

Artificial Intelligence in Pharmaceutical Industry

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Abstract: *Artificial intelligence (AI) is rapidly transforming the pharmaceutical industry, offering a range of opportunities to improve drug discovery, development, and manufacturing processes. AI-powered tools are being used to analyze vast amounts of data, identify patterns and relationships, and make predictions that can accelerate the development of new drugs and improve their efficacy and safety.*

Keywords: In drug discovery, AI is being used

I. INTRODUCTION

Artificial Intelligence (AI) is a stream of science related to intelligent machine learning, mainly intelligent computer programs, which provides results in the similar way to human attention process. [1] In general, AI is used for analyzing the machine learning to imitate the cognitive tasks of individuals. AI technology is exercised to perform more accurate analyses as well as to attain useful interpretation. [2] Various useful statistical models as well as computational intelligence are combined in the AI technology. [3] The progress and innovation of AI applications are often associated to the fear of unemployment threat. However, almost all advancements in the applications of AI technology are being celebrated on account of the confidence, which enormously contributes its efficacy to the industry. AI technology becomes a very fundamental part of industry for the useful applications in many technical and research fields. The emergent initiative of accepting the applications of AI technology in pharmacy including drug discovery, drug delivery formulation development and other healthcare applications have already been shifted from hype to hope. [4-5] The uses of AI models also make possible to predict the in vivo responses, pharmacokinetic parameters of the therapeutics, suitable dosing, etc. [6] According to the importance of pharmacokinetic prediction of drugs, the uses of in silico models facilitate their effectiveness and inexpensiveness in the drug research. [7] There are two key classes of AI technology developments. [8] [12-13] The machine learning employs suitable statistical methodologies with the capability to learn with or devoid of being unequivocally programmed. In addition, de novo design promotes the invention of newer drug molecules with regard to optimal or desired qualities. In the current review article, the uses of AI in pharmacy, especially in drug discovery, in case of the drug delivery formulation development, polypharmacology and hospital pharmacy are discussed. [13] The COVID-19 pandemic may further accelerate utilization of AI/ML in clinical trials due to increased reliance on digital technology in patient data collection. With this paper, we attempt a general review of the current status of AI/ML in drug development and also present new areas where there might be potential for a significant impact. We hope that this paper will offer a balanced perspective, help in separating hope from hype, and finally inform and promote the optimal use of AI/ML. [14]

II. HISTORY

Allen Newell, Herbert A Simon, was developed the Logic Theorist. It was born in 1956 that Dartmouth college had organized the famous conference [16]. It has been forecasted that the revenue from AI market will be increasing by as much as ten-fold between the years 2017 and 2022. Natural language processing market, which has several applications including text prediction, and speech and voice recognition has been said to achieve a growth of 28.5% in the year 2017. Worldwide revenue from big data and business analytics was US\$ 122 billion in the year 2015 and it is being expected that the figures will rise to more than US\$ 200 billion by the year 2020. [17] Artificial intelligence has a rocky history spanning back to the 1950s. For a long time it was seen as a field for dreamers, but that started to change in 1997 when IBM's Deep Blue co to defeat chess champion Garry Kasparov. By 2011, IBM's new Watson

supercomputer was able to win the US\$1m prize in the US game-show Jeopardy. Since then, Watson has expanded into healthcare and drug discovery, including a partnership with Pfizer in 2016 to accelerate drug discovery in immunology. In December 2016 IBM in collaboration with Pfizer introduced IBM Watson, a cloud-based such as medical lab reports and helps researchers with the ability to identify relationships between distinct data sets through dynamic visualizations Pfizer introduced IBM Watson, a cloud-based such as medical lab reports and helps researchers with the ability to identify relationships between distinct data sets through dynamic visualizations. [18]

III. CLASSIFICATION OF AI

AI can be classified into two different ways: according to calibre and their presence. According to their ability, AI can be categorized as:

Artificial Narrow Intelligence (ANI) or Weak AI: It performs a narrow range task, i.e., facial identification, steering a car, practicing chess, traffic signalling, etc.

Artificial General Intelligence (AGI) or Strong AI: It performs all the things as humans and also known as human level AI. It can simplify human intellectual abilities and able to do unfamiliar task.

Artificial Super Intelligence (ASI): It is smarter than humans and has much more activity than humans drawing, mathematics, space, etc. According to their presence and not yet present, AI can be classified as follows:

Type 1: It is used for narrow purpose applications, which cannot use past experiences as it has no memory system. It is known as reactive machine. There are some examples of this memory, such as a IBM chess program, which can recognize the checkers on the chess playing board and capable of making predictions.

Type 2: It has limited memory system, which can apply the previous experiences for solving different problems. In automatic vehicles, this system is capable of making decisions there are some recorded observations, which are used to record further actions, but these records are not stored permanently.

Type 3: It is based upon "Theory of Mind". It means that the decisions that human beings make are impinged by their individual thinking, intentions and desires. This system is non-existing AI.

iv). Type 4: It has self-awareness, i.e., the sense of self and consciousness. This system is also non-existing AI. [19-20]

3.1 Technologies Used in AI

Natural language processing (NLP): program computers to process and analyze large amounts of natural language data.

Support vector machine (SVM): Given a labeled training data (supervised learning), the algorithm outputs an optimal hyperplane which categorizes new examples.

Heuristics: mental shortcuts that ease the cognitive load of making a decision. Eg., using a rule of thumb, an educated guess, an intuitive judgment, a guesstimate, profiling, or common sense.

Artificial neural networks (ANN): Started in way back in 1940s, is an information processing model that is inspired by the way biological nervous systems, such as the brain, process information. An artificial neuron is a mathematical function. ANN takes data samples rather than entire data sets to arrive at solutions, which saves both time and money. ANNs have three layers that are interconnected (PYTHON). Neural networks learn things in exactly the same way as the brain, typically by a feedback process called back-propagation (back prop). ANNs are used in Self Driving cars, Character Recognition, Image Compression and Stock Market Prediction. It is depicted schematically in Figure 2. Software of artificial neural networks (ANNs) models the pattern recognition capacities of brain neural networks. Like a single neuron in the brain, artificial neuron system receives feedback from many external sources, processes it, and makes decisions. Interestingly, ANN simulates the biological nervous system and uses adaptive biological neurons analogues. ANN represents a promising modeling technique, especially for data sets having non-linear relationships which are frequently encountered in pharmaceutical processes. The various applications of ANNs can be summarized into classification or pattern recognition, prediction and modeling (Figure 2). Based on their pattern of association ANNs are classified as supervised 'associating networks, Unsupervised feature-extracting networks and Non-adaptive unsupervised networks. The potential applications of ANN methodology in the pharmaceutical sciences range from interpretation of analytical data, image recognition, drug and dosage form design through biopharmacy to clinical pharmacy. [21-22]

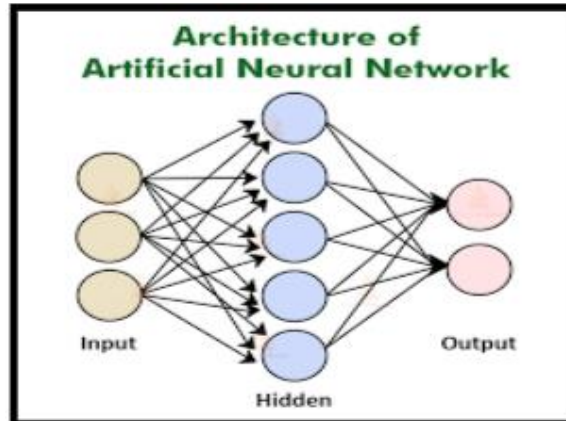


Fig 2: Typical illustration of artificial neural network

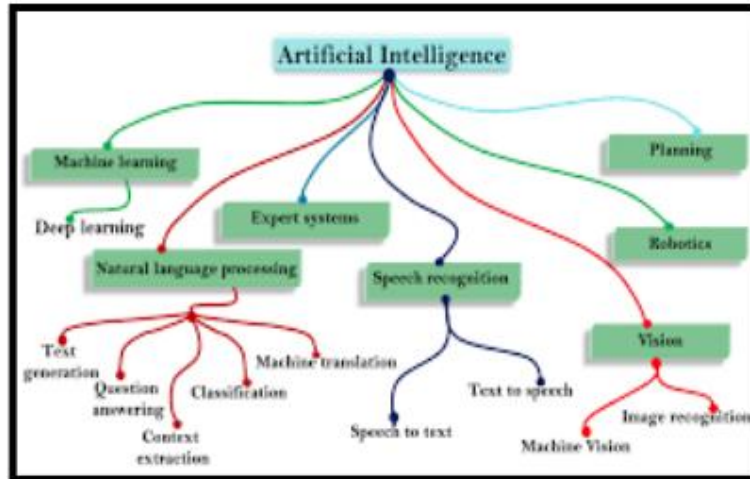


Fig 3: Ways and techniques of achieving AI

Achieving AI

AI is achieved using the following tools and techniques and are shown in Figure 3.

Machine Learning (ML)

It is a method where the target (goal) is defined and the steps to reach that target are learned by the machine itself by training (gaining experience). For example to identify a simple object such as an apple or orange. The target is achieved not by explicitly specifying the details about it and coding it but it is just as we teach a child by showing multiple different pictures of it and therefore allowing the machine to define the steps to identify it like an apple or an orange.

Tools of AI

Robot pharmacy:

The objective of improving the safety of patients, UCSF Medical Center uses robotic technology for the preparation and tracking of medications. According to them, the technology has prepared 3, 50, 000 medication doses without any error. The robot has proved to be far better than humans both in size as well as its ability to deliver accurate medications. The abilities of the robotic technology include preparation of oral as well as injectable medicines which include chemotherapy drugs that are toxic. This has given freedom to the pharmacists and nurses of UCSF so that they can utilize their expertise by focusing on direct patient care and working with the physicians. [24].



Fig. 4: Robot pharmacy

MEDi Robot:

MEDi is a short form for medicine and engineering designing intelligence. Tools of AI The pain management robot was developed as part of a project led by Tanya Beran, professor of Community Health Sciences at the University of Calgary in Alberta. She got the idea after working in hospitals where children scream during medical procedures. The robot first builds a rapport with the children and then tells them what to expect during a medical procedure, although the robot cannot think, plan, or reason, it can be programmed such that it shows to have AI. [25-26]

Erica robot:

Erica is a new care robot that has been developed in Japan by Hiroshi Ishiguro, a professor at Osaka University.) It was developed in collaboration with the Japan Science and Technology Agency, Kyoto University, and the Advanced Telecommunications Research Institute International (ATR). It can speak Japanese and has a blend of European and Asian facial feature. [27] Like any normal human being, it likes animated films, desire to visit south-east Asia, and wants a life partner who would chat with it. The robot cannot walk independently; however, it has been developed with the ability to understand and answer questions with human-like facial expressions. Erica is the “most beautiful and intelligent” android as Ishiguro fixed up the features of 30 beautiful women and used the average for designing the robot’s nose, eyes, and so on. [28]

TUG robots:

Aethon TUG robots are designed to autonomously travel through the hospital and deliver medications, meals, specimens, materials, and haul carry heavy loads such as linen and trash. It has two configurations, i.e., fixed and secured carts as well as exchange base platform that can be used to carry racks, bins, and carts.

The fixed carts are used for delivering medications, sensitive materials, and laboratory specimens, whereas, the exchange platform is employed to Vyas, et al.: Artificial Intelligence: New era in pharmacy profession Asian Journal of Pharmaceutics • Apr-Jun 2018 • 12 | 75 transport materials that can be loaded on different racks.

The TUG can deliver several types of carts or racks thus making it a very flexible and utilizable resource. [29]

Automated control process system [ACPS]:

The elements of [ACPS] include:

- Sensing process variables’ value.
- Transmission of signal to measuring element.
- Measure process variable.
- Presenting the value of the measured variable.
- Set the value of the desired variable.
- Comparison of desired and measured values.
- Control signal transmission to final control element. and
- Control of manipulated value.

Manufacturing Execution System(MES)

The benefits of using MES include compliance with guaranteed legal regulations, minimized risks, increased transparency, shortened production cycles, optimized resource utilization, controlled, and monitored production steps, and optimized up to batch release. [31]

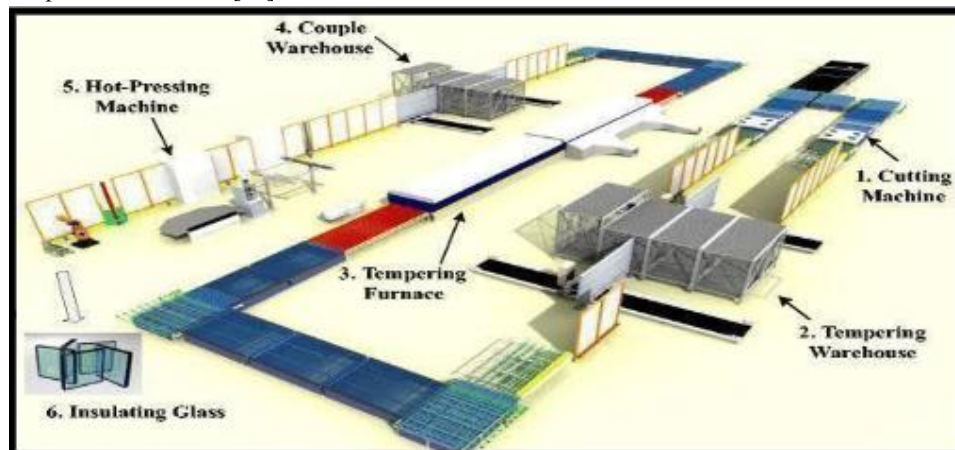


Fig. 5: Manufacturing Execution Systems

Development of Novel Peptides from Natural food

The Irish start up Nerites leverages AI and other novel technologies facilitate the discovery of new and more robust food and healthy ingredients. BASF (Baden Aniline and Soda Factory”) will take advantage of this partnership to develop novel functional

peptides derived from natural foods. In practice, BASF uses Nuritas AI and DNA analysis capabilities to predict, analyze, and validate peptides from natural sources. The main goal of BASF is to discover and deliver to the market peptide-based therapies that’ll help treat conditions like diabetes.

Treatment and Management of Rare diseases

Advances in AI, renewed interest in rare disease treatments. Currently, there are over 350 million people with over 7,000 rare diseases around the world. However, it’s not all gloom and doom for patients with rare diseases as Heal, a UK-based biotech firm, has secured \$10 million in Series A funding to use AI to develop innovative drugs for rare conditions. Thera chon, another Swiss biotech company that leverage AI to develop drugs for the treatment of rare genetic diseases, has received \$60 million in funding. [31]

Recent Development in AI:

AI Market in Health care:

According to venture capital firm Rock Health, 121 health AI and machine learning companies raised between 2011 and 2017. The value of 10 promising AI applications and found that they could create up to \$150 billion in annual savings for U.S. health care by 2026. Reducing health costs by Image processing, safeguarding patients’ personal records against cybercriminals and assisting in surgeries. AI-enabled workflow assistants are aiding doctors free up their schedules, reducing time and cost. AI helps pathologists in analyzing tissue samples and thus, in turn, making more accurate diagnosis. As per Harvard Business Review and Accenture, there are 10 potential applications of AI which could change the health care industry (Table 1 and Figure 7). [32]

Health Application	Motivation for adoption
Robot assisted surgery	Technological advances in robotic solution for more types of surgery
Virtual nursing assistants	Increasing pressure caused by medical labor shortage
Administrative workflow	Easier integration with existing technology infrastructure
Fraud detection	Need to address increasingly complex service and payment fraud attempts

Dosage error reduction	Prevalence of medical errors, which leads to tangible penalties
Connected machines	Proliferation of connected machines/devices
Clinical trial participation	plethora of data; outcomes-driven approach
Preliminary diagnosis	Interoperability/data architecture to enhance Accuracy
Autonomous image Diagnosis	Storage capacity, greater trust in AI technology
Cyber security	Storage capacity, greater trust in AI technology

Table 1: Ten potential health applications and potential motivation for adoption

Advantages of 3D Printed Drug Delivery:

- High drug loading capability compared to conventional dosage forms.
- Accurate and Precise dosing of potent drugs which are administered at small doses for activity.
- Reduced production cost due to less wastage of materials.
- Suitable drug delivery for difficult to formulate active ingredients like poor water solubility and narrow therapeutic windows drugs.
- Medication can be tailored to a patient in particular based on age, gender, genetic variations, ethnic differences and environment.
- Treatment can be customized to improve patient adherence in case of multi-drug therapy with multiple dosing regimen.
- 3D printers capture minimal space and are affordable.[34]

Advantages of AI Technology:

Error 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.

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.

Daily application: AI is very useful for our daily acts and deeds. For examples, GPS system is 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.

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 moods disturb the efficiency of judgement and this problem can be overcome by the uses of machine intelligence

Repetitive tasks: In general, human beings can perform single task at a time. In contrast to the human beings, machines are capable of performing multi-tasking jobs and can analyze more rapidly in comparison to the human beings.

Various machine parameters, i.e., speed and time can be adjusted according to their requirements.

Medical uses: In general, the physicians can assess the condition of patients and analyze the adverse effects and other health risks associated with the medication with the help of AI program. Trainee surgeons can gather knowledge by the applications of AI programs like various artificial surgery simulators (for examples, gastrointestinal simulation, heart simulation, brain simulation, etc.

No breaks: Unlike human beings who have the capacity of working for 8 h/day with breaks, the machines are programmed in such a way that these are capable of performing the work in a continuous manner for long hours devoid of any kinds of conons.[45]

IV. APPLICATION

In Formulation:

Controlled release tablets: The first work in the use of neural networks for modeling pharmaceutical formulations was performed by Hussain and coworkers at the University of Cincinnati (OH, USA). In various studies they modelled the in vitro release characteristics of a range of drugs dispersed in matrices prepared from various hydrophilic polymers. In all cases, neural networks [46] with a single hidden layer were found to offer reasonable performance in the prediction of drug release. In a more recent study involving the formulation of diclofenac sodium from a matrix tablet prepared from cetyl alcohol, personnel from the pharmaceutical company KRKA dd (Smerjeska, Slovenia) and the University of Ljubljana (Slovenia) have used neural networks to predict the rate of drug release and to undertake optimization using two- and three dimensional response surface analysis. [47]

In Product Development:

The pharmaceutical product development process is a multivariate optimization problem. It involves the optimization of formulation and process variables. One of the most useful properties of artificial neural networks is their ability to generalize. These features make them suitable for solving problems in the area of optimization of formulations in pharmaceutical product development. ANN models showed better fitting and predicting abilities in the development of solid dosage forms in investigations of the effects of several factors (such as formulation, compression parameters) on tablet properties (such as dissolution). ANNs provided a useful tool for the development of micro emulsion-based drug-delivery systems in which experimental effort was minimized. [48]

Challenges in Adoption of AI in Pharma companies:

While AI has an extensive potential to help redefine the pharmaceutical industry, the adoption itself is not an easy walk in the park.

Challenges that pharma companies face while trying to adopt AI:

- The unfamiliarity of the technology – for many pharma companies, AI still seems like a “black box” owing to its newness and esoteric nature.
- Much of the data is in a free text format – that means pharma companies have to go above and beyond to collate and put this data into a form that’s able to be analyzed. Pharma will simply look at artificial intelligence as a basic, everyday, technology. [49]



Fig. 13: Challenges to adoption of AI in pharma

V. FUTURE SCOPE

Machine learning techniques can manage complex analyzes with huge, heterogeneous, and high-dimensional information collections with no manual input, which has proved helpful in the writing business applications. Combining machine learning, particularly deep learning, with human skill and experience might be the best way to coordinate numerous enormous data stores. The amazing information-mining capacity of AI innovation has given new essentiality to computer supported medication plans that incorporate multiple clinical considerations are better than piecemeal

information, which can speed up prescription processes.. The coordinated development of mechanization and innovations resulting from combining technologies should lead to advancements in medication resulting from improved analysis of large and complex datasets. This will be necessary to shorten drug development cycles, reduce costs, and improve success rates: the ultimate goal of implementing AI in this context. [50]

VI. CONCLUSION

The main potential of AI in the pharmaceutical industry is to reduce costs and increase efficiency. Extensive research has demonstrated that dynamic learning can distinguish profoundly exact AI models while using half or less information than traditional AI and information sub- sampling approaches. Although the reason for this increased productivity is not fully understood, it appears that reduced repetition and predisposition, as well as gaining more significant information to traverse choice limits, are key components in this improved execution. 3D printing technology can make complex formations as cost and time efficient. It may improve its applications in Pharmaceutical Research and Biotechnological fields. 3D printing involves wide technical range in pharmaceutical field with novel drug delivery system, generation of new excipients, improvements of drug compatibility and customized dosage forms. In future 3D printing can be regulated and followed by pharmaceutical and all other sectors with needed level of safety and security concerns.

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