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Comprehensive Review on the role of Artificial intelligence (AI) in drug discovery and drug development

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Abstract:

Artificial Intelligence or AI, has become a potent technology that might change the way healthcare works, from medicine delivery to drug discovery. This paper looks at how AI is already being used and will be used in the future in the pharmaceutical business, with an emphasis on medication delivery and research. It talks about a lot of different things, such as smart drug delivery networks, sensors, drug repurposing, statistical modeling, and simulating biological and biotechnological systems. It also looks at how The review talks about how AI may be used in medication formulation and distribution, clinical trials, drug safety, and pharmacovigilance. It talks about the rules and problems that come up when using AI in the pharmaceutical industry, such as privacy, data security, and how easy it is to understand AI models. The study continues with a look at the future, pointing out new trends, talking about the flaws and biases in AI models, and stressing how important it is to work together and share information. It gives a full picture of how AI might change the pharmaceutical sector and make patient care better, as well as areas where further research and development is needed.

Introduction

When computers are programmed to mimic human intelligence in terms of thought and behavior, we call this "artificial intelligence" (AI). A common definition of artificial intelligence is a method by which computers can mimic many of the sophisticated human skills. It was during a symposium in 1956 when John McCarthy and Marvin Minsky first brought up the topic of artificial intelligence (AI) [Arshad *et al*.2021:Sheikh *et al*., 2023]. Data digitization has been on the increase in the pharmaceutical business recently. The challenge of learning, analyzing, and using such data to solve complex healthcare concerns is a downside of digitization [Amisha *et al*., 2019]. This promotes the adoption of AI because of its ability to automate the management of large data sets [Haleem et al., 2022]. The term "artificial intelligence" (AI) refers to a set of computer programs and networks designed to simulate human intellect. Having said that, technology is not dangerous enough to supplant people Davenport et al., 2019; Wirtz et al 2019. The phrase "artificial intelligence" (AI) refers to computer systems and programs designed to automatically do certain tasks by analyzing, understanding, and learning from given data. New developments in the pharmaceutical sector are always taking place, as this review shows. Its applications in medicine are

constantly growing, as this essay demonstrates. Rapid progress in AI-guided automation will likely cause a sea change in how people work, according to the McKinsey Global Institute Smith et al ., 2000; Lamberti et al .,2019.

Fig. 1. Artificial Intelligence

Reasons for Using AI

1. Building Expert Systems: The overarching goal is to design smart, automated systems that can advise

and mentor humans to help them make the right choices.

2. Emulating Human Intelligence in Computers: AI aims to mimic human cognitive processes, making computers act intelligently and making judgments, particularly in challenging and complicated circumstances, much like humans. When it comes to automating tasks and reducing worker stress, algorithms are crucial.

3. AI Finds Use in Many Different Areas: AI has many different uses in many different areas, such as computer science, psychology, statistics, cognitive science, engineering, ethics, healthcare, space technology, logic, and linguistics, among many others.

4. Computer science applications: optimization, logic, control theory, language analysis, neural networks, classifiers, statistical learning methods, and probabilistic methods for uncertain reasoning are just a few of the complex computer science solutions built using mechanisms like Search and AI. A branch of AI and computer science, machine learning (ML) enables computers to autonomously gain knowledge and improve their understanding via experience. With the use of machine learning, it is now able to manage suppliers and paperwork, coordinate the transfer of products, and anticipate predicted supplier demand.

Classification of AI Methods

a. Artificial Narrow Intelligence (ANI): ANI is a subset of AI that isn't smart enough to play chess, drive, or recognize faces; it can only do very specific jobs.

b. AGI: It's a lot like human intelligence; it can do a lot of different things, learn from experience, and solve different kinds of problems.

c. **Artificial Super Intelligence (ASI):** It's even more advanced than human intelligence; it can do things like complex math, draw, and do scientific research Tarle et al.,2023; Shah et al.,2021.

Artificial intelligence and its possible uses in the pharmaceutical industry

There has been a surge of interest in medicinal chemistry's potential to use artificial intelligence (AI) as a game-changer in the pharmaceutical industry in recent years Kolluri et al.,2022. Historically, drug development has depended on labor-intensive procedures such as high-throughput screening and trial-and-error research, which is a challenging and time-consuming process. There is hope, however, that AI methods such as natural language processing and machine

learning (ML) may make this process faster and more precise by allowing for the efficient and accurate analysis of massive volumes of data Qureshi et al., 2023. A recent study Xu, Y et

al.,2021 detailed the use of deep learning (DL) to reliably predict the effectiveness of medicinal compounds. Artificial intelligence methods have also been used to forecast the toxicity of potential new medications Visan et al., 2024. These and other research have shown that AI may improve drug development processes in terms of efficiency and effectiveness. However, there are limitations and challenges to applying AI to develop new bioactive compounds. Additional study is necessary to fully understand the pros and downsides of AI in this domain, along with any ethical considerations Pu, et al., 2019. Regardless of these challenges, it is expected that the development of new therapeutics will be heavily reliant on artificial intelligence.

Limitations and drawbacks of the existing drug discovery process

Methods in medicinal chemistry rely on large-scale testing techniques and trial-and-error processes at the moment Rees et al., 2020. In order to identify the ones that possess the required properties, these procedures include screening through a large number of potential medicinal compounds. Although effective, these methods are not always cheap, take a long time, and often provide false findings. The difficulty in accurately predicting their physiological reactions and the availability of suitable test substances may further

limit them Wess et al., 2001. Algorithms based on artificial intelligence (AI), including supervised and unsupervised learning approaches, evolutionary algorithms, and rule-based algorithms, may be able to fix these problems. In most cases, these methods rely on analyzing large datasets with several potential uses Abbasi et al., 2023; Shi et al.,2024. For instance, as compared to more traditional approaches, these methodologies provide more precise and efficient predictions of the safety and effectiveness of new medicinal compounds Hansen et al., 2015; Askr et al., 2023. Artificial intelligence (AI) systems may also help identify novel drug development targets, such as disease-related proteins or genetic pathways Lysenko et al., 2018. This might lead to the development of new and better medications by expanding the breadth of drug discovery beyond the limitations of conventional approaches You et al., 2019. Therefore, while traditional methods of pharmaceutical research have had some success in the past, they are limited by their reliance on empirical trial and error and their inability to accurately predict the behavior of new, potentially bioactive compounds Jung et al., 2022. In contrast, AI-based approaches can improve the efficiency and accuracy of drug discovery processes, leading to the creation of stronger drugs.

The use of AI in the pharmaceutical industry and its potential effects on medication discovery and affordability

The development of novel compounds endowed with targeted properties and functionalities is yet another significant use of AI in the pharmaceutical industry. Finding and altering preexisting molecules is often a labor-and time-intensive process that conventional methods depend on. However, artificial intelligence (AI) based approaches may facilitate the efficient and rapid development of novel molecules exhibiting the necessary properties and functions. New therapeutic molecules with desired qualities, such as solubility and activity, may be proposed by training a deep learning (DL) algorithm on a dataset of existing medicinal compounds and their relevant attributes. Evidence like this suggests these strategies might be useful for the efficient and rapid development of novel medication candidates. DeepMind has recently contributed significantly to artificial intelligence research with the development of AlphaFold, a revolutionary software platform for enhancing our knowledge of biology [Nussinov et al., 2022]. By combining protein sequence data with AI, this powerful system can forecast the appropriate three-

dimensional structures of the proteins. Many believe that this new development in structural biology will revolutionize the process of drug discovery and individualized healthcare. The development of Alpha Fold represents a giant leap forward for the use of artificial intelligence in Fig. 2. Framework of AI technique application to drug discovery and evaluation, structural biology and surrounding biological fields.

Modern research in the field of de novo drug creation is making use of ML methods and MD simulations to improve the efficiency and precision of the process. The idea of integrating various techniques is being researched in order to take advantage of their synergy [Mouchlis et al., 2021]. Deep learning and interpretable machine learning (IML) are also used in this attempt. When researchers use AI and MD together, they can create drugs faster and more efficiently than previously.

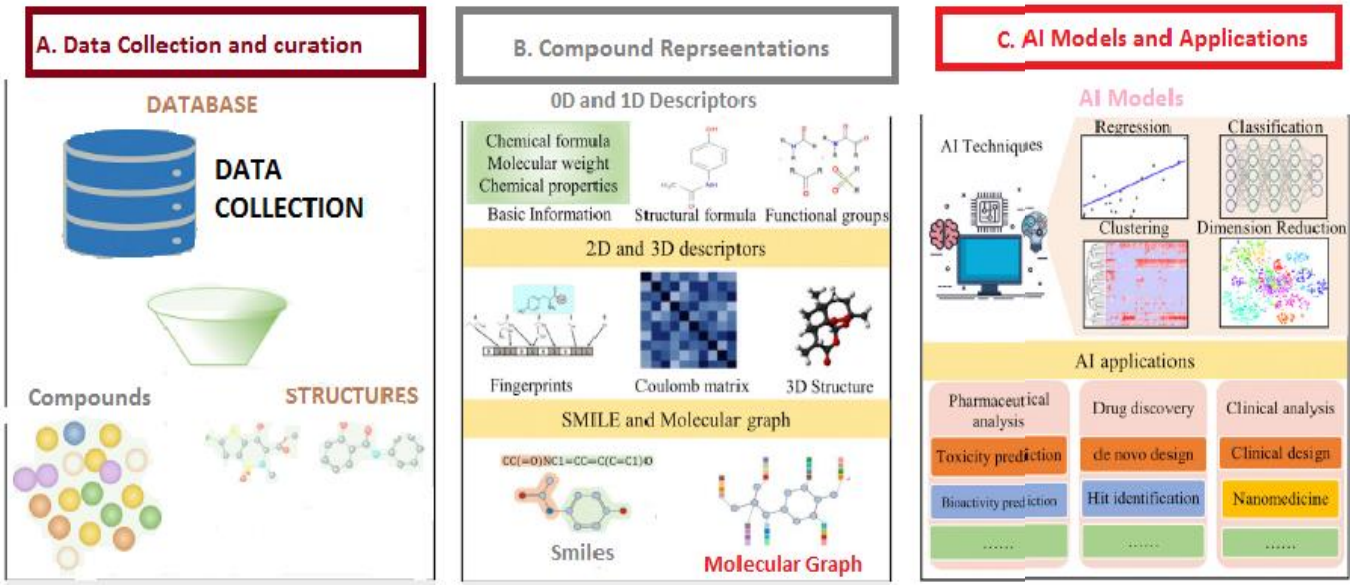

Fig. 2. Framework of AI technique application to drug discovery and evaLuation

Utilization of AI Technology

Artificial intelligence (AI) in drug discovery: The process of discovering new medications is notoriously complex and time-consuming, sometimes taking ten to fifteen years. Because of the high failure rate of potential new drugs to pass both clinical trials and regulatory clearance, pharmaceutical sector productivity is falling. The pharmaceutical industry is increasingly turning to artificial intelligence (AI) to solve this problem, as it may reduce costs and speed up the development of new medications. The pharmaceutical industry is making use of AI to expedite the discovery of novel compounds, verify medication targets, and improve drug designs. Synthesis planning, compound property assessment, and chemical

structure prediction with targeted effects are all made easier with the use of machine learning and silicon approaches. The massive amounts of data generated by the drug development process make deep learning an ideal tool for data management. [Kalyane et al., 2020] in

Because of Al, there have been major shifts in the fields of drug research and development.

Among Al's many significant contributions to this field are the following:

Identifying Objects

Genetic, protein, and medical record data are just a few examples of the many kinds of data that artificial intelligence (AI) systems may analyze. This is useful for finding possible therapeutic targets. By identifying these targets and understanding the role of molecules in disease, Al contributes to the creation of medications that may influence biological processes.

Simulating the Aspect-Relationship (SAR)

Through the use of Al models, the relationship between a compound's chemical structure and its biological function may be established. Scientists are able to create compounds with the necessary attributes, such as high efficacy, selectivity, and good pharmacokinetic

properties, allowing them to optimize the therapeutic potential.

New Drug Development

Artificial intelligence systems may suggest new chemical structures that look like medicinal drugs

by modifying generative models and using reinforcement learning. Artificial intelligence (AI) broadens the chemical realm and helps create new medical opportunities by learning from chemical databases and experimental data.

Reusing Pharmaceuticals

Algorithms can sift through mountains of scientific data in search of new medications with therapeutic potential. Al speeds up the medication development process and cuts expenses by finding new applications for old pharmaceuticals.

Accurately Anticipated Harm

By analyzing a substance's properties and molecular structure, Al systems can forecast the drug's toxicity. Machine learning algorithms may learn from toxicological datasets and then detect potentially harmful structural elements or foretell negative outcomes. This aids in the quest for safer medications by reducing the likelihood of adverse events during clinical trials. [Banerjee et al., 2022]

Application of AI in Manufacturing

Using AI in the context of Quality by Design (QBD) concepts in manufacturing has made the hitherto haphazard process of formulating new products much more methodical and rational. Artificial intelligence (AI) has several potential uses in the pharmaceutical sector, including optimizing process design and controls, analyzing trends to drive continuous improvement, and intelligent monitoring and maintenance. Modern manufacturing processes may be used with AI to assist pharmaceutical production and obtain desired outcomes. Examples of potential applications of artificial intelligence in pharmaceutical manufacture include as following:

Planning and Efficiently Scaling Operations

Applying artificial intelligence (AI) techniques, such as machine learning, to process data allows for the rapid identification of optimum processing parameters or ways to scale up operations. This leads to less development time and less waste.

Skilled in Managing Procedures

This technology allows for the dynamic control of the manufacturing process to get the required results. It is also possible to create process controls that can foretell how a manufacturing process

will unfold by integrating AI methods with data collected in real-time from

sensors. Many pharmaceutical companies have begun using APC technologies, which integrate AI methods with knowledge of the fundamental physical, chemical, and biological changes happening throughout manufacturing.

Keeping an Eye on Processes and Finding Problems

It is possible to conduct maintenance procedures to reduce process downtime when equipment operation deviates from the norm. It is also possible to employ AI algorithms to track the quality of products and their packaging. One example is vision-based quality control, which use artificial intelligence software to analyze images of vials, labels, and packaging made of glass. The software can identify whether a product isn't up to par in terms of quality.

Evaluating Current Trends

Despite the fact that customer complaints and variance reports sometimes include large amounts of text, artificial intelligence (AI) remains an essential tool for analyzing them. AI paves the way for the discovery of clusters of connected problems and their prioritization for further development. Being able to recognize patterns in production variations is very helpful since it allows you to understand all the reasons behind it. [Beneke et al., 2019] in The most effective formulation or technique

may be predicted using expert systems, NNS, and AI technology to determine the optimal values for complex research variables Paul et al., 2021 in Fuzzy models and artificial neural networks (ANNs) were used by researchers to tackle the issue of tablet capping on the manufacturing line. The correlation between machine settings and tablet capping occurrences was probed and analyzed using these state-of-the-art computational approaches. The most recent advancements in artificial intelligence, such as tablet-classifiers and meta-classifiers, are used to ensure the finest quality of the end product. In order to detect any deviations or faults in the tablet manufacturing process, these state-of-the-art technologies are crucial Chan et al., 2019.

Using AI for Pharmaceutical Formulation

The three-dimensional (3D) conformation of a target protein is critical in structure-based drug development. Understanding the three-dimensional chemical environment of the ligand-binding site on target proteins is crucial for the development of novel pharmacological drugs. In the past, researchers have sought this objective by using methods such as de novo protein creation and

homology modeling. The discipline has made extensive use of these

technologies to get insights into the structure of the target protein and to logically create potential therapeutic medicines. DeepMind, 2023 Alpha Fold, a remarkable AI tool, can accurately predict the three-dimensional structure of therapeutic target proteins, according to recent advancements in structure-based drug discovery. The remarkable performance of this technique has shown its capacity to revolutionize protein structure prediction and its consequences for medication creation Yang, et al., 2022.

Artificial intelligence's function in medication repurposing

The term "drug repurposing" describes the practice of applying commonly used pharmaceuticals or pharmacological combinations to new and unexpected medical contexts. Repurposing medicines is giving new uses for old medications or pharmacological combinations that are currently on the market. This approach is crucial for speeding up the pre-clinical phase of developing new drugs as it is less costly and takes less time than the traditional way of starting the drug discovery process from scratch. A more expedited alternative to de novo drug production, pharmaceutical repurposing has grown in prominence since the COVID-19 pandemic. In spite of its high cost and lengthy duration, the de novo drug development approach yields effective results. A

more expedited and cost-effective approach would be to repurpose currently-approved pharmaceuticals that have shown pharmacokinetics and mechanisms. Governments and pharmaceutical corporations are interested in this technology since it saves time and money. Artificial intelligence streamlines the process of drug repurposing while cutting costs and saving time. Alam, et al., 2024 in As a result of careless testing and research, drug repurposing has been discovered on several occasions. As an example, Pfizer used sildenafil citrate, originally intended for the treatment of hypertension, to manufacture Viagra, a novel medicine for the treatment of erectile dysfunction Zhou, et al., 2020.

The five-stage process is typical in conventional drug development.

i. Research conducted before to clinical trials;

ii. Clinical trials themselves;

iii) FDA monitoring;

iv) Post-market safety monitoring and development; and

v) Discovery and development

Repurposing medications, on the other hand, is a simple four-step process:

i. Research in the medical field

ii. Acquiring compounds

iii. Identifying compounds

iv. Clinical Research and FDA post-market safety monitoring and development. [Mak, et al., 2019]

Using AI in a scientific study

Poor methods of patient recruitment and selection, together with difficulties in adequately monitoring patients during the study, are common causes of clinical trial failures. Finding enough qualified participants to join in a clinical trial within the allotted period is the main cause of trial delays. Research shows that a significant majority of studies do not achieve their enrollment targets. Applying AI techniques to improve patient intake and selection processes holds great potential for addressing these difficulties. These AI-driven solutions not only enable more comprehensive patient characterisation, but they can also gather and analyze data simultaneously from several clinical trial locations Kate, et al., 2023. Approximately one-third of Phase II trial compounds actually make it to Phase III at this point. This kind of inquiry, which costs a billion dollars, takes ten to fifteen years to complete. Preclinical development also loses money on unsuccessful studies.

Artificial Intelligence and the Chemistry of New Drugs Synthesising

The selection of compounds is one of the most crucial and challenging tasks after chemical discovery. The standard approach for this is

retrosynthesis. Synthia, formerly known as Chematica, is a software tool that suggests potential synthesis pathways for eight important medicinal targets in order to make this process easier. This is achieved by increasing efficiency, decreasing expenses, and raising yield by programming of a set of rules into the computer. In addition, Synthia has offered synthetic alternatives to patented products and has been beneficial in producing materials that were previously unavailable Vora, et al.,2023. Through the automation of experimental operations, AI-based automated chemical synthesis technologies are reshaping research by eliminating the need for human labor. Peptides, oligonucleotides, natural products, and pharmaceuticals are among the many things that these systems can synthesize. Furthermore, automated synthesis is becoming more efficient. More and more people are making use of high-throughput experiments (HTEs), which allow for the simultaneous execution of hundreds of reactions. At room temperature, these HTEs may conduct low-volatile solvent reactions using 24-or 96-well reactors. There are a lot of reaction variables in metal-catalyzed cross-coupling reactions, which is one area where HTEs are quite interesting. Palladium catalyst tolerance in certain processes may be predicted using the RF methodology developed by Ahneman and colleagues. This

approach outperforms the more conventional linear regression analysis while also shedding light on the catalyst inhibition mechanism. Isani, et al., 2023

Using AI in a research study of 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. Finding enough qualified participants to join in a clinical trial within the allotted period is the main cause of trial delays. Research shows that a significant majority of studies do not achieve their enrollment targets. 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 Kalyane, et al., 2020. Approximately one-third of Phase II trial compounds actually make it to Phase III at this point. This kind of inquiry, which costs a billion dollars, takes ten to fifteen years to complete. Preclinical development also loses money on unsuccessful studies. 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 Patel, et al., 2022.

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 Singh, et al., 2022; Kolluri et al., 2022. 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 skills 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 to make improvements.

Classification in machine learning

Machine learning may be categorized into three primary categories.

1. Supervised Learning: Supervised learning is used when the dataset

comprises input variables and corresponding output target values. The input function is transformed into the output function by the algorithm. The aims are to identify the risk generator and optimize clinical trials.

2. Unsupervised Learning: The antithesis of supervised learning constitutes this. This signifies that in the absence of a matching output variable, and when data is only provided as input, unsupervised learning is executed. Clustering is one of the most prevalent kinds of unsupervised algorithms. This method predicts outcomes for unknown inputs by using the intrinsic groupings identified in the data. This method is used to predict client purchase behaviors.

3. Reinforcement of learning: It is analogous to the Technique of unsupervised learning. The machine learning directive is to establish a decision hierarchy. An artificial intelligence is presented with a situation akin to a game. Illustrations include

a. Guiding agents on video game gameplay.

b. Executing robotic activities with a specific objective in focus. Sah, 2020; Dara, et al., 2021.

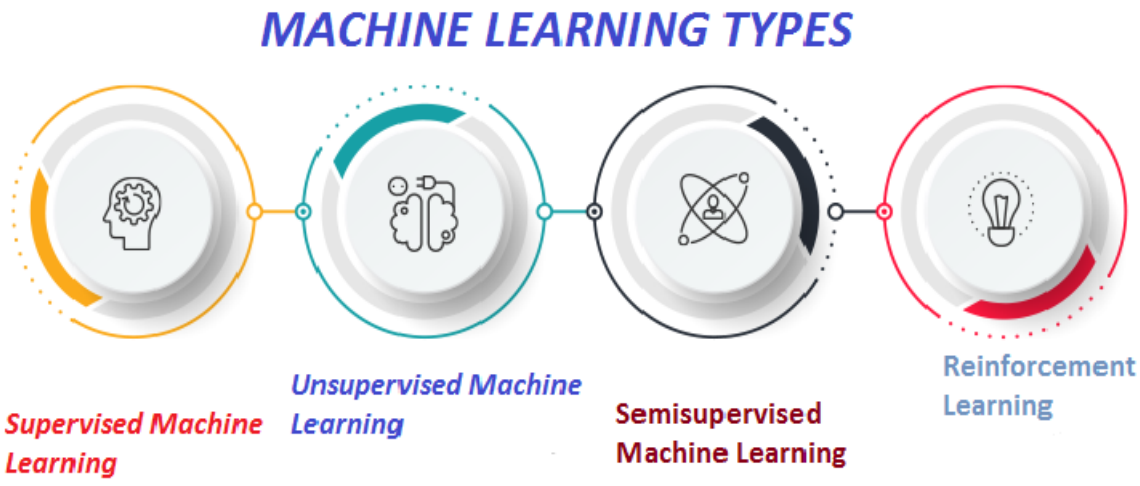

Fig. 3. Types of Machine Learning

Challenges and Constraints of AI Application in Pharmaceutical Research

Despite AI's possible benefits in drug research, several challenges and limitations must be considered. The presence of suitable data constitutes a significant barrier. Substantial quantities of data are typically required for AI-driven methodologies to facilitate their training Basu et al., 2020. The precision and reliability of the outcomes are often influenced by the restricted volume, inconsistent quality, or substandard nature of the available data Kleinberg, 2018. Ethical considerations present a significant obstacle, as AI-driven solutions may engender inquiries related to bias and fairness (refer to the subsequent section) Silvia et al., 2020. Predictions generated by a machine learning system can be flawed or unjust if the

training data is skewed or not representative Shimao, et al., 2022. It is essential to consider the ethical and equitable application of AI in the development of new medicinal compounds Sandfort et al., 2019. The obstacles encountered by Al within the realm of chemical medicine can be addressed through an array of strategies and methodologies. Employing data augmentation Askr et al., 2023 represents a method that involves generating synthetic data to enhance existing datasets.

The current AI-based approaches cannot supplant traditional experimental methods, nor can they replicate the expertise and experience of human researchers Schraagen et al.,2021; Gilpin et al.,2019. Artificial intelligence is limited to generating forecasts grounded in the data at hand; it is incumbent upon human researchers to subsequently authenticate and elucidate the findings Qureshi et al., 2023. Nonetheless, the amalgamation of artificial intelligence with conventional experimental techniques has the potential to enhance the methodology of discovering novel pharmaceuticals Jarrahi, 2018. Through the integration of artificial intelligence's predictive capabilities with the expertise and insights of human researchers Paul et al., 2021, one can significantly expedite the advancement of novel pharmaceuticals.

Conclusion

The extensive use of Al methods to various stages of drug research and development has been seen in recent years. The emergence of Al methods has greatly accelerated drug development. A fascinating new area of use for Chat Generative Pre-Trained Transformer (Chat GPT) is in the realm of drug research. Because it may provide methods for finding potential targets, developing new drugs, and enhancing their effects. Several obstacles must be overcome during the lengthy, costly, and labor-intensive process of new drug development, which begins with the identification of a novel therapeutic molecule and continues until the treatment is introduced onto the market. Using a variety of complex models and software, artificial intelligence may save time, money, and human labor by predicting novel lead compounds and their pharmacokinetic and pharmacodynamic properties. Additionally, it has the potential to increase the therapeutic effectiveness of the pharmacological molecule while decreasing its adverse drug reactions (ADRs). First and foremost, there must be access to high-quality data to train models using Al methods. The increasing amount of chemical and biological data cannot be fully used due to the issue of poor data quality. Unprocessed data may be better managed and organized with

the help of data curation. Collaboration between pharmaceutical companies and academic institutions to develop data standards and frameworks for data clearing and collection is necessary to reach this objective. Data quantity is also an important factor while using Al algorithms. Another prevalent issue with drug discovery models that rely on AI techniques is their lack of interpretability. The interpretability of a model is the extent to which its methods can be understood by others. In most cases, the proposed models are inadequate for understanding the pharmacological and biological relevance of these compounds. The drug development and research business has used Al tools despite the aforementioned constraints. Al's approaches will revolutionize this sector.

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