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Need for Artificial Intelligence in Pharmaceutical Industry and its Limitations

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Abstract

AI is often being touted as the means to bring about the fourth Industrial Revolution and its role in almost all sectors of our society is almost certain. This brings about an urgent need for evaluating benefits and limitations of AI and machine learning across various sectors. Pharmaceutical industry has pioneered in embracing the use of AI in all of its core areas but the success as of yet seems very limited. The major advantage of AI is that it reduces the time that is needed for drug development and, in turn, it reduces the costs that are associated with drug development, enhances the returns on investment and may even cause a decrease in cost for the end user along with improved drug safety. So in this article we will review the scope and limitations of AI in the pharmaceutical industry.

Keywords: AI; Drug discovery; Drug design; ML; Clinical trial

Introduction

Artificial intelligence is the simulation of human intelligence patterns and processes by machines and computer systems. As a general rule, AI frameworks work by breaking down large amounts of specified training data for correlations and patterns, and using these patterns to make forecasts about future states.

AI programming focuses on the following cognitive skills:

a) Learning

b) Reasoning

c) Self-correction

d) Planning

e) Knowledge representation

f) Automated decision making

All through the world, countless investigations are being done on AI [1]. A lot of cash is being pumped in to make a framework that can work indefinitely more productively and at a substantially less time than a typical individual. Be it an educational setup, a manufacturing firm, a government office, or a research firm; AI finds itself relevant in each field. Examples of AI include speech recognition, language processing, self-driving cars, personalised social media feeds, personalised web searches.

Applications of AI in Pharmacology and why it is needed in Pharmacology

Drug development (Figure 1) and designing is an expensive and lengthy process. Some estimates state that it takes on an average 10 years and approximately 2.6 billion USD to develop a single molecule. With the current pandemic the world experienced the dire need for development of therapeutics and vaccines in an unprecedented short duration and many reputed organisations like Pfizer, Bayer, and Novartis etc. turned their attention to AI/ML for the task [2]. Also, COVID 19 pandemic hampered the supply chain management across the sectors including drug and vaccine production. And like in many other industries, this is a potential area where AI can play a critical role.

Various aspects of drug manufacturing can also benefit from AI, some of which are listed below:

1) Drug discovery and drug design- One of the most time-consuming processes in the pharmaceutical industry can benefit immensely from AI and ML applications. There are more than 10^60 drug-like molecules and experimental studies can only test 10^5 components per day. AI and computational drug discovery can speed up this process and end up cutting a lot of time and cost involved in the process. AI cannot just guide speedy compound identification, but also contribute to suggestions of synthesis routes of these molecules alongside the forecast of the desired chemical structure and an understanding of drug-target interactions [3].

2) AI can revitalise nano-medicine and dose optimisation- diagnostic nano-materials are used to assemble a patient-specific disease profile, which is then leveraged, through a set of therapeutic nanotechnologies, to improve the treatment outcome. However, high intra-tumor and inter-patient genetic variations make this a very demanding task. Integration of AI approaches using pattern analysis and classification algorithms for improved diagnostic and therapeutic

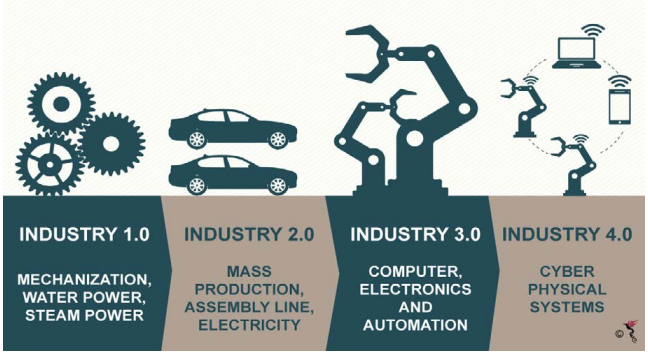

Figure 1: Representative image of the progress through industrial revolutions.

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accuracy, can help overcome complications and barriers in patient-specific approaches. AI can also boost nano-medicine design process by optimising material properties according to predicted interactions with the target drug, biological fluids, immune system, vasculature and cell membranes, all influencing therapeutic efficacy [4].

3) AI can prove to be instrumental in quality control, quality assurance and automated manufacturing protocols and thereby preventing wastages and streamlining pharmaceutical manufacturing processes and supply chains [5].

4) Clinical trial design and monitoring- arguably one of the most time consuming processes in drug discovery is participant recruitment for clinical trials. AI and ML can help in enrolment, matching/stratification and protocol designing for clinical trials and consequently save a lot of time and money. Moreover, AI can help monitor ongoing trials and ensure adherence to protocols and compliance among the participants. An added advantage with AI and digitisation of clinical trials is that these trials are no longer geo-restricted and as a result the outcome will be more globally representative rather than to a particular ethnic cohort [6].

5) Marketing- like all the industries, pharmaceutical industry too needs to have marketing strategies. AI is already used by many e-commerce sites for effective marketing and this same strategy can benefit the pharmaceutical industry immensely [7].

6) Prediction of toxicity- The prediction of the toxicity of any drug molecule is vital to avoid toxic effects. Cell-based in vitro assays are often used as preliminary studies, followed by animal studies to identify the toxicity of a compound, increasing the expense of drug discovery [8].

7) Pharmacovigilance- AI and ML can and will play a pivotal role in speedy and cost effective processing of ICSR (Individual Case Safety Report) and PMS (Post Marketing Surveillance) data, enabling better drug safety and personalised therapy (Figures 2 and 3).

Limitations of AI in its Current State

Despite all the promises, AI comes with its own set of limitations. Like all early stage techs, AI is still evolving and in its early stages of development and it has a lot to prove. One of the most limiting factors with AI is the requirement of comprehensive training data. This training data requires a lot of human input and humans do make errors and hence AI is also not infallible. One major apprehension is potential job losses with AI taking over but personally I believe that it would require an up-gradation of skill set as this would create a new set of jobs in the sector. When used in de novo drug design, AI can predict

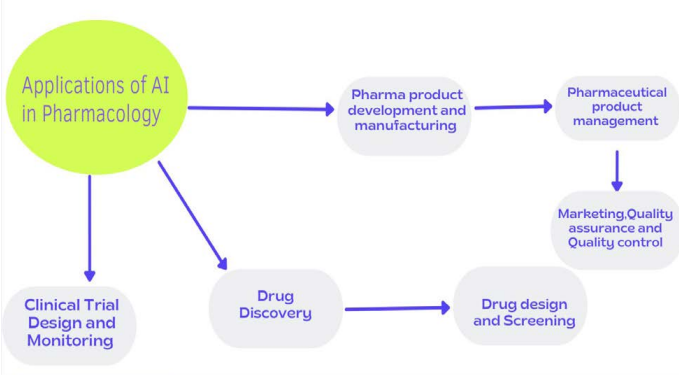

Figure 2: Possible areas of application of AI in pharmacology.

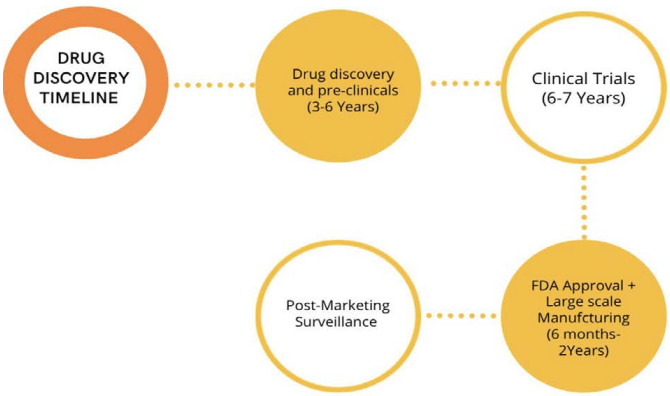

Figure 3: Drug discovery timeline.

models/structure that we may currently be unable to manufacture [9].

AI and ML being completely IT based may prove to be challenging for medical field workers and on the flip side IT professionals lack medical knowledge. This means that an interdisciplinary approach to train doctors and IT professionals will have to be developed. Like all tech, at some point we will require a regulatory system for AI as well and the repercussions of that are as yet unclear and uncertain [10].

Conclusion

It is guaranteed that AI will influence all spheres of our lives and it is evolving and becoming smarter every day. And AI is sure to revolutionise the pharmaceutical industry too. It is more of a question about 'when' rather than 'will'. There is still a lot to do before AI can bring about a meaningful change. AI is a promising strategy to immensely reduce the cost and time of drug discovery by providing evaluations of drug molecules in the early phases of development. In the current big data era, clinical and pharmaceutical data continue to grow at a rapid pace, and novel AI techniques to deal with big data sets are in high demand. The recent deep learning modelling studies have shown advantages compared to traditional machine learning approaches for this challenge. The next decade may witness seamless integration between human intelligence and AI systems and the pharmaceutical industry cannot remain immune to it. Although there are no drugs currently on the market created with AI-based approaches and explicit difficulties remain with regards to the implementation of this technology, it is likely that AI will become an invaluable tool in the pharmaceutical industry in the near future.

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