WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.453
Volume 13, Issue 11, 144-156. Review Article ISSN 2277–7105

A REVIEW ON ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL INDUSTRY

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Article Received on 05 April 2024,
Revised on 25 April 2024,
Accepted on 15 May 2024
DOI: 10.20959/wjpr202411-32453

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ABSTRACT

Artificial Intelligence (AI) and AI technologies are playing a vital role in the Pharmaceutical Industries. Many technologies of Artificial Intelligence are involved in various field of the Pharmaceutical industries like drug development, designing of dosage form, invention of novel drugs, manufacturing, nanotechnology, clinical technology etc. this advancement in the technology will make ease of the human jobs and save time. Using this AI technology will also decrease the chances or human errors reducing the effort and hence the results will be reliable.

KEYWORDS: Artificial Intelligence, technology, Pharmaceutical Industry, Dosage form, Drug Design.

Definition

Artificial intelligence is the technology that enables computers to mimic and display intelligence similar to that of humans. Interaction, language, education, interpretation, image processing, logic and decision-making are all included in this. AI imitates cognitive functions in machines to produce behavior that is similar to that of humans.

INTRODUCTION

Artificial intelligence use in pharmaceutical technology has increased over the years, and the use of technology can save time and money while providing a better understanding of the relationships between different formulations and processes parameters.[1] The pharmaceutical sector is an important one that is essential to preserving lives. It functions through ongoing innovation and the integration of new technology to meet the demands of the global healthcare system and handle medical crises like the most recent pandemic. Innovation is typically the result of extensive research and development across a range of domains, including production technology, packaging issues, and customer-focused marketing strategies.[2]

In the field of medicine, artificial intelligence is the application of automated algorithms to carry out operations that would typically need human intelligence. In vivo responses can also be evaluated using information models and the evaluation of therapeutic drugs, appropriate drugs, etc. Pharmacokinetics can also be predicted. In drug development, the use of computer models boosts their effectiveness and affordability based on the significance of pharmacokinetic prediction. In the field of artificial intelligence technology development, there are two primary factions. Conventional computational techniques fall under the first group. In these techniques, professionals like mechanical engineers attempt to replicate human experience and report their findings. The second method makes use of artificial neural networks (ANNs) to build systems that can replicate the operations of the human brain. In particular, a variety of artificial neural networks, such as recurrent neural networks (RNN) and deep neural networks (DNN), control the development of artificial intelligence technology. In Merck Kaggle and NIH Tox21 issues, DNN problems have been demonstrated to be more predictive than basic machine learning techniques. Machine learning may learn with or without training by utilizing the proper statistical approaches.[3]

HISTORY OF AI

It is possible that this 1995 AI program, created by Newell and Simon, was the first of its kind. John Mc Carthy is recognized as the father of artificial intelligence and is credited for eventually coining the term.

Introduction of AI

- The origins of artificial intelligence (AI) can be found in the 1956 attempts of classical philosophers to characterize human thought as a symbolic system.
- The term artificial intelligence (AI) was not, however, properly defined until 1956, at a symposium at Hanover, New Hampshire's Dartmouth College.

AI Maturation (1943-1952)

- Year 1943: Warren McCulloch and Walter Pits completed the initial research that is currently known as artificial intelligence in 1943.A model of artificial neurons was proposed by them.

- 1949 saw the development of an update rule by Donald Hebb that altered the strength of the connections between neurons. Hebbian learning is the current term for his rule.
- 1950: Alan Turing, an English mathematician, made significant contributions to machine learning. In his book "Computing machinery and intelligence," Alan Turing makes a test-related proposal. A Turing test is used to determine whether a machine is capable of displaying intelligent behavior comparable to that of a person.

AI birth (1952-1956)

- 1955 saw the creation of the first artificial intelligence program, known as "Logic theorist," by Allen Newell and Herbert A. Simon. This program found new and more elegant proofs for various theorems and had proven 38 out of 52 mathematical theorems.
- 1956: At the Dartmouth conference, American computer scientist John McCarthy coined the term artificial intelligence (AI). AI was originally recognized as a legitimate academic area.

The golden years: Initial Zeal (1956-1974)

- 1966: The focus of the researchers was on creating algorithms that could resolve mathematical puzzles. In 1966, Joseph Weizenbaum invented the first chatbot, called ELIZA.
- Year 1972: WABOT-1, the first intelligent humanoid robot, was created in Japan.

The Initial AI Winter (1974-1980)

- The first artificial intelligence winter occurred from 1974 and 1980. The term "AI winter" describes a period of time when computer scientists struggled with a severe lack of government funding for AI research.
- There was less interest in AI publicity during AI winter.

An AI explosion (1980-1987)

- Year 1980: AI returned with the "Expert system" following a period of hibernation. An expert system was designed to mimic a human expert's decision-making process.
- The American Association of AI's inaugural national conference took place at Stanford University in 1980.

The Second Winter of AI (1987-1993)

- The second artificial intelligence winter occurred from 1987 to 1993.

- Once more, the government and investors stopped sponsoring AI research because the results were inefficient and the cost was too high. Expert systems like XCON were incredibly economical.

The Advent of Sentient Entities (1993-2011)

- Year 1997: IBM Deep Blue defeated Gary Kasparov, the global chess champion, in this year, making history as the first computer to defeat a world champion.
- In 2002, artificial intelligence (AI) made its debut in homes through the Roomba vacuum cleaner.
- Year 2006: AI entered the business sphere and remained there till 2006. AI has also being used by companies like Netflix, Facebook, and Twitter.

Big data, artificial general Intelligence and Deep learning (2011 to Present)

- Year 2011: IBM's Watson triumphed in the 2011 Jeopardy competition, which required it to solve puzzles and challenging questions. Watson demonstrated its ability to comprehend normal language and quickly find answers to challenging problems.
- In 2012, Google released "Google Now," an Android app feature that allowed users to receive information in the form of a prediction.
- Year 2014: In the iconic "Turing test," chatbot "Eugene Goostman" emerged victorious in a competition.
- 2018: The IBM "Project Debater" did remarkably well when debating difficult subjects with two expert debators.[4]
- Important machine learning advances have been dubbed GPT-3 (issued by OpenAI in 2020) and Gato (published by DeepMind in 2022).
- After testing the GPT-4 big language model on a wide range of tasks in 2023, Microsoft Research came to the conclusion that "it could reasonably be viewed as an early (yet still incomplete) version of an artificial general intelligence (AGI) system.[5]

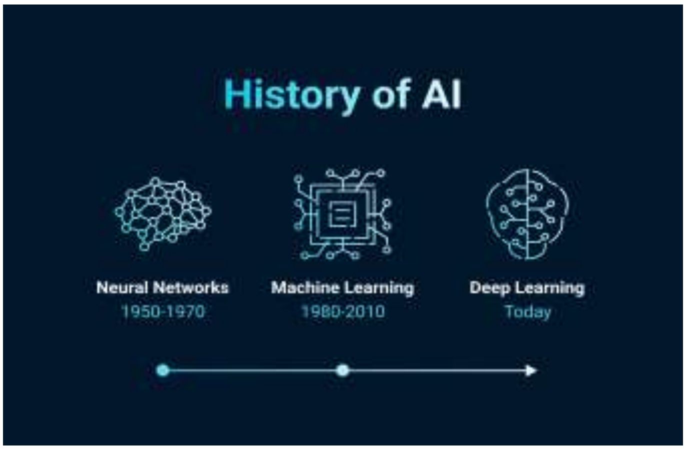

Fig. 1: History of AI

The current state of Pharmaceuticals and Ai's role

Because of their many benefits, small molecules are the subject of ongoing research in the pharmaceutical business to improve goods and consumer satisfaction. While the preparation of synthetic derivatives is inexpensive, the chemical synthesis process is straightforward. There are thus a lot of stable and effective small-molecule-loaded formulations available in the pharmacy industry. Generic molecules compete with many novel small molecules, with the exception of treating uncommon disorders. Complex data and clinical trials are necessary before these molecules may be introduced to the market. These procedures put more financial pressure on businesses to innovate more. To make up for the problem brought on by tiny molecules and the inadequate distribution of research and discoveries, the biomolecular medication business is nevertheless expanding quickly. Reactivity and conformation are the foundations of small-molecule activities.[6,7,8,9,10,11,12]

To eliminate system bias concerns and make successful decisions, human intervention is still necessary for a careful review of certain parameters and cross-verifications. However, given AI's enormous potential for use, a great deal of effort may be able to lessen its drawbacks and improve its effectiveness and dependability.[13]

- **AI learning under supervision**

A sort of machine learning known as "supervised learning" involves training an algorithm on a labeled dataset with an already-known desired outcome. By examining the patterns and connections found in the labeled data, the algorithm gains the ability to translate input data into the appropriate output. This method is frequently applied in many different fields, including predictive modeling, natural language processing, and picture recognition.[14] The applications are,

- **Drug Design and Discovery:** It is possible to forecast the characteristics or activity of novel therapeutic options using supervised learning algorithms. The model may identify patterns and connections between desired outcomes and molecular properties by training on a dataset of known substances and the actions that go along with them. This helps in drug discovery and design by enabling the prediction of novel compounds' activity, potency, or toxicity.[15]

- **Predictive Maintenance and Quality control:** Supervised learning can be applied to pharmaceutical manufacturing to support both of these processes. The model can be trained to forecast equipment failure, product quality deviations, or process anomalies using data from production processes, equipment sensors, or quality testing results. This enables proactive maintenance and quality assurance.[16]

- **Identification of drug target:** By examining biological data, supervised learning algorithms can assist in the identification of possible drug targets. The model can learn patterns and indicate possible targets for more research by being trained on data pertaining to genomic, proteomic, or transcriptomic traits and their relationship to treatment response or illness progression.[17]

- **Prognosis and Diagnosis of disease:** Based on medical data, supervised learning algorithms can be used to forecast patient outcomes or make illness diagnoses. The model is able to predict the course of the disease or the response to treatment by training on labeled datasets that comprise patient characteristics, clinical data, and disease outcomes.[18]

- **Detection of adverse event:** Pharmacovigilance data can be used to identify and categorize adverse events linked to medications using supervised learning algorithms. The model can be trained using labeled adverse event data in order to find patterns and potential safety signals, which will aid in the identification and characterisation of adverse occurrences.[19]

- **Predictive clinical trial modelling:** Clinical trial results can be predicted by supervised learning. The model can be trained to predict patient response, treatment efficacy, or safety outcomes using historical clinical trial data, which includes patient characteristics, treatment interventions, and trial outcomes. This data can improve patient selection and serve as a guide for trial design.[20]

- **Unsupervised artificial intelligence learning**

When an algorithm receives no labeled data, it is said to be engaged in unsupervised learning. Rather, its job is to find patterns and connections on its own in the data. This method is frequently applied in exploratory data analysis and is helpful for identifying hidden clusters or structures in a dataset. The methodology being discussed is widely referred to as "data-driven methodology.[21] "The unsupervised artificial intelligence learning is utilized as described below.

- **Grouping:** Data points are grouped by grouping algorithms according to their similarities, which makes it possible to find logical groups or clusters within the data.[22]

- **Diminution of dimensionality:** Principal component analysis (PCA) and t-distributed stochastic neighbor embedding (t-SNE) are two dimensionality reduction approaches that are used to minimize the complexity of high-dimensional datasets while retaining significant information.[23]

- **Identification of anomalies:** Algorithms for detecting anomalies are used to find uncommon or uncommon data points that substantially differ from the predicted trends. Anomaly detection is a helpful tool in the pharmaceutical sector that can be used to find problems with data quality, identify potential safety concerns, and discover adverse events.[24]

- **Association regulation of mining:** The Apriori algorithm is one example of an association rule mining tool that looks for intriguing relationships or associations between objects in a collection. Association rule mining can be used in the pharmaceutical industry to analyze data on adverse events, drug-drug interactions, and co-occurrence patterns between drugs and medical problems.[25]

- **Subject matter modeling:** From massive text corpora, latent topics or themes are extracted using topic modeling methods like latent Dirichlet allocation (LDA). The pharmaceutical industry can uncover important research subjects, new trends, or patient feelings by using topic modeling to examine scientific literature, clinical trial results, and social media data.[26]

- **Utilizing AI Tools in Drug Discovery**

Artificial intelligence has the power to revolutionize the search for new drugs. It can increase its efficacy and efficiency, which will benefit pharmaceutical companies creating novel pharmaceuticals to patients in dire need of appropriate therapies. AI can be applied at several phases of the drug-finding process. Among the instances are:

- AI-powered high-throughput virtual screening
- AI-based prediction of target protein structure
- Using AI to predict bioactivity
- AI-powered toxicity prediction, plus more[27]

- **AI in development of drug**

Then, a special medicinal component needs to be included in an appropriate dose form that satisfies the necessary delivery requirements. In this situation, artificial intelligence (AI) can replace the traditional method of trial and error.[28] QSPR can be used to handle a wide range of computational problems in the formulation design domain, including problems with instability, dissolving, porosity, and many more.[29] Using rule-based algorithms, decision-support systems select the kind, quantity, and sort of excipients based on the physicochemical characteristics of the medication. They also monitor the entire process and make occasional adjustments using a feedback loop.[30]

- **AI in formulation of drugs:** In addition to normal dosage forms, pharmaceutical sciences have seen the emergence of diverse formulations, such as solid dispersions, extrudates, pellets, nanoparticles, and liposomes. These methods are referred to as "formulation techniques" because they facilitate the creation of formulations or add functionality to typical dosage forms like tablets. Because AI applications in formulation techniques can effectively address a variety of API issues, such as low solubility, stability, bioavailability, and production capability, it is even more worthwhile to investigate these methods in order to create next-generation drug products with desired efficacy and health outcomes.[31]

- **Formulation of Controlled-Release tablets:** Chem software is used to teach the ANN model complex and specific skills from the input and output data units. Researchers employ a powerful artificial neural network (ANN) model to predict the optimal tablet formulations based on two ideal in vitro dissolution-time profiles and two desirable in vivo release profiles.[32]

- **Formulation of immediate release tablets:** Turkoglu created a direct compression tablet formulation using hydrochlorothiazide to increase tablet strength. In a different study, Kesavan and Peck created a model of a caffeine tablet formulation to explain the properties of the granule and tablet (Disintegration time, Hardness and Friability), as well as the diluting agent and binder content in each formulation and processing variables (Type of granulator, method of adding binder). It was shown by these two analyses that neural networks outperformed conventional statistical techniques. Thus, researchers using a range of genetic algorithms and neural networks have reevaluated Kesavan and Peck's findings.[33] This talk demonstrated how the optimal formulation was decided by the relative importance of the output qualities, the constraints imposed on the various component tiers, and processing factors. Researchers analyzed the same data using neuro-fuzzy computing, and they often produced useful rules that emphasized the salient features of each item.[34]

CONCLUSION

To conclude, Artificial Intelligence (AI) in Pharmaceutical industry has introduced new era of opportunities. Although it has several advantages, few disadvantages where due to Artificial Intelligence unemployment rate will get increased, machines can replicate human brain but they do not have moral or emotions as that of human, the cost of Artificial Intelligence is high and unlike humans, machines do not learn from experiments. Hence Artificial Intelligence can be used in the Pharmaceutical industry for the development with humans and not by replacing human.

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