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ARTIFICIAL INTELLIGENCE IN PHARMACY

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Abstract
Computer science's artificial intelligence (AI) field develops tools for machines to analyze complex data and perform tasks more effectively. The amount of research on artificial intelligence has skyrocketed, and its application to healthcare services and research is developing at a faster rate. This paper explains in detail the potential benefits and drawbacks of artificial intelligence (AI) in pharmaceutical and healthcare research, utilizing specific algorithms and deep and machine learning integration. Examine the data that medical systems employ. AI has gained recognition in recent years for its use in a number of pharmaceutical science domains, particularly pharmacological research, where it serves as an efficient instrument for data mining based on vast amounts of pharmacological data and machine learning techniques. Therefore, artificial intelligence (AI) has been applied to de novo drug design, activity scoring, virtual screening, and in silico assessment of a pharmacological molecule's absorption, distribution metabolism, excretion, and toxicity.

Keywords: Artificial neural networks, Drug discovery, Drug delivery research, Hospital pharmacy.

Introduction

The use of artificial intelligence (AI) in medicinal chemistry has gained significant attention inrecent years as a potential means of revolutionizing the pharmaceutical industry.AI is a stream of science related to intelligent machine learning, mainly intelligent computer programs, whichprovides results in a similar way to the human attention process.**(1)** This process generally comprises obtaining data, developing efficient systems for the uses of obtained data, illustratingdefinite or approximate conclusions, self-correlations and adjustments. In general, AI is used for analyzing machine learning to imitate the cognitive tasks of individuals. In this perspective,various useful statistical models, as well as computational intelligence, are combined in AI technology Recently, AI technology becomes a very fundamental part of the industry for usefulapplications in many technical and research fields.

In this review, we briefly discuss the significant contribution of AI/ML in target identification and drug discovery. When focusing on the pharmaceutical sector, the role of AI cannot be ignored due to its wider applications across various stages. The influence of AI across all stages of pharmaceutical products from drug discovery to product management is very evident.**(5)** In drug discovery, AItechnologies are used in both the drug screening and drug design; the algorithm includes, to name a few, ML, deep learning, AI-based quantitative structure–activity relationship (QSRL) technologies, QSLRML, virtual screening (VS), support vector machines (SVMs), deep virtualscreening, deep neural networks (DNNs), recurrent neural networks (RNNs), etc. Neural networks in AI are inspired by biological neural networks where there is an input and output response after processing the information received. Artificial neural networks (ANN) have several connected units for processing the information. DNNs are similar to ANN wherein there are several layers of data processing units. RNNs process the data in a sequence wherebythe output data of the previous analysis is processed as input data for the next phase of analysis. SVMs are used for classification and regression of input data.**(6)** In pharmaceutical product development, AI is being used to choose the appropriate excipients, selecting the development process, and ensuring the specifications are achieved as per the compliance during the process.The model expert system (MES), ANNs, etc. are used in pharmaceutical product development. In manufacturing, AI is used in automated and

personalized manufacturing, matching manufacturing errors to set limits. AI technologies such as meta classifier and tablet classifierare used to achieve the desired quality in the final product. The incorporation of AI in clinicaltrials helps in selecting subjects and monitoring the trial, the dropouts are reduced because of close monitoring.

Mostly concerning safety and the dangers that may be potentiated by the creation of machinesthat could match human cognitive capabilities. One of the five predictions made by Forbes for AI in 2019 is that it may become an issue of national politics(4). Aside from concerns that AIs may be used as weapons for war and mass destruction, certain people have expressed concernsthat the creation of AI systems that are smarter than humans, through general AI could be more fatal and be the end of the human race itself. They believe we may not be able to predict how AI systems that are more intelligent than us will behave and that humans may end up being controlled by these super-intelligent machines. Scientists believe most of the safety concerns about future super-intelligent AI systems may be resolved.

1. History of artificial intelligence:

The origins of artificial intelligence (AI) may be traced back to myths, legends, and rumours of man-made creatures that were given intellect and consciousness by skilled artisans. Philosophers who attempted to characterize human mind as the mechanical manipulation of symbols provided the groundwork for contemporary AI. In the 1940s, this study led to the creation of the programmable digital computer (9). According to reports, the natural language processing industry, which encompasses a variety of appliances including text prediction, voice, and speech recognition, grew by 28.5% in 2017. Big data and business analytics generated $122 billion in global revenue in 2015, and it is predicted that thisfigure will surpass $200 billion by 2020. The 1950s are when artificial intelligence first Jeopardy.Since then, Watson has increased its involvement in healthcare and medication research, including a 2016 cooperation with Pfizer to quicken immuno-oncology drug discovery. In December 2016, IBM partnered with Pfizer to launch IBM Watson, a cloud-based medical laboratory reporting tool that enables researchers to identify relationships between different datasets through dynamic visualizations

2. AI General overview

The term AI (also known as machine intelligence) is very commonly confused and used interchangeably with robotics and automation. (9) While robotics is simply the creation of machines that can carry out difficult repetitive tasks, AI refers to the exhibition of human-likebehaviors or intelligence by any computer or machine. Traditionally, robots were not built to possess these “intelligent capabilities” even though they may be able to move or carry objects independently using a designed program and surface sensors in a process known as automation. AI, in essence, is the field of computer science that specializes in the creation of intelligent machines, developed with the ability to perform tasks that will ordinarily be associated with a human being.AI is frequently applied to the development of digital computers or computer- controlled robots with the capacity to autonomously execute intellectual and cognitive human- like processes. Such intellectual and cognitive processes include learning, reasoning, problem- solving, perception, and language.

AI classification;

a) According to caliber
b) According to the presence

Based on their caliber, AI system is classified as follows:

Weak intelligence or Artificial narrow intelligence (ANI): This system is designed and trained to perform a narrow task, such as facial recognition, driving a car, playing chess, and traffic signaling. E.g.: Apple SIRI virtual personal assistance, tagging in social media.

Artificial General Intelligence (AGI) or Strong AI: It is also called Human-Level AI. It can simplify human intellectual abilities(6). Due to this, when it is exposed to an unfamiliar task, it can find the solution. AGI can perform all the things as humans.

3. Artificial Super Intelligence (ASI): It is brainpower, which is more active than smart humans in drawing, mathematics, space, etc; in every field from science to art. It ranges from the computer just little than the human to a trillion times smarter than humans.

- The role of ML in predicting drug efficacy and toxicity: One of the key applications of AIin medicinal chemistry is the prediction of the efficacy and toxicity of potential drug comparend Hintze, an AI scientist classified the AI technology based on its presence and not yet present. They are as follows:

Type 1: This type of AI system is called a Reactive machine. E.g. Deep Blue, the IBM chess program which hit the chess champion, Garry Kasparov, in the 1990s. It can identify checkerson the chessboard and can make predictions; it does not have the memory to use pastexperiences(7). It was designed for narrow purposes use and is not useful in other situations. Another example is Google’s AlphaGo.

Type 2: This type of AI system is called a Limited memory system. This system can use past experiences for present and future problems. In autonomous vehicles, some of the decision- making functions are designed by this method only. The recorded observations are used to record the actions happening in the future, such as changing the lanes by car. The observationsare not in the memory permanently.

Type 3: This type of AI system is called as "theory of mind". It means that all humans have their thinking, intentions, and desires which impact the decisions they make. This is a non-existAI.

Type 4: These are called self-awareness. The AI systems have a sense of self and consciousness. If the machine has self-awareness, it understands the condition and uses the

ideas present in others' brains. This is a non-existing AI.. Classical protocols of drug discovery often rely on labor-intensive and time-consuming experimentation to assess the potential effects of a compound on the human body. This can be a slow and costly process, and the results are often uncertain and subject to a high degree of variability(8). AI techniques such as ML are able to overcome these limitations. Based on the analysis of a large amount of information, ML algorithms can identify patterns and trends that may not be apparent to human researchers. This can enable the proposal of new bioactive compounds with minimum side effects much faster than using classical protocols.

Limitations of current methods in drug discovery :

Currently, medicinal chemistry methods relies heavily on a hit-and-miss approach and largescale testing techniques8 . These techniques involve examining large numbers of potential drug compounds in order to identify those with the desired properties. However, these methods can be slow, costly, and often yield results with low accuracy.**(12)** In addition, they can be limited by the availability of suitable test compounds and the possibility to accurately predict their behavior in the body.

The role of ML in predicting drug efficacy and toxicity :

One of the key applications of AI in medicinal chemistry is the prediction of the efficacy and. toxicity of potential drug compounds. Classical protocols of drug discovery often rely on laborintensive and time-consuming experimentation to assess the potential effects of a compound on the human body. This can be a slow and costly process, and the results are often uncertain and subject to a high degree of variability. AI techniques such as ML are able to overcome these limitations. Based on the analysis of a large amount of information, ML algorithms can identify patterns and trends that may not be apparent to human researchers. Another importantapplication of AI in drug discovery is the identification of drug-drug interactions that take placewhen several drugs are combined for the same or different diseases in the same patient, resulting in altered effects or adverse reactions. **(13)**This can be identified by AI-based approaches by analyzing large datasets of known drug interactions and recognizing patterns

and trends. This has been recently addressed by a ML algorithm to accurately predict the interactions of novel drug pairs . The role of AI to identify possible drug-drug interactions in the context of personalized medicine is also relevant, enabling the development of custommadetreatment plans that minimize the risk of adverse reactions

3. The role of collaboration between AI researchers and pharmaceutical Scientist;

The role of collaboration between AI researchers and pharmaceutical scientists is crucial in the development of innovative and effective treatments for various diseases. By combining their expertise and knowledge, they can create powerful algorithms and machine learning models aimed to predict the efficacy of potential drug candidates and speed up the drug discovery process. This collaboration can also help improve the accuracy and efficiency of clinical trials,

as AI algorithms can be used to analyze the data collected during these trials to identify trendsand potential adverse effects of the drugs being tested. . An illustrative example is the collaboration between the pharmaceutical company Merck and the AI company Numerate to develop AI-based approaches for medicinal chemistry. Many new companies are currently arising around this area and their impact is expected to be significant at the short term.**(11)** By working together, they can help to identify new targets for drug development and improve the effectiveness of existing treatments, ultimately benefiting patients and improving their qualityof life.

4. Challenges and limitations of using AI in drug discovery ;

Despite the potential benefits of AI in drug discovery, several challenges and limitations that must be considered. One of the key challenges is the availability of suitable data. AI-based approaches typically require a large volume of information to be trained. In many cases, the amount of data accessible may be limited, or the data may be of low quality or inconsistent, which can affect the accuracy and reliability of the results. Ensuring the ethical and fair use ofAI for the development of new therapeutic compounds is an important consideration that mustbe addressed(10) . Several strategies and approaches that can be used to overcome the obstacles faced by AI in chemical medicine. One approach is the use of data Arguementation, which involves the generation of synthetic data to supplement existing datasets. Current AI-based approaches are not a substitute for traditional experimental methods, and they cannot replace the expertise and experience of human researchers. AI can only provide predictions based on the data available, and the results must be validated and interpreted by human researchers.

5. Ethical considerations in the use of AI in the pharmaceutical industry

As said in the previous section, it is important to consider the ethical implications of using AI in this fields. One key issue is the potential for AI to be used to make decisions that affect

people's health and well-being, such as decisions about which drugs to develop, which clinicaltrials to conduct, and how to market and distribute drugs. Another key concern is the potential for bias in AI algorithms, which could result in

unequal access to medical treatment and unfair treatment of certain groups of people. This could undermine the principles of equality and justice.[11]The use of AI in the pharmaceutical industry also raises concerns about job loss dueto automation. .

AI AND DEVELOPMENT OF PHARMACEUTICALS:

Companies are collaorating with AI vendors and leveraging AI technology in their manufacturing processes for research and development and overall drug discovery. Reports show nearly 62 percent of healthcare organizations are thinking of investing in AI shortly, and

72 percent of companies believe AI will be crucial to how they do business in the future.According to researchers, the use of these technologies improves decision-making, optimizes innovation, improves the efficiency of research/clinical trials, and creates beneficialnew tools for physicians, consumers, insurers, and regulators.Research works are carried out daily to find new active principles for the currently incurable diseases and conditions; increasethe safety profile of already existing drugs; combat drug resistance and minimize therapeutic failure. Hence, there is an increase in the size and variety of biomedical data sets involved in drug design and discovery. [8]

AI in pharmacy practice in hospital and community pharmacies; Machine learning models allowe-mails to be personalized at a speed and accuracy greater than that of any human being. Chatbots can be used to increase the efficiency of service delivery. Chatbots are capable of mimicking interactions between customers and customer care of sale staffs. Chatbots are capable of automatically resolving customer complaints and queries and the difficult questionsare transferred to human staff. In retail pharmacy, this principle can be applied. The chatbots can be programmed to mimic pharmacist-patient interaction.

Implications for pharmacists and their practice:

AI can strongly influence and shift pharmacists' focus from the dispensing of medications toward providing a broader range of patient-care services. The pharmacist can leverage AI to help people get the most from their medicines and keep them healthier.

AI approaches in polypharmacology:

Now a day, 'one-disease-multiple-targets' concept governs over the 'one-disease-one - targets' concept for the advanced realization of pathological process in various disorders at their molecular basis. The phenomenon of 'one-disease-multiple-targets' is known as polypharmacology. Which are accessible for the accomplishment of a variety of important and useful information related to the structure of crystals, chemical features, biological properties, molecular pathways, binding affinities, disease concern, drug targets, etc.

DIAGNOSIS BASED ON AI:

Artificial intelligence (AI) is utilized in healthcare facilities in numerous ways, such as organizing.medication types for individual patients and selecting suitable or accessible methods of administration or treatment regimens. In accuracy of medicine: The impact of artificial intelligence on genetic evolution and genomics is beneficial. The Advanced Genomics AI platform is efficient in detecting genomic data and medical records patterns that indicate mutations and correlations that cause diseases. This approach equips healthcare professionals All the previous data and reports, clinical expertise, etc., are considered in the designing of the treatment plan as suggested by this technology. IBM Watson for Oncology, the software as a service, is a cognitive computing decision support system that analyzes patient data against thousands of historical cases and insights gleaned from working thousands of hours with Memorial Sloan Kettering Cancer Center physicians and provides treatment options to help oncology clinicians make informed decisions. These treatment options are supported by literature curated by Memorial Sloan Kettering, and over 300 medical journals and 200 textbooks, resulting in almost 15 million pages of text.

Assisting in repetitive tasks: AI technology also assists in some repetitive tasks, such as examining the X-ray imaging, radiology, ECHO, ECG, etc., for the detection and identificationof diseases or disorders.

Barriers to AI integration in pharmacy practice;

conAs is the case with any technology, AI technology could face various barriers that impedeits adoption, functioning, and improvement . The adoption of AI technology could be hindered by the lack of awareness and knowledge of AI applications in pharmacy Understanding and familiarizing pharmacists with AI technology is crucial for its successful adoption in the pharmacy field. Another important barrier to AI technology adoption is data privacy and security concerns. AI has not achieved impeccable privacy protection and safety yet AI systems carry the danger of violating patients' privacy and security since they depend on the usage of

personal data to perform the required tasks. (12)The extensive data requirements of many AI models, coupled with cerns about potential data leaks, hinder the widespread adoption of AI technologies. Moreover, the integration of AI technology into the field of pharmacy can be greatly affected by regulatory constraints.

Artificial intelligence in drug discovery:

AI technologies in the healthcare industry have enabled pharmaceutical companies to expedite their drug discovery process. Moreover, it automates target identification and facilitates medication repurposing by evaluating off-target

chemicals. This results in quicker drugdevelopment and reduced repetition.
Give tasks in both the AI and health care sectors.Leading Neural networks and ANNs:
The learning algorithm of neural networks (from input data) takes two different forms mainly.
The classes of neural networks are

i) *Unsupervised learning:* Here the neural network is submitted with input data havingrecognised pattern. It is used for organizational purpose. The unsupervised learning algorithm uses 'Self Organizing Map' or 'Kohonen'. This is known sets as very useful modeling for the searching of relationships amongst the complex data.

ii) *Supervised learning:* This kind of neural network is illustrated with the sequences of harmonizing inputs and outputs. It is used for learning relationship-connection between the inputs and the outputs. It shows its usefulness in formulation to measure the cause and effects linking between input-output. It is the most frequently employed ANNs and is entirely linked with the back propagation learning rule. This learning algorithm is known as the outstanding methodology for the prediction as well as classification jobs.

Fuzzy logic and neurofuzzy logic:

According to the conventional logic, proposal may be true or false. The hypothesis behind the logic lies either in or totally outside the "true" set. When the hypothesis lies within the "true" set, the membership function is denoted as "1" and when the hypothesis lies outside the "true"set, the membership function is denoted as "0". (4) The basic concept of fuzzy logic is promotedby Lotfi Zadeh in the 1960s.26 In contrast to the conventional logic, the fuzzy logic is not limited to be 0 or 1. However, any continuous value in-between these limits can be taken here.When 20°C temperature is taken as "comfortable", according to the conventional logic temperature of 19 or 21°C, which remain outside this set, are "uncomfortable".

Advantages of artificial intelligence:

ror minimization: AI assists to decrease the errors and increase the accuracy with more precision. Intelligent robots are made of resistant metal bodies and capable of tolerating the aggressive atmospheric space, therefore, they are sent to explore space.

i) *Difficult exploration:* AI exhibits its usefulness in the mining sector. It is also used in the fuel exploration sector. AI systems are capable of investigating the ocean by defeating the errors caused by humans.

ii) *Daily application:* AI is very useful for our daily acts and deeds. For examples, GPS systemis broadly used in long drives. Installation of AI in Androids helps to predict what an individual is going to type. It also helps in correction of spelling mistakes.

iii) *Digital assistants:* Now-a-days, the advanced organizations are using AI systems like 'avatar' (models of digital assistants) for the reduction of human needs. The 'avatar' can follow the right logical decisions as these are totally emotionless.Human emotions and moodsdisturb the efficiency of judgement and this problem can be overcome by the uses of machineintelligence.

conclusion

As AI technological approaches believe like human beings imagining knowledge, solving problems, and making decisions, there has been a noticeable increase in interest in the past few years in using AI technology for the analysis and interpretation of some important fields of pharmacy, such as drug discovery, dosage form designing, polypharmacology, hospital pharmacy, etc It has been shown to be beneficial to use automated databases and workflows for efficient analysis using AI techniques.

Author contributions

All authors are contributed equally.

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Declaration of Competing Interest

The authors have no conflicts of interest to declare.

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