilance. Utilizing real-world data analysis, artificial intelligence systems can significantly improve drug safety monitoring [23]. ML and natural language processing (NLP) are used by AI to predict and identify adverse drug events (ADEs). Use of diverse data sources, including electronic health records, is becoming more necessary due to the rise in medication-related issues.

One of the proposed models that analyzed 10,000 datasets from WebMD and Drugs.com and obtained state-of-the-art performance in ADE detection and extraction was the DL-based approach with Bidirectional Encoder Representations from Transformers (BERT) models. It addressed the problems that physicians run across when writing prescriptions by showcasing the potential of deep learning for healthcare activities and information extraction [24].

Established in 1978 in Uppsala, Sweden, the Uppsala Monitoring Centre (UMC) is a global drug monitoring center in collaboration with the WHO. It manages multiple databases, including VigiFlow, VigiBase, and VigiLyze, on behalf of the WHO. The public can access VigiAccess, an open access database. PV provides additional methods for the analysis of case reports, including VigiGrade, VigiMatch, and VigiRank [25]. Marketing authorization holders (MAHs) in India are mandated to report the Individual Case Safety Report (ICSR) of any marketed drug to the Central Drugs Standards Control Organization (CDSCO) and the National Coordination Centre for Pharmacovigilance Programme of India (NCC-PvPI) (Pharmacovigilance Gsr 287 € dated 8-03-2016, REGD.D.L.-33004/99). These reports are sent to WHO-UMC, Sweden, via a different program called VigiFlow [34].

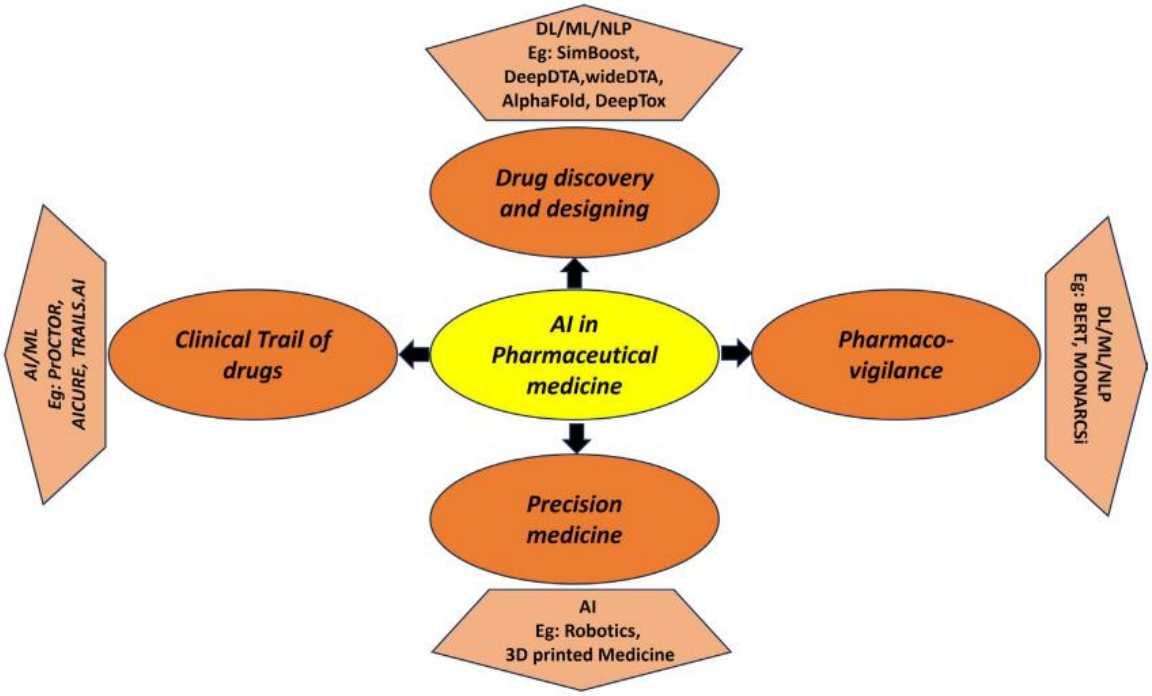
Using AI, the Pharmacovigilance Programme of India first inserted case-related structured and unstructured content as XML, DOCX, PDFs, and images. Through the use of NLP and ML, information is extracted from ICSR in a compliant manner. Furthermore, because ICSR is frequently of poor quality, AI is used in decision-making. AI could be essential for running correlations, classifying medications, tracking individual or unlisted adverse occurrences, and more [39]. A causality decision support tool called the Modified Naranjo Causality Scale for ICSRs (MONARCSi) was created using the Naranjo causality score as a foundation. High

positive and negative predictive values (79 and 88%, respectively), an F1 score of 71%, and high specificity (93%) and moderate sensitivity (65%) were all displayed, indicating that

Precision medicine

Precision medicine emphasizes the significance of combining established clinical indices with molecular profiling to provide customized therapeutic, diagnostic, and predictive approaches for individual patient populations. A more precise taxonomy that takes into account recent advancements in molecular biology will unavoidably result from the push toward a deeper understanding of disease [27]. Because it enables medical professionals to create personalised treatment plans that are precisely matched to the individual characteristics of each patient, personalised medicine has the innate potential to completely transform the therapeutic environment [26]. The tangible benefits of precision medicine are becoming more and more apparent, such as the prompt diagnosis of conditions and the rise in the use of customized therapeutic approaches in the medical field [28]. The integration of high-throughput genotyping with electronic health records (EHRs) offers scientists a significant opportunity to derive new phenotypes from actual clinical and biomarker data. This convergence has prompted extensive research into the effects of precision medicine on contemporary healthcare, particularly focusing on genotype-guided treatment strategies.

It may be particularly useful to identify the characteristics of medications and chemicals to use some of the chemistry-focused websites with large databases, such as DeepChem (https://deepchem.io/about.html). The creation of a novel medication would be a possibility if an existing medication or molecule was unable to control a target. Artificial intelligence has been employed to create novel structures that could aid in the development of more efficacious therapies, like pharmaceuticals or mechanical devices, as well as to assist in selecting suitable chemical syntheses [30]. "Magistral" production, as opposed to "officinal" or conventional pharmaceutical manufacturing, is a recent development in the ability to produce remedies in real-time based on the unique demands of the patient [31]. One may imagine production that is exact and efficient thanks to robotics technology powered by AI.



Drawbacks of AI

The effective implementation of any kind of information technology in the healthcare industry faces a number of obstacles. Data collecting, technology advancement, therapeutic application, and ethical and societal difficulties are some of the obstacles. The first problem is that ML and DL models require big datasets to identify or forecast a wide range of activities with accuracy. According to Lubarsky et al. [32], the sectors with the easiest access to enormous datasets have witnessed the greatest improvements in machine learning's ability to produce more exact and accurate algorithms. Access to information is a big problem for the healthcare industry. Baowaly et al. claim that problems with data security and privacy arise from AI-based solutions.

Because health records include sensitive information, hackers frequently target them during data breaches. AI ethics have been questioned ever since the technology's creation. The true issue is accountability, not the data security and privacy concerns mentioned above. Because of the seriousness of the repercussions, the existing system requires that those who make poor decisions—especially in the medical field—be held accountable. It might be challenging to hold the doctor responsible because they had no input into the development or supervision of the algorithm. However, it can appear that the developer is at fault, with little bearing on the therapeutic environment [33]. AI has long raised concerns among the public that jobs in the healthcare industry may disappear. Certain individuals are unfriendly and doubtful of AI-based initiatives due to their fear of being replaced [33].

Conclusion:

The field of pharmaceutical medicine has benefited greatly from the introduction of artificial intelligence. It has shown great potential in a number of areas, including patient management, clinical experimentation, and drug discovery. Making Use of AI Powered tools reduce time and cost restrictions while accelerating the drug development process and making it easier to identify new therapeutic targets. In the field of pharmaceutical development, these creative uses have led to increased efficacy and decreased costs. Moreover, patient classification and the personalization of medication interventions could benefit from the incorporation of AI. Successful and economical trials can be carried out by utilizing a patient-centric strategy and integrating AI with RCTs to help with clinical outcome prediction and validation. Better overall health outcomes and increased therapeutic efficacy may arise from this.

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