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Review Article

A COMPREHENSIVE REVIEW ON ROLE OF ARTIFICIAL INTELLIGENCE (AI) IN DRUG DISCOVERY AND DRUG DEVELOPMENT

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Abstract

The modeling of human behavior in connection to the intellectual processes involved in problem solving is known as artificial intelligence (AI). Human cognitive science reading, observation, planning, interpretation, reasoning, correction, speech recognition, linguistics, and other sources are examples of these mechanisms. Artificial Intelligence (AI) streamlines processes by enabling computers to learn from prior experiences, map efforts and actions to outcomes, detect faults and rectify them, adapt to new and random input values, and carry out human-like jobs with ease through comprehensive scenario analysis. By evaluating, filtering, sorting, forecasting, scoping, and figuring out massive data volumes to adhere to the finest implementation practices for generating an ideal solution, artificial intelligence (AI) streamlines work. As of 2019, the main uses of AI in the pharmaceutical industry include: drug discovery and development; drug-adherence and dosage; using AI to make sense of clinical data and produce better analytics; finding more reliable patients for clinical trials more quickly; introducing automated robot pharmacies to fill prescriptions and dispensing; and marketing, logistics, and supply chain. Above all, artificial intelligence has the potential to save lives by reducing expenses and developing novel, efficient treatments. Thus, biotech businesses ought to begin utilizing AI's benefits as soon as possible. Therefore, adopting AI and machine learning solutions will benefit the sector greatly. It can be effectively applied to build a robust, long-lasting pipeline of novel medications. We would be able to develop medications more quickly and more cheaply if we could harness the power of contemporary supercomputers and machine learning. This paper provides a thorough analysis of the state of artificial intelligence in pharmaceutical sciences, with a focus on the pharmaceutical industry. In summary, human-machine cooperation is the way of the future, and as technology develops, human clinical professionals will also need to adapt, learn, and develop. It is the evolution of medicine, not its extinction, even though future experts will need to be proficient in both medicine and technology.

Keywords: Pharmaceutical sciences, Pharmaceutical industry, startups, Deep learning, Machine Learning, Artificial Intelligence, Neural Networks, Drug Development.

INTRODUCTION

Artificial Intelligence (AI)

The term artificial intelligence (AI) describes the replication of human intelligence in computers that have been designed to think and act like people. Artificial Intelligence is sometimes defined as a technique that allows machines to simulate a wide range of complex human abilities. The first mention of artificial intelligence (AI) occurred in 1956 at a conference that John McCarthy and Marvin Minsky hosted [1,2]. The pharmaceutical industry has seen a sharp rise in the digitalization of data in recent years. But with digitalization also comes the difficulty of learning, examining, and using that information to address intricate clinical issues [3]. Because AI can manage massive volumes of data with greater automation, this encourages the usage of AI [4]. Artificial Intelligence (AI) is a technology system that mimics human intelligence through a variety of sophisticated tools and networks. However, it does not pose a danger to entirely replace the physical presence of humans [5, 6]. Artificial Intelligence (AI) uses hardware and software that can analyze, comprehend, and learn from the input data to make decisions on its own for achieving predetermined goals.

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As this overview explains, advancements in the pharmaceutical area are ongoing. As this article explains, its uses in the pharmaceutical industry are always expanding. The McKinsey Global Institute predicts that the swift advancements in AI-guided automation would probably transform society's work culture entirely [7, 8].

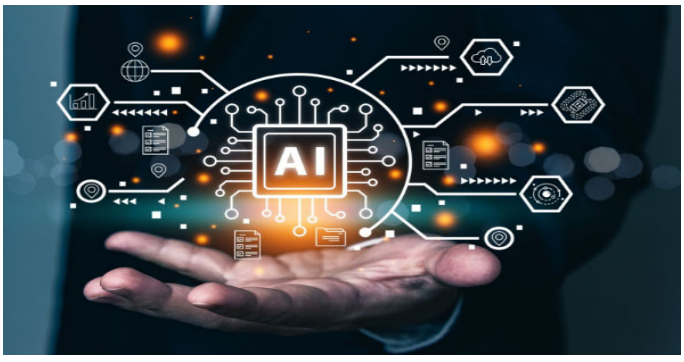

Fig. 1. Artificial Intelligence

Objectives of AI

1. **Creating Expert Systems:** The main objective is to create intelligent, automated systems that can guide and advice

people in order to assist them make the best decisions possible.

2. **Developing Human-like Intelligence in Computers:** Artificial Intelligence (AI) seeks to imitate human cognitive patterns, enabling computers to behave human-like and provide intelligent decisions, especially in complex and demanding environments. Algorithms play a vital role in task automation and worker stress reduction.
3. **Applications in a Range of Domains:** Artificial Intelligence (AI) finds application in a number of fields, including computer science, psychology, statistics, cognitive science, engineering, ethics, the natural sciences, medicine, space technology, logic, and linguistics.
4. **Computer science applications:** a number of mechanisms, including Search and AI is used to build a variety of complex computer science solutions, including optimization, logic, control theory, language analysis, neural networks, classifiers, statistical learning methods, and probabilistic methods for uncertain reasoning. Machine learning (ML), a subfield of artificial intelligence and computer science, allows computers to automatically learn from experience and improve their interpretation of it. Predicting expected supplier demand, coordinating the transfer of goods, and managing suppliers and paperwork are all made possible by machine learning.

Types of Artificial Intelligence (AI)

a. **Artificial Narrow Intelligence (ANI):** This type of AI lacks overall human-like intelligence and is only capable of performing narrow tasks, such as face recognition, driving, or chess.
b. **Artificial General Intelligence (AGI):** Similar to human intelligence, AGI is capable of performing a wide range of activities, learning from experience, and resolving a variety of issues.
c. **Artificial Super Intelligence (ASI):** beyond human intelligence, ASI can perform tasks such as complex mathematics, drawing, and scientific research.[9,10]

AI and its potential applications in drug development

Recent years have seen a major increase in interest in the application of artificial intelligence (AI) in medicinal chemistry as a possible game-changer for the pharmaceutical sector [11]. Drug discovery, the process of finding and creating novel drugs, is a difficult and drawn-out process that has historically relied on labor-intensive methods like high-throughput screening and trial-and-error research. However, by enabling more accurate and efficient analysis of vast amounts of data, artificial intelligence (AI) techniques like machine learning (ML) and natural language processing provide the potential to improve and speed up this process [12]. The authors of previous article have recently reported on the successful application of deep learning (DL) to accurately forecast the efficacy of pharmaceutical substances [13]. The toxicity of medication candidates has also been predicted by AI-based techniques [14]. These and other studies have demonstrated AI's potential to increase the efficacy and efficiency of drug discovery procedures. Nevertheless, there are obstacles and restrictions associated with using AI to create novel bioactive substances. To properly grasp the benefits and constraints of AI in this field, more research is required in addition to ethical issues [15]. Notwithstanding these obstacles, it is anticipated that in the coming years, artificial intelligence will play a major role in the creation of novel drugs and treatments.

Drawback and limitations in current methodology of drug discovery

Presently, large-scale testing procedures and a trial-and-error methodology are mostly relied upon in medicinal chemistry methodologies [16]. These methods entail looking through a lot of possible medication molecules to find the ones that have the necessary qualities. But these techniques can be expensive, time-consuming, and frequently produce inaccurate results [14]. Furthermore, they may be constrained by the accessibility of appropriate test chemicals and the challenge of precisely forecasting their physiological responses [17]. These issues may be resolved by a variety of AI-based algorithms, such as reinforcement learning, supervised and unsupervised learning techniques, and evolutionary or rule-based algorithms. These techniques are usually predicated on the examination of substantial volumes of data that have multiple applications [17–19]. For example, these methods can more accurately and efficiently predict the toxicity and efficacy of novel therapeutic molecules than can be achieved with conventional techniques [20, 21]. Additionally, new targets for drug development, such as particular proteins or genetic pathways implicated in illnesses, might be found using AI-based algorithms [22]. This has the potential to broaden the scope of drug discovery beyond the constraints of more traditional methods and could ultimately result in the creation of new and improved drugs [23]. Consequently, although conventional approaches to pharmaceutical research have demonstrated some degree of success in the past, they are constrained by their dependence on empirical trial and error and their incapacity to precisely forecast the behavior of novel, potentially bioactive chemicals [24]. On the other hand, AI-based methods can result in the production of more potent drugs by increasing the efficacy and accuracy of drug discovery procedures.

How artificial intelligence can impact drug discovery and possible cost effectiveness

Creating new molecules with particular characteristics and functions is another important way that AI is being used in medication discovery. Conventional techniques frequently rely on the labor- and slow-intensive process of identifying and modifying already-existing molecules. On the other hand, AI-based methods can make it possible to quickly and effectively develop unique compounds with desired characteristics and activities. In order to propose new therapeutic molecules [25] with desirable properties like solubility and activity, for instance, a deep learning (DL) algorithm was recently trained on a dataset of known drug compounds and their corresponding properties. This shows the potential of these methods for the quick and effective design of new drug candidates. Recently, Deep Mind has developed Alpha Fold, a ground-breaking software platform for improving our understanding of biology, which has made a substantial contribution to the field of AI research [26]. It is a potent algorithm that predicts the relevant three-dimensional structures of the proteins using protein sequence data and AI. It is anticipated that this advancement in structural biology would transform medication discovery and customized treatment. In terms of the application of AI in structural biology and the biological sciences generally, Alpha Fold is a major advancement.

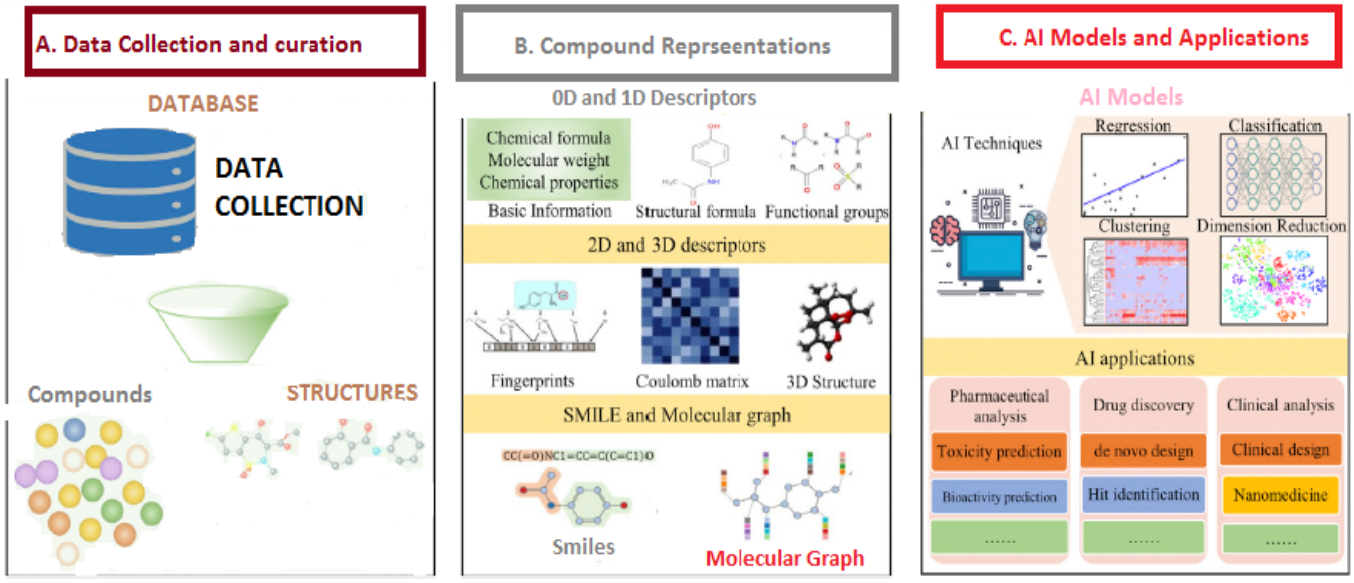

Fig. 2. Framework of AI technique application to drug discovery and evaluation

De novo drug design is a subject that is currently using ML approaches and molecular dynamics (MD) simulations to increase accuracy and efficiency. To capitalize on the synergies between these approaches, the strategy of merging them is being investigated [27]. This endeavor also involves the application of interpretable machine learning (IML) and deep learning techniques. Researchers are able to build medications more effectively and efficiently than ever before by combining the power of AI and MD.

Applications of artificial intelligence

AI in Drug Discovery: Finding new drugs is a difficult and drawn-out process that frequently takes ten to fifteen years. The pharmaceutical industry's productivity is dropping because so few prospective drug candidates make it through clinical studies and regulatory approval. Artificial Intelligence (AI) is being embraced by the industry more and more to address this, as it can expedite medication discovery while cutting expenses. AI is being used in drug development to optimize drug designs, validate drug targets, and find interesting molecules fast. Machine learning and silicon techniques aid in the efficient planning of synthesis, evaluation of compound characteristics, and prediction of chemical structures with desired effects. AI in the form of deep learning is particularly helpful in managing the enormous volume of data produced throughout the drug discovery process. [28]

Drug development and research have changed significantly as a result of AI**.**

The following are some of the most important contributions of AI in this domain

Target Detection

Artificial intelligence (AI) systems are capable of analyzing a variety of data types, including genetic, protein, and medical record data. This aids in the identification of potential therapy targets. AI helps in the development of drugs that can affect biological processes through determining these targets and comprehending how molecules function in illnesses.

AI-powered virtual screening

Finds drugs more quickly by effectively screening large chemical libraries. It helps researchers pick compounds for experimental testing and saves important time and resources by identifying possible therapeutic candidates that can bind to particular targets.

Modeling the Structure-Activity Relationship (SAR)

AI models can be used to connect the biological function of compounds with their chemical structure. In order to maximize therapeutic potential, that enables scientists to produce molecules with desired qualities including high effectiveness, selectivity, and favorable pharmacokinetic properties.

De Novo Drug Design

By manipulating generative models and reinforcement learning, artificial intelligence systems can propose novel chemical structures that bear resemblance to therapeutic compounds. Through its ability to learn from chemical databases and experimental data, artificial intelligence (AI) expands the chemical domain and facilitates the development of new medicinal possibilities.

Repurposing Drugs

AI systems can search through vast amounts of scientific data to identify current drugs that may be used as treatments for different diseases. AI reduces costs and expedites the drug research process by repurposing existing drugs for novel uses.

Predictable Toxicity

AI systems are able to predict the toxicity of drugs by looking at the characteristics and chemical structure of a substance. While receiving instruction on toxicological databases, machine learning algorithms are capable of identifying hazardous structural features or predicting adverse consequences. This helps minimize negative outcomes during clinical trials and help researchers find safer drugs. [29]

Application of AI in Manufacturing

Quality by Design (QBD) principles has replaced the traditional trial-and-error method of formulation development with a more systematic and logical procedure thanks to AI [30]. The pharmaceutical industry can benefit greatly from artificial intelligence in a number of ways, such as process design and control optimization, trend tracking to encourage ongoing progress, and intelligent monitoring and maintenance. AI can be applied to support pharmaceutical manufacture, and modern manufacturing methods can be employed to achieve desired results. Artificial intelligence could be utilized in the production of pharmaceuticals, as demonstrated by the following examples:

Design and Scaling of Processes

It is possible to quickly identify the optimal processing parameters or scale-up processes by using AI models, such as machine learning, that are developed from process data. As a result, waste and development time are decreased.

Proficient Procedure Management

With the use of this technology, the production process can be dynamically controlled to provide the desired outcomes. By combining real-time sensor data with AI approaches, process controls that predict the course of the manufacturing process can also be developed. APC technologies, which combine AI techniques with an understanding of the underlying chemical, physical, and biological transformations occurring in the production process, have been used by a number of pharmaceutical producers.

Process Monitoring and Defect Identifying

When machinery operation deviates from normal, maintenance measures may be initiated to minimize process downtime. AI methods can also be used to monitor product quality, including packaging quality. As one illustration, vision-based quality control uses AI-based software to examine pictures of glass vials, labels, and packaging. Any deviations from a product's required quality criteria are detected by the program.

Trend Assessment

Even in cases where customer complaints and variance reports involve a significant amount of text, artificial intelligence (AI) can be a crucial tool in their analysis. AI makes it feasible to find groups of related issues and rank them in order of importance for ongoing development. The capacity to identify patterns associated with production variations is a major benefit as it facilitates a comprehensive knowledge of the underlying reasons.[30] Expert systems, NNS, and AI technologies predict the ideal values for complicated variables under study to produce the best formulation or procedure. [31]The problem of tablet capping on the production line was addressed by researchers using fuzzy models and artificial neural networks (ANNs). These cutting-edge computational methods were applied to investigate and examine the relationship between machine configurations and tablet capping incidents. Cutting-edge AI tools like tablet-classifiers and meta-classifiers are used to guarantee the highest levels of quality for the final result. These cutting-edge technologies are essential for spotting possible mistakes or variations in the tablet production process. [32]

Application of AI in Drug Design

In structure-based drug discovery, a target protein's three-dimensional (3D) conformation is crucial. This is important since creating new pharmacological compounds frequently centers on comprehending the three-dimensional chemical environment of the target protein's ligand-binding site. Researchers have historically used techniques like homology modeling and de novo protein design to accomplish this goal. These methods have been widely applied in the field to guide the logical creation of possible therapeutic drugs and to obtain insights into the structure of the target protein. [33] Recent developments in the field of structure-based drug discovery have shown that the amazing artificial intelligence tool Alpha Fold is capable of precisely predicting the three-dimensional structure of target proteins for drugs. This technology has performed incredibly well, demonstrating its ability to completely change how we approach protein structure prediction and the implications this has for drug design. [34]

AI role in Drug Repurposing

Utilizing well-known medications or pharmacological combinations in unforeseen medical circumstances is known as drug repurposing. Drug repurposing is the process of presenting novel effects of pharmaceuticals or combinations of drugs based on already-approved treatments. Because it is less expensive and time-consuming than the conventional method of beginning the drug discovery process from scratch, this strategy is essential for accelerating the pre-clinical stage of the development of novel medications. Since the COVID-19 outbreak, repurposing medications has gained popularity as a quicker method of discovering therapeutic drugs or drug combinations than de novo drug manufacturing. Although it takes a long time and is expensive, the de novo drug discovery process works well. Repurposing already-approved drugs with proven pharmacokinetics and mechanisms offers a quicker and less expensive solution. This method attracts the interest of governments and pharmaceutical companies while saving time and money. Drug repurposing is made easier by AI technology, which also reduces expenses and time. [35] Drug repurposing has frequently been found by accident during haphazard testing and investigation. For instance, Pfizer repurposed sildenafil citrate, which was first developed as a medication to treat hypertension, to create Viagra, a new medication to treat erectile dysfunction. [36]

Conventional drug development usually involves five phases

i Pre-clinical research,
ii Clinical research
iii FDA monitoring
iv FDA post-market safety monitoring and development
v Discovery and development

However, the process of repurposing drugs involves just four steps:

i Clinical research
ii Compound acquisition
iii Compound identification

iv Clinical Research and FDA post-market safety monitoring and development. [37]

AI in a research study

Clinical trial failures are often caused by inefficient techniques for patient recruiting and selection, as well as challenges in effectively monitoring participants during the investigation. The primary reason for clinical trial delays is the difficulty of finding enough eligible individuals to enroll in the designated amount of time. Studies show that up to 86% of trials fail to reach their enrollment goals. There is a lot of promise for tackling these issues with the application of artificial intelligence (AI) tools to enhance patient intake and selection procedures. In addition to collecting and analyzing data concurrently from several clinical trial sites, these AI-powered platforms also allow for a more complete patient characterization. [38] Currently, only around one-third of trial chemicals in Phase II reach Phase III. These billion-dollar investigations take ten to fifteen years to finish. Studies that don't work out also cost money for preclinical development.

AI and Drug Synthesis

One of the most important and difficult jobs after discovering molecules is to synthesis the chosen compounds. Retro synthesis is the conventional method used to do this. Synthia, a software application originally known as Chematica, has been created to facilitate this procedure by proposing possible synthesis routes for eight crucial therapeutic targets. This is accomplished by programming a set of rules into the computer, which raises yield, lowers costs, and increases efficiency. Furthermore, Synthia has shown to be useful in creating previously unproduced materials and providing substitute synthetic processes for patented goods. [39] By doing away with the necessity for human labor, automated chemical synthesis technologies based on artificial intelligence are revolutionizing research through automation of experimental processes. These systems are capable of carrying out a wide range of processes, including the synthesis of peptides, oligonucleotides, natural products, and medicines. Additionally, the efficiency of automated synthesis is being enhanced. High-throughput experiments (HTEs), which enable the simultaneous operation of dozens or even hundreds of reactions, are being used by an increasing number of individuals. These HTEs may use 24- or 96-well reactors and perform low-volatile solvent reactions at room temperature. One area of great interest in HTEs is metal-catalyzed cross-coupling reactions, which include a multitude of reaction variables. Palladium catalyst tolerance in certain processes may be predicted using the RF methodology developed by Ahneman and colleagues. This method provides insights into the catalyst inhibition mechanism and performs better than traditional linear regression analysis. [40]

AI in a clinical trial

Clinical trial failures are often caused by inefficient patient recruiting and selection procedures as well as challenges in effectively monitoring participants during the study. The primary reason for clinical trial delays is the difficulty of finding enough eligible individuals to enroll in the designated amount of time. Studies show that up to 86% of trials fail to reach their enrollment goals. There is a lot of promise for tackling these issues with the application of artificial intelligence (AI) tools to enhance patient recruiting and selection procedures. In addition to collecting and analyzing data concurrently from several clinical trial sites, these AI-powered platforms also allow for a more complete patient characterisation. [41] Currently, only around one-third of trial chemicals in Phase II reach Phase III. These billion-dollar investigations take ten to fifteen years to finish. Studies that don't work out also cost money for preclinical development. More than thirty AI algorithms have been approved by the US FDA for use in the diagnosis of various medical conditions, including stroke and diabetic retinopathy. The more than 300 clinical trials registered under the names "Artificial Intelligence," "Machine Learning," or "Deep Learning" attest to AI's ability to enhance healthcare through early diagnosis and other advantages. Researchers may be able to use AI to build AI-assisted randomization schemes with a wide variety of factors and anticipate trial outcomes sooner, hence reducing the chance of participant damage. In summary, AI has the ability to improve patient care and accelerate medical advancements. [42]

Role of Machine learning with artificial Intelligence

Machine learning is a subfield of artificial intelligence and computer science, allows automatically learn from experience and improve their interpretation of it Predicting expected supplier demand, coordinating the transfer of goods, and managing suppliers and paperwork are all made possible by machine learning. As digital technologies are increasingly being used to gather patient data, the COVID-19 pandemic may hasten the application of AI/ML in clinical trials. [43,44] The development of modern AI techniques has given pharmaceutics and biomedical science access to highly reliable computational methods. Artificial intelligence (AI) mimics or enhances human performance by simulating human intelligence in computer models. In the pharmaceutical sector, the process of developing new drugs is very costly, time-consuming, and governed by various regulations. The advent of artificial intelligence (AI), deep learning (DL), machine learning (ML), and computational chemistry has significantly altered the success rate of medication development.AI is being used by a huge number of startups and pharmaceutical businesses for medication research and development in the last ten years. Numerous pharmaceutical corporations have either acquired AI technologies or formed partnerships with them, such as Novartis and Pfizer with IBM Watson.

Explanation of machine learning:

It is based on an AI application that teaches computer programs or algorithms the fundamentals of automatically becoming familiar with a task and developing skill without the need for scripting. It enhances computer programs' capacity to handle data and apply it for learning. A system requires programmers to write and review appropriately in order to redact improvements.

Classification of machine learning

Machine learning can be divided into three main types.

1. **Supervised Learning:** Supervised learning is applied when the data consists of input variables and output target values. The input function is converted to the output

function via the algorithm. Determining the risk generator and pursuing clinical trial optimization are the objectives.

2. **Unmonitored Learning:** The opposite of supervised learning is this. This indicates that when there is no corresponding output variable and the data is solely available as an input, unsupervised learning is performed. Among the most popular categories of unsupervised algorithms is clustering. Using the intrinsic groups found in the data, this technique forecasts the result for unknown inputs. One use of this tactic is forecasting the purchasing habits of customers.
3. **Reinforcement of learning:** It is comparable to the method of unsupervised learning. The machine learning directive is to construct a decision order. An artificial intelligence is provided with a scenario that resembles a game. Examples are

   a Instructing agents on how to play video games.
   b Performing robotics tasks with a predetermined goal in mind. [45, 46]

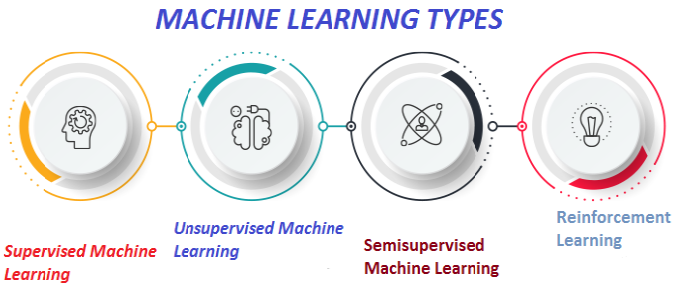

Fig. 3. Types of Machine Learning

Limitations and Difficulties of AI Use in Drug Discovery

Notwithstanding AI's potential advantages in drug research, there are a number of obstacles and restrictions to take into account. The availability of appropriate data is one of the main obstacles [47]. Large amounts of data are usually needed for AI-based techniques in order to train them [48]. The accuracy and dependability of the results can frequently be impacted by the limited quantity, variable quality, or poor quality of the data that is available [49]. Ethical issues also pose a barrier, since AI-based solutions may give rise to questions regarding prejudice and justice (see the part below this one) [50].Predictions made by an ML system, for instance, may be unfair or erroneous if the training data is biased or unrepresentative [51]. It is crucial to take into account the ethical and equitable use of AI in the creation of novel medicinal molecules [52]. The challenges AI faces in the context of chemical medicine can be solved using a variety of tactics and techniques. Utilizing data augmentation [53] is one strategy; it entails creating artificial data to complement preexisting datasets.

Traditional experimental methods and the expertise and experience of human researchers cannot be replaced by current AI-based approaches [54,55]. AI can only make predictions based on the data available; human researchers must then validate and interpret the results [56]. However, integrating AI with traditional experimental methods can improve the process of finding new drugs [57]. By combining the predictive power of AI with the knowledge and experience of human researchers [58], it is possible to accelerate the development of new medications [59].

Conclusion

We have seen in recent years how widely AI approaches are being applied to different phases of drug research and development. Drug development has advanced significantly as a result of the explosion of AI approaches. In the field of drug research, the use of Chat Generative Pre-Trained Transformer (Chat GPT) is another intriguing area. Given that it can offer techniques for locating possible targets, creating novel medications, and maximizing the effects. New drug discovery is a labor-intensive, expensive, and time-consuming process that entails several challenges from the point of identification of a novel drug molecule until the time the medicine is released into the market. Artificial Intelligence can predict new lead molecules along with their pharmacokinetic and pharmacodynamic parameters using a wide range of sophisticated software and models, saving time, money, and human labor. It can also lower the adverse drug reactions (ADRs) of the drug molecule, increasing its therapeutic efficacy. The availability of high-quality data that can be utilized to train models based on AI techniques is the first important element. The problem of poor data quality prevents the full use of the growing volume of biological and chemical data. Data curation is a solution that may be used to manage and organize unprocessed data. To achieve this goal, pharmaceutical corporations and academic institutions should work together to create frameworks and data standards that would aid in the clearing and gathering of data. Quantity of data is also crucial for the use of AI algorithms. The lack of interpretability of AI technique-based drug discovery models is another common problem. The degree to which others can comprehend the procedures a model employs to arrive at its conclusions is known as its interpretability. The suggested models are generally insufficient for deciphering their biological and pharmacological significance. Despite the mentioned difficulties, the drug research and discovery sector has used AI tools. It seems sense that AI methods will completely transform this industry.

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