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Joining hands AI & Pharmaceutical Industry: Emerging Trend

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Abstract: Artificial Intelligence (AI) is the simulation of human behaviour in relation to the processes of intelligence involved in problem solving. Such mechanisms include human cognitive science reading, observation, preparation, interpretation, reasoning, correction, speech recognition, linguistics, and other sources. AI simplifies tasks by making machines learn from past experiences, mapping efforts and actions to results, identifying errors, correcting them, adjusting to new and random input values, and effortlessly performing human-like tasks through in-depth scenario analysis. AI simplifies work by analysing, filtering, sorting, predicting, scoping, and determining large data volumes to follow the best implementation procedures for producing an optimal solution. AI plays an important role in various fields of pharmacy like drug discovery, drug delivery formulation development, poly-pharmacology, hospital pharmacy, etc. The article is describing the drugs discovery, tools of AI, manufacturing execution systems automated control processes systems, AI to predict new treatment, development of novel peptides from natural foods, treatment and management of rare diseases, drug adherence and dosage, challenges to adoption of AI in pharma

Index Terms: **Artificial intelligence, Hospital pharmacy, Drug Discovery, challenges to adoption of AI in pharmacy, Artificial neural network.**

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. This process generally comprises obtaining data, developing efficient systems for the uses of obtained data, illustrating definite or approximate conclusions and self-corrections/adjustments. AI technology is exercised to perform more accurate analyses as well as to attain useful interpretation. Recently, 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. The

uses of AI models also make possible to predict the in vivo responses, pharmacokinetic parameters of the therapeutics, suitable dosing, etc. According to the importance of pharmacokinetic prediction of drugs, the uses of in silico models facilitate their effectiveness and inexpensiveness in the drug research.8 There are two key classes of AI technology developments. The first one comprises the conventional computing methodologies including expert systems, which can simulate the human experiences and illustrating the conclusions from the principles, like expert systems. The second one comprises the systems, which can model the mode of brain functioning employing the artificial neural networks (ANNs). In the current review article, the uses of AI in pharmacy, especially in drug discovery, drug delivery formulation development, poly-pharmacology and hospital pharmacy are discussed.

History

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 computer was able 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 immuno-oncology. 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.

Differences between machine learning and artificial intelligence

“Machine learning” (ML) is the branch of AI where the goal is defined and the steps to achieve this goal are fed into the system along with the rules and alternative actions to be considered. This information is automatically learned by the system that improves itself based on experience. The program that generates the algorithm integrates the input and the output for efficient performance. The main aim is to produce accurate results than to produce the desired ones. It does not involve randomization based on changing parameters; rather it is based on fixed values. The goal of ML is to learn from a predetermined set of data and produce mechanical solutions for better machine performance, no decision-making is involved. It is completely algorithm-based with structured data formats for inputs and outputs. It involves knowledge building without the discretion of what is right or wrong. The important functionality of ML involves pattern recognition in huge data sets and acting on them. Artificial Intelligence (AI) is based on the ability of a machine to acquire knowledge and apply it skilfully based on various real-life scenarios and real-time data. In AI the goal is to act instead of a human in a human-like manner in order to execute specific independent or interdependent tasks. AI may incorporate multiple programming integrations, validations, and pattern recognition methods to behave in an expected way. The main aim of AI is to produce a result through intelligent data analysis, mining, and deeper understanding It involves producing results based on smart real time processing and automation where the parameters are dynamic. The goal of AI is to simulate human intelligence in producing realistic solutions to complex problems through better decision-making It is based on the machine’s response to circumstances and complex problems without a fixed algorithm in place. It involves multiple levels and forms of analysis to seek an optimal solution. It leads to the wisdom of learning using intelligence and self-

imposed discretion of right and wrong. AI involves smart learning by a computer through awareness of past iterations and application of alternative information processing and cognitive analysis that demand distinct capabilities.

Milestone in AI

The first use of the phrase- 'Artificial Intelligence' was appeared in 1956. However, the concept of AI was employed since 1950 with the uses of problem-solving as well as symbolic methodologies

Objectives of AI

- **Multi-Domain Application:** AI will help in multiple domains of implementation like Computer Science, Cognitive Science, Statistics, Psychology, Medical Science, Engineering, Ethics, Natural Sciences, Healthcare, Space Technology, Logic, Linguistics, E-commerce, and more.
- **Creation of Expert Systems:** It involves the creation of automated systems that exhibit intelligent behaviour and advice humans on the right course of action.
- **Applications in Computer Science:** AI helps in developing several mechanisms to solve many difficult problems in the field of computer science like Search and Optimization, Logic, Control Theory, Language Analysis, Neural Networks, Classifiers, and Statistical Learning Methods, and Probabilistic Methods for uncertain reasoning.
- **Implementation of Human Intelligence in Computers:** It will help create identical cognitive patterns in computers which will help them behave like humans and take appropriate actions to solve complex problems. This will enable automated processes and reduced human workload through the application of algorithms.

Pros of Artificial Intelligence

AI simplifies work by analysing, filtering, sorting, predicting, scoping, and determining large data volumes to follow the best implementation procedures for producing an optimal solution. Performing mundane tasks is faster and effective with reduced errors when performed efficiently by AI systems. Accurate results can be obtained by the implementation of highly-responsive AI systems in technology-driven complex tasks and difficult/uncertain explorations. They function in all environments without being bound physically, environmentally, or emotionally. Simulations are worked on in real-time by AI systems as if they are real-life scenarios for better and realistic results. The Security and Protection of data and crucial information is maintained by AI systems and loopholes are automatically fixed or notified about High-Quality analysis and results are delivered by AI systems that are well-integrated with various technology systems. It can be categorized into list points.

1. **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
2. **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
3. **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.
4. **Difficult exploration:** AI exhibits its usefulness in the mining sector. It is also used in the fuel exploration sector. AI systems can investigate the ocean by defeating the errors caused by humans.
5. **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
6. **Increase technological growth rate:** AI technology is widely used in most of the advanced technological innovations worldwide. It can produce different computational modelling programs and aims for the invention of the newer molecules. AI technology is also being used in the development of drug delivery formulations.

Disadvantages of AI technology

1. **Expensive:** The launch of AI causes huge money consumption. Complex designing of machine, maintenance and repairing are highly cost effective. For the designing of one AI machine, a long period of time is required by the R&D division. AI machine needs updating the software programmes, regularly. The reinstallations as well as recovery of the machine consume longer time and huge money.
2. **No replicating humans:** Robots with the AI technology are associated with the power of thinking like human and being emotionless as these add some advantages to perform the given task more accurately without any judgement. If unfamiliar problems arise, robots cannot take the decision and provide false report.
3. **Unemployment:** The widespread uses of AI technology in all the sectors may cause large scale unemployment. As because of the undesirable unemployment, human workers may lose their working habits and creativity.
4. **No original creativity:** Machines with AI technology have neither sensitivity nor the emotional intelligence. Humans can hear, see, feel, and think. They can use their creativity as well as thoughts. These features are not achievable by the uses of machines.

5. **No improvement with experience:** Human resource can be improved with experiences. In contrast, machines with AI technology cannot be enhanced with experience. They are unable to identify which individual is hard working and which one is nonworking.

AI used in Drug discovery

Traditional drug discovery methods are target-driven, i.e., a known target is used to screen for small molecules that either interact with it or affect its function in cells. These approaches work well for easily druggable targets that have a well-defined structure and whose interactions inside the cell are understood in detail. However, these methods are extremely limited due to the complex nature of cellular interactions as well as limited knowledge of intricate cellular pathways.

AI can overcome these challenges by identifying novel interactions and inferring functional importance of different components of a cellular pathway.

- AI utilizes complex algorithms and machine learning to extract meaningful information from a large dataset, e.g., a dataset of RNA sequencing can be used to identify genes whose expression correlates with a given cellular condition
- AI can also be used to identify compounds that could bind to 'undruggable targets', i.e., proteins whose structures are not defined. Through iterative simulations of interactions of different compounds with small pieces of a protein, a predictive set of compounds can be easily identified in a relatively small amount of time.

Benefits of applying AI to drug discovery

The application of AI to drug discovery has the potential to revolutionize the current time scale and scope of drug discovery.

1. AI does not rely on predetermined targets for drug discovery. Therefore, subjective bias and existing knowledge is not a factor in this drug development process.
2. AI utilizes the latest advances in biology and computing to develop state-of-the-art algorithms for drug discovery. With the rapid increase in processing power and reduction in processing cost, AI has the potential to level the playing field in drug development.
3. AI has a higher predictive power to define meaningful interactions in a drug screen. Therefore, the potential for false positives can be reduced by carefully designing the parameters of the assay in question.
4. Most importantly, AI has the potential to move drug screening from the bench to a virtual lab, where results of a screen can be obtained with greater speed and promising targets can be shortlisted without the need for extensive experimental input and manpower hours.

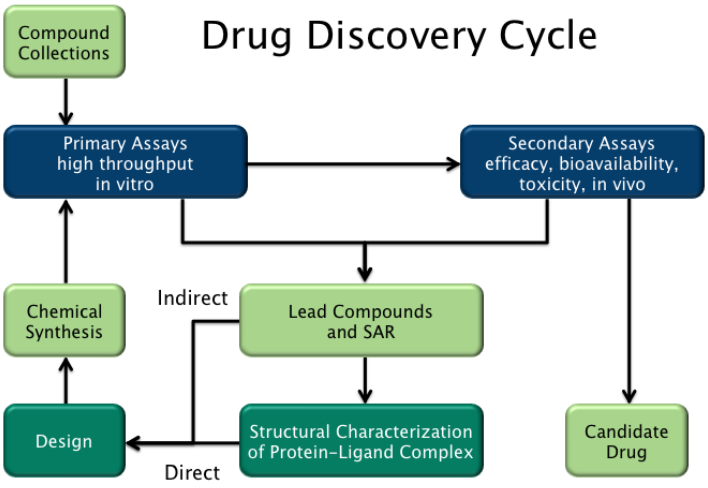

Figure 1

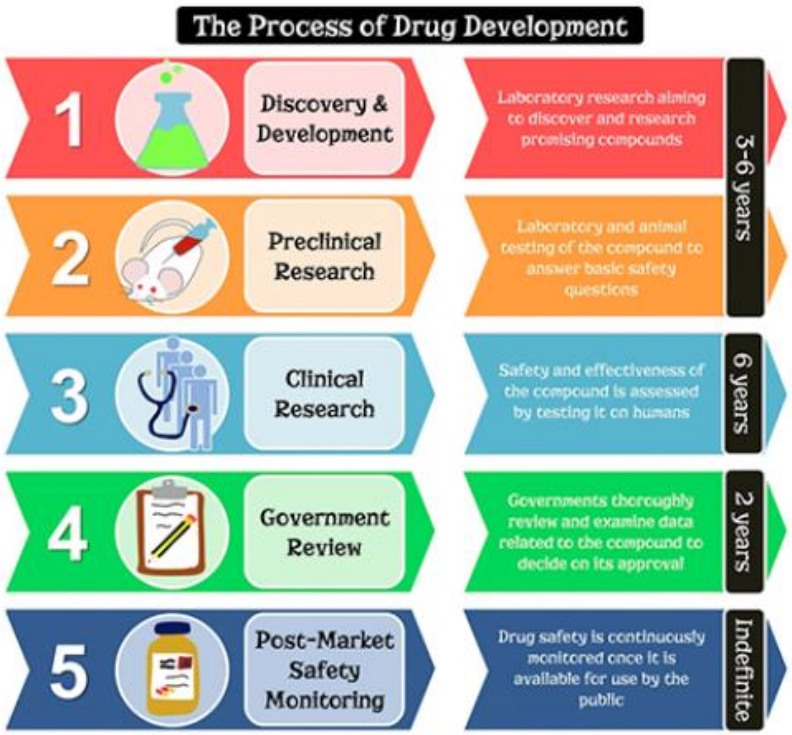

Figure 2

Table No. 1: Traditional V/S AI-based drug discovery methods

S. No.	TRADITIONAL	AI-BASED
1	Target-driven	Data-driven
2	Work well for easily druggable targets that have a well-defined structure and whose interactions inside the cell are understood in detail	Complex algorithms and machine learning can extract meaningful information from a large dataset
3	Extremely limited due to the complex nature of cellular interactions and limited knowledge of intricate cellular pathways	Identify compounds that could bind to undruggable targets i.e., proteins whose structures are not defined

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:

1. **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.
2. **Artificial General Intelligence (AGI) or Strong AI:** It performs all the things as humans and known as human level AI. It can simplify human intellectual abilities and able to do unfamiliar task.
3. **Artificial Super Intelligence (ASI):** It is smarter than humans and has much more activity than humans drawing, mathematics, space, etc.

Adoption of AI in Pharma

The drug discovery procedure begins from the available results attained from different resources like high throughput screening modelling, fragment screening modelling, computational modelling and existing data reported. Pharmaceutical Industry can accelerate innovation by using technological advancements. The recent technological advancement that comes to mind would be artificial intelligence, development of computer systems able to perform tasks normally requiring human intelligence, such as visual perception, speech recognition, decision-making, and translation between languages. There are numerous others like:

a) Personalizing the treatment
b) Help build new tools for the patient, physicians etc.
c) Clinical trials research: applying predictive analytics to identify candidates for the trial through social media and doctor visits.

Challenges that pharma companies face while trying to adopt AI

a) Lack of proper IT infrastructure – that is because most IT applications and infrastructure currently in use were not developed or designed with artificial intelligence in mind. Even worse, pharma firms must spend lots of money to upgrade their IT system.
b) The unfamiliarity of the technology – for many pharma companies, AI still seems like a "black box" owing to its newness and esoteric nature.
c) Much of the data is in a free text format – that means pharma companies must go above and beyond to collate and put this data into a form that is able to be analysed. Despite all these limitations, one thing is for certain: AI is already redefining biotech and pharma. And ten years from now, Pharma will simply look at artificial intelligence as a basic, every day, technology

Benefits of adapting AI

a) Rapid analysis of data
b) Effective use of incomplete data sets
c) Enhancement of product quality and performance at low cost
d) Ability to accommodate constraints and preferences and ability to generate understandable rules
e) Development of new products
f) Shorter time to market
g) Improved customer response

Table No. 2: Potential health applications and potential motivation for adoption

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	Patent cliff; 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	Increase in breaches; pressure to protect health data

Applications

1. 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 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. Immediate release tablets: Work in this area began only some three years ago with two studies. One by Turkoglu and coworkers from the University of Marmara (Turkey) and the University of Cincinnati11 used both neural networks and statistics to model tablet formulations of hydrochlorothiazide. The networks produced were used to prepare three-dimensional plots of massing time, compression pressure and crushing strength, or drug release, massing time and compression pressure to maximize tablet strength or to select the best lubricant. Although trends were observed no optimal formulations were given. The trends were comparable to those generated by statistical procedures. Comparable neural network models were generated and then optimized using genetic algorithms. It was found that the optimum formulation depended on the constraints applied to ingredient levels used in the formulation and the relative importance placed on the output parameters. A high tablet strength and low friability could only be obtained at the expense of disintegration time. In all cases lactose was the preferred diluents and fluidized bed the preferred granulating technique.

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.

Future of Artificial Intelligence

Companies like Google and Uber are already using AI capabilities to power self-driven cars. AI will have a great bearing on the automated transportation field by aiding handicapped drivers and preventing accidents. More evolved AI systems will support in hazardous factory-based jobs and may replace humans as well. Climatic change predictions can be made by AI systems using data sciences and environmental technologies. Around 80 percent of customer service operations will be handled by effective and timely AI systems.

Personalized health management will be made easier through AI systems symptom-identification and medical data processing abilities. Cyborg technology can help patients utilize artificial prosthetics for a better living by communicating with a robotic system. In space technology, AI can study orbital paths during successful launches and suggest actions based on its observations. Coming to Pharma Industry, AI is the future of pharma but the technology is available now. Artificial Intelligence can cut costs down, create new, effective treatments and above all else, help save lives. So, biotech companies should start making use of the advantages of AI at the earliest. Terms of compound design, scope and increase given to us by AI and machine learning will mean that we can tap into a much wider chemical space, giving us a much wider and more diverse range of chemicals to better enable us to pick the best drug discovery molecules. In terms of the industry's choice of patients for clinical trials, the software will also help companies detect any problems with drugs far earlier in terms of efficacy and safety. The industry therefore has a lot to gain from embracing solutions to AI and machine learning. It can be used to create a strong, sustainable pipeline of new medicines to good effect. Using the power of modern supercomputers and machine learning would make it possible for us to produce medicines faster and at reduced costs.

Conclusion

Human being is the most sophisticated machine that can ever be created. The human brain, which is working hard to create something that is much more efficient than a human being in doing any given task and it has great success to extent in doing so. The AI tools like Watson for oncology, tug robot and robotic pharmacy has changed the profession considerably. The bigger the health care sector gets more sophisticated and more technologically advanced infrastructure it will need. Artificial intelligence is the design and application of algorithms for analysis of learning and interpretation of data. Artificial intelligence (AI) of health industry is a set of multiple technologies that allow machines to feel, understand, act, and learn to perform administrative and clinical health care functions. In conclusion, the future lies in cooperation between humans and machines, and alongside technological advances, human clinical experts will need to adapt, learn, and grow. Although potential experts will have to be both medical and technology experts, it is evolution of medicine, not extinction. There are various AI and machine learning applications in pharmaceutical applications, including disease identification/diagnosis, personalized treatment/behavioural modification, drug discovery/manufacturing, radiology and radiotherapy, smart electronic health records, prediction of epidemic outbreaks, sales, marketing, predictive analytics, and so on. In addition, AI and ML-based analytics are superior for advertising, particularly because success often needs many ongoing complex decisions with a high degree of judgment.

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