WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.084
Volume 12, Issue 6, 289-305. Review Article ISSN 2277– 7105

EMBRACING ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN PHARMACEUTICAL INDUSTRY

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Article Received on
28 Feb. 2023,

Revised on 19 March 2023,
Accepted on 09 April 2023

DOI: 10.20959/wjpr20236-27791

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ABSTRACT

For more than 200 years, the world has been through revolutions before the advent of mechanization then electronics then the digital revolution, all profoundly changed the world's economies and sparked a surge of new ideas and opportunities across sectors but this revolution of artificial intelligence, data science and machine learning could be even more disruptive. In this review, we discuss the application of artificial intelligence (AI) in many areas of the pharmaceutical industry, such as drug discovery and development, clinical testing, production and formulation of dosage forms, and clinical trials, among others; such usage reduces human effort while meeting objectives in a short amount of time. Although there are ethical issues about the use of AI in healthcare and pharmaceutical industry, it is obvious that no machine or system will able to match the intelligence and emotion of the human being.

KEYWORDS: Artificial intelligence, AIML, Machine learning, Pharmaceutical Industry.

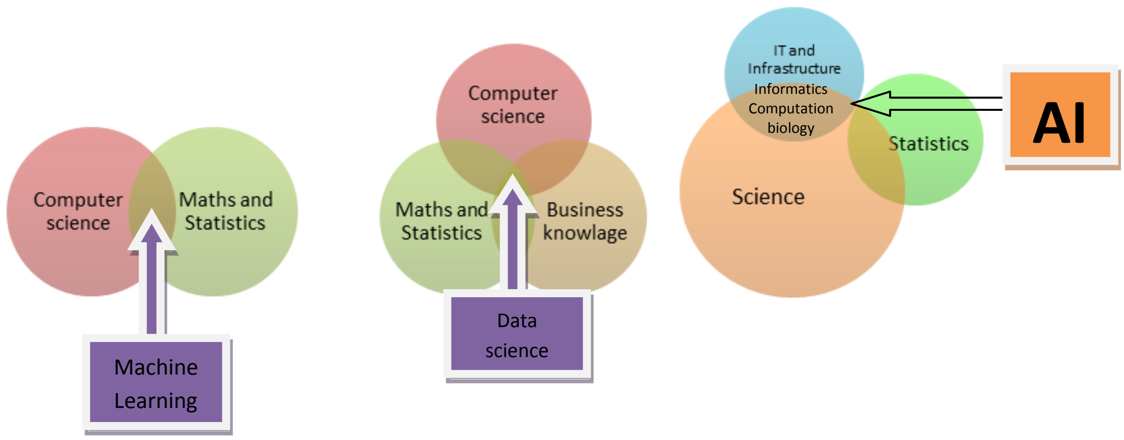
1. INTRODUCTION

Over the last decade, pharmaceutical industry has become aware of the capability benefits of leveraging artificial intelligence and its collective subfields which include machine learning, deep learning, big data, data science and advanced analytics.[1] These technologies are being used across the pharmaceutical industry in order to improve data-driven decision making, increase automation, and acquire insights into data. Artificial intelligence refers to a computers or a computer-enabled system's ability to analyze data and create results that are comparable to the thought process of human in learning, solving problems and decision making. AI is a branch of science that deals with machines that can perform tasks like logic, reasoning, planning, learning, sensory understanding, interaction and perception.[2]

The objective of an AI is to generate a system that can solve complicated issues using logic and reasoning comparable to that of humans. It is a more advanced form of computer-assisted technique that involves gathering data from a variety of sources then making ready rules accordingly to be accompanied for handling the required data, and drawing feasible consequences to determine suitable consequences and conclusions. The latest breakthroughs in the fields of artificial intelligence and machine learning have resulted in nothing short of astonishing innovation. Artificial intelligence algorithms-based solutions are finding use in a wide range of fields.

The pharmaceutical sector has been one of the most recent beneficiaries of this trend. The redeem from lower level technical experts has now been echoed by the top levels of many organizations, as instance by Vas Narasimhan's (CEO of Novartis) goal to evolve AI to place it at the "heart of the company"[3] and Alex Bourla's (CEO of Pfizer) aim to win the digital race in pharma using machine learning and AI to speed up R&D.[4] Artificial intelligence (AI) can be used to improve data processing in almost every aspect of the pharmaceutical and healthcare industries. AI functions as a machine learning system that responds to and analyses data in real time, allowing researchers to acquire data more efficiently. Furthermore, the more data AI responds to, the smarter it will become. The application of AI in the pharmaceutical and healthcare industries has revolutionized how scientists create new medications and combat disease in recent years. Designing treatment regimens, checking the accuracy of medicine, and drug development are only a few of the key uses of AI in pharmaceutical industry.[5] To speed up drug discovery, major pharmaceutical firms are implementing AI software or working with AI-based start-ups. AI is also being utilized more and more to identify medication efficacy and analyze adverse drug occurrences. It may also assist regulatory agencies in expediting medication approval processes.

A number of AI-based tools have been developed such as IBM Watson for oncology, Robot pharmacy (for preparation and dispensing of medicines for individual patients), Erica robot (understands and answers questions with human-like facial expressions)etc.[6] Various statistical and mathematical tools are being employed in AI, so that the computer software and processes can resemble the human behavior. Artificial intelligence algorithms are used in every step of the process, from identifying hit series to determining the lead molecule and, lastly, the creation of medicinal molecules, including clinical trials. It is making the transition to healthcare, powered by increasing availability of healthcare data and rapid progress of analytics techniques.[7] Neural networks are a type of computational and mathematical model that uses data to derive relationships between it without requiring the user to have any prior knowledge of the desired data.[8] It does not give any predictions but generate a variety of outcomes that would best suit the experimental data and therefore comply with its given criteria. Furthermore, this approach is modified to create Artificial Neural Networks (ANN), which is useful in addressing challenges in pharmaceutical research, development, and formulation.[9] A number of studies have already shown that AI can perform as well as or better than humans in key healthcare activities like disease diagnosis. Algorithms are already beating radiologists in terms of detecting dangerous tumors and advising researchers on how to build populations for expensive clinical trials. The pharmaceutical industry has seen a significant growth in data digitization in recent years. However, the difficulty of obtaining, analyzing, and using knowledge to solve complicated healthcare issues arises with digitalization. This encourages the adoption of AI since it is capable of handling enormous amounts of data with more automation.



2. AI and ITS subfields

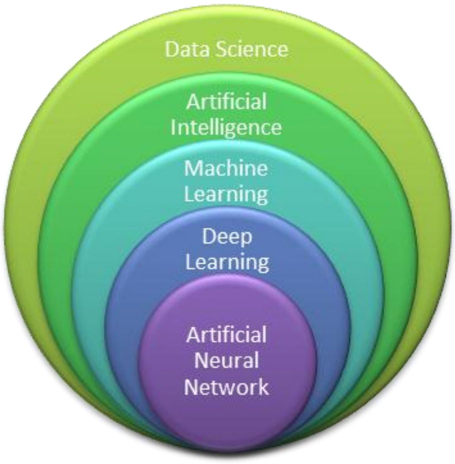


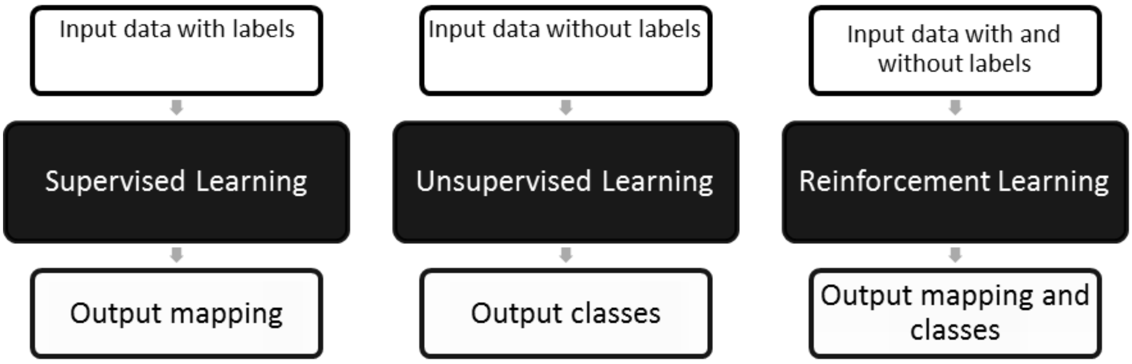
Figure 1: Artificial Intelligence is a sub-field of Data Science. AI includes the field of Machine Learning (ML) and its subset Deep Learning (DL).

3. Machine learning

The words Artificial Intelligence and Machine Learning are frequently used interchangeably. As a result, many people may be confused about what a machine learning model is and how it differs from an AI model. Both AI and machine learning are branches of computer science that contribute to the development of intelligent systems. However, while these two concepts are related, they are not synonymous terms. AI is a broad term that refers to the development of machines that can mimic human behavior and intelligence. On the other hand, ML is a very specialized field of AI that aims to create software that can automatically learn from past data to gain knowledge through experience and improve its learning behavior over time to make predictions based on fresh data.[10]

Machine learning is a subfield of artificial intelligence. Machine learning has been the most effective type of AI in recent times, and it is at the heart of many of the present applications. The fundamental principle of ML is that a machine uses data to "learn" from it. As a result, machine learning systems can use knowledge and training from enormous data sets fast to excel at tasks such as people recognition, audio recognition, object detection, translation, and many more.[11] When given with data and fresh experiences, machine learning allows systems to identify patterns and establish their own rules rather than following pre-programmed instructions.

3.1. Machine learning is classified into three sections



Supervised learning

Supervised learning is the most popular type of machine learning algorithm since it is the easiest to understand and apply. It has been described as being similar to a teacher using lesson cards to educate a little child. It is associated with the development of predictive approaches generated from regression as well as classification methods that provide such predictions using data from input and output sources. The output data include disease diagnostic methods in the classified category, drug efficacy, and absorption, distribution, metabolism, and excretion (ADME) predictions in the regression analysis.[12] It's also used to identify risk factors and provide recommendations for improving clinical trials.

Unsupervised learning

Unsupervised learning is the exact opposite of supervised learning in that the algorithm learns from itself and does not use labels that have been pre-programmed. The algorithm understands the data and then learns to group/cluster/organize the input data. This sort of algorithm finds patterns in data and restructures it into something useful. It is a valuable type of machine learning in that it gives insights into data that humans may overlook or that haven't been allocated in supervised learning methods.[13] It is an effective algorithm in research articles, which is beneficial for medications and medical research.

For example, there may be a big database containing all of the articles on a certain subject, and an unsupervised learning algorithm would know how to arrange the papers in such a manner that it was always aware of development in various fields of medicine. If the article was connected to the network, the ML may recommend specific references you should cite or perhaps additional papers you should read to assist your paper justify its hypothesis. Imagine how valuable this sort of machine learning might be in a clinical trial context, and how critical clinical data transparency would become if data provided from other drug firms was not only accessible and in the public domain, but also hocked into an unsupervised learning environment. This sort of machine learning has potential not only for clinical trials but also for drug discovery, as shown by firms like Benevolent AI, which recently struck a relationship with AstraZenca.[14]

Its main function is to make decisions based on the environment and then carry them out to achieve excellent results. The output of this form of ML is drug design using a de novo approach, which falls under the decision-making category, and experimental drug design, which falls under the execution category. As a result, both may be accomplished using the modeling approach and the application of quantum chemistry.[15]

For example, Brite Health is a startup that uses machine learning to improve patient involvement in clinical studies. This firm uses apps for volunteers or patients and dashboards for site administration.[15] Millions of clinical data points are used to train the app and dashboard. These trained data points are built to discover important signals that tend to correlate with patient disengagement from clinical studies, and it alerts the user as well as the next planned activity and site visit. This promotes patient involvement while also preventing disengagement. The dashboard at the site gets any information of disengagement from all enrolled patients and assists in monitoring them to avoid any small or big violations. Through curative material and a conversational Chatbot, the app system also delivers study documents for reference and personalised communication. As a result, this firm employs supervised machine learning for patient interaction via the App and Dashboard, while also employing reinforcement learning via the Chatbot.

4. Current market scenario of AI in pharmaceutical industry

The pharmaceutical industry is one of the largest in the world, with billions of dollars invested annually in the discovery of novel compounds and medications. Pharmaceutical firms are gradually moving their approach toward AI and big data for drug development and clinical trial design in order to reduce related failures and, as a result, lower R&D costs.

According to the healthcare industry professionals surveyed in GlobalData's recent study, artificial intelligence (AI) and big data will continue to disrupt the pharmaceutical business. In the next two years, 28 percent of firms will use AI and big data to optimize drug discovery and development processes, while 32 percent will use big data to simplify sales and marketing, according to the study 'Smart Pharma'. According to 36 percent of 198 pharmaceutical industry professionals surveyed, AI is expected to be the emerging technology that will have the greatest impact on the industry in next decade.[16]

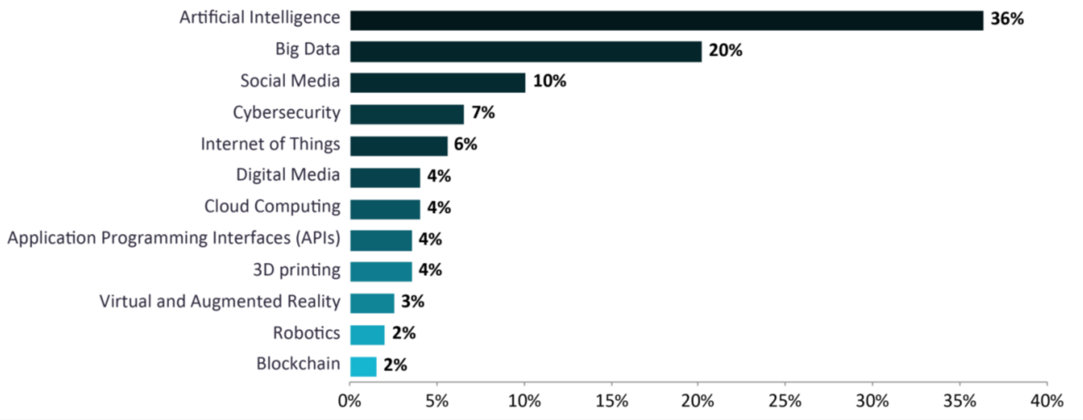


Figure 2: Technologies that will have the greatest impact on the pharmaceutical industry in 2021(%).[16]

The thematic approach to sector activity groups important business information on hiring, acquisitions, patents, and other topics by subject to determine which firms are better placed to whether the disruptions coming to their industries. These themes, of which AI is one, are best described as "any issue that keeps a CEO up at night," and tracking them allows firms to see who is leading the way on certain challenges and who is trailing behind. Novartis, GlaxoSmithKline, and Merck & Co are categorized as major players in the AI industry, with an additional 19 firms designated as leaders, according to these criteria. Due to a lack of AI investment, ten firms are considered vulnerable.[17] There were 44 AI deals in pharma in the first quarter of 2019. By the first quarter of 2021, that number was 85. According to a research by Deep Pharma Intelligence, overall VC financing in AI-biotech firms increased by about 23 percent in 2020 (as of November) compared to 2019, surpassing $1.9 billion, which is higher than in 2015, 2016, and 2017 combined.[18]

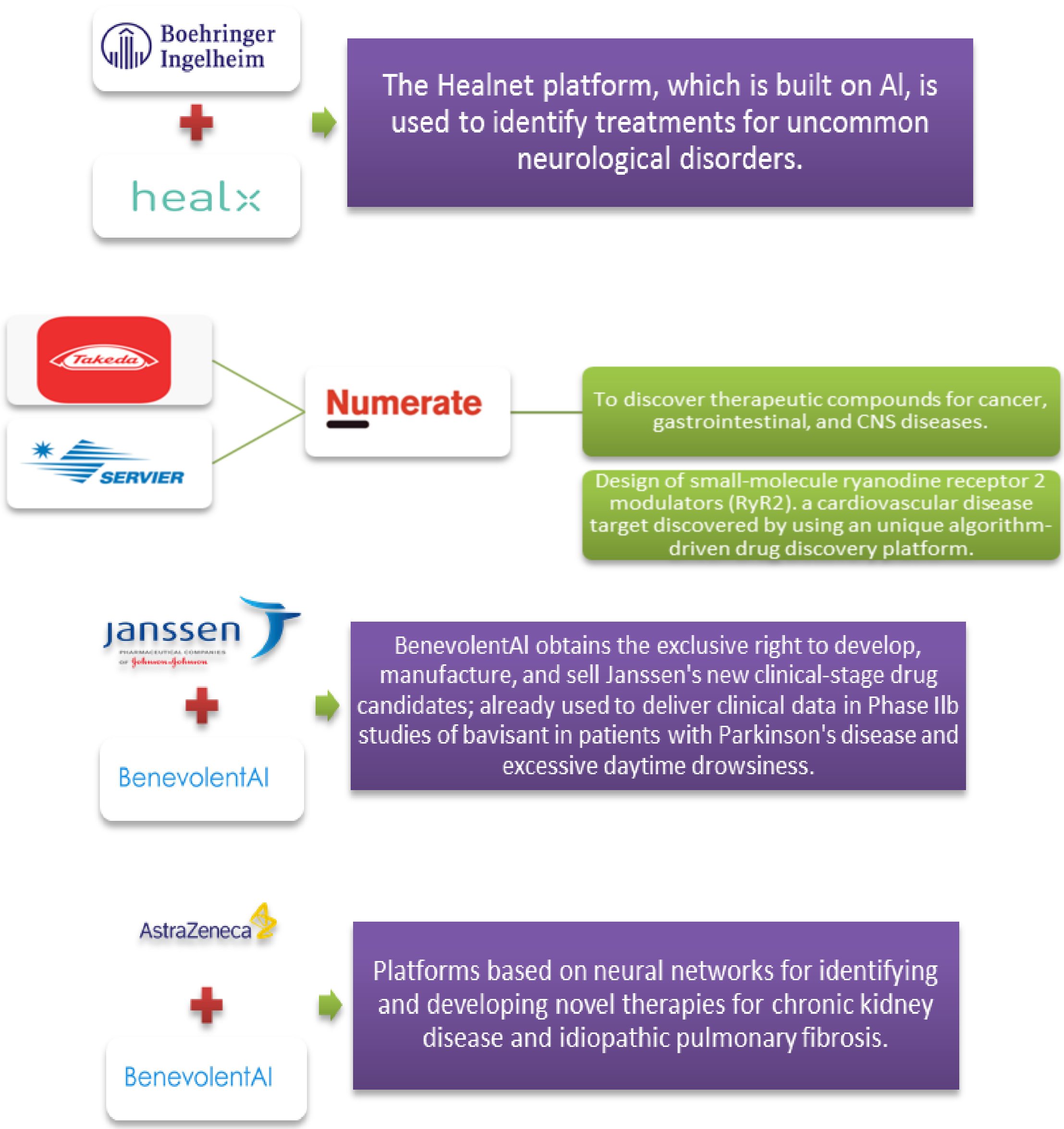
The year 2020 was a good year for AI drug development funding. The total yearly investment value hit new heights in 2020, despite the fact that the number of financing rounds peaked in 2018 and has been declining since then. In fact, from $10.7 million in 2015 to $51.7 million in 2020, the average financing amount has risen.

The strong levels of investment activity seen last year continued into the first half of 2021, with fewer but larger investment rounds. The investment value has already surpassed $2.1 billion in the first half of 2021, accounting for 71% of the entire value last year. This year's big series A and B fundings included Cellarity ($123 million), Dyno Therapeutics ($100 million), Enveda Biosciences ($51 million), Engine Biosciences ($43 million), and BigHat Biosciences ($19 million). In the AI drug development business, series C and D investment rounds are on average 3.5 times larger than series A and B fundraising rounds. As a result, Series C and D funding make a substantial contribution to the industry's total investment value. In the first half of 2021, some of the most notable series C and D investment rounds included Insitro ($400 million), Insilico Medicine ($255 million), and Exscientia ($100 million). Exscientia's series C was followed by a series D, which included an extra $225 million and the option to raise an additional $300 million at their discretion. With a total of $11.8 billion in financing and $2.1 billion already committed this year, final quarter of 2021 is on track to be a landmark year for AI in drug development.[19]

AstraZeneca Plc is in the forefront of the artificial intelligence employment competition, with 676 new roles advertised between January 2020 and June 2021. The company's highest hiring period was in April 2021, when it posted 73 new AI-related job openings. Johnson & Johnson was the second most aggressive artificial intelligence employer, after AstraZeneca Plc, with 616 new roles advertised. With 545 new job ads, Takeda Pharmaceutical Co Ltd came in third.[20] With internal investment in data integration and AI, pharma companies can overcome the challenges and not only stand to gain a competitive advantage but can also fundamentally improve the quest for new and better medicines.

5. Leading pharmaceutical Companies and Their association with artificial intelligence (AI) organizations


Lilly
Atomwise
Atomwise and Eli Lilly and Company have struck a multi-year deal to use Atomwise's patented artificial intelligence (AI) technology to help Lilly's preclinical drug development activities. also to develop drugs on novel protein targets.
Pfizer
XtalPi
Quantum mechanics and machine learning techniques are combined with cloud computing to predict the 3D structure of molecules, as well as their mechanical and chemical characteristics and how they attach to protein receptors.
Pfizer
IBM Watson Health
Use of machine learning, natural language processing, and cognitive reasoning technologies in immuno-oncology to discover novel therapeutic targets, combination treatments, and patient selection strategies.
Microsoft
NOVARTIS
Research on cell and gene-based treatments, generative chemistry, visual segmentation and analysis for smart and personalized therapy delivery of therapies, and optimization of cell and gene therapies at scale.
BAYER
Sensyne Health
Clinical development of novel cardiovascular disease therapies using Sensyne Health's unique clinical AI technology.
SANOFI
Exscientia
To discover and develop bispecific small compounds for the treatment of diabetes and its comorbidities



6. Key ethical issues and challenges for ai adoption in pharma

Despite the potential of artificial intelligence and machine learning to change the pharmaceutical industry, using these technologies has its own set of challenges. The following are some of the problems that pharma firms encounter when attempting to implement AI:

Data governance: - AI systems rely on careful data governance to manage, make available, and integrate data. Hundreds of different equipment for biochemical tests, analytical chemistry, sequencing, gene expression, genomics, patient data, clinical data, and wearable sensors may be used by large pharma, each with its own database. Even single experiments may add cell source data, drug candidate data, protocol information, raw and processed data, intermediate and final results, plus metadata. Academic collaborations and industrial consortiums bring additional data resources from the outside. Because of the diversity of data, data governance and integration is critical and a major problem for the sector.[21]

Lack of a single, Unifying problem: - The pharmaceutical industry's objective of rapidly discovering new medications to enhance patients' lives does not correspond to a single AI challenge. Instead, AI is helping to discover better targets and screens, improve modeling, priorities safety indications, increase patient participation in clinical trials, and solve a variety of other issues.

Unlike Amazon's and Netflix's recommender engines, which generate 35 percent and 75 percent of their income,[22] pharma cannot focus on a single solution but must tackle hundreds of critical challenges, thereby decentralizing resources.

Insufficient skillsets: - technological gap between collecting data from databases, cleaning it, applying existing machine learning techniques, and visualizing the results is filled by data science. This is a crucial necessity since, unlike traditional software, commercial off-the-shelf solutions must be tailored for unique business challenges and educated on appropriate data, which necessitates specialist skill.[23] Data scientists require subject area skills in addition to machine learning math, statistics, and programming. The pharmaceutical sector, which is filled with PhDs, has a lot of scientific knowledge, but this combination of talents is uncommon. This shortfall is exacerbated by competition from technological firms that pay a premium for machine learning expertise. Even such individuals, however, lack the underlying scientific and pharma expertise required to understand the challenges and advance solutions.

Scientific approach: - To effectively use AI approaches, the present pharma strategy must transition from an expert-driven scientific process to a data-driven collaboration between scientists and AI. The scientific process of examining data, developing hypotheses, and experimentally verifying these hypotheses is used in every phase of R&D, from defining the targets, screening, and optimization, through clinical trials. Human mind is not well adapted for generating complicated multivariable hypotheses with millions of datapoints, even if humans excel at postulating simple hypotheses with modest datasets. Furthermore, major pharma's present search for novel drugs includes high-throughput instruments to generate more data, electronic health records (EHR), genome-wide association studies (GWAS), expression data, and so on. With data mining, modelling, simulation, and knowledge bases, hypothesis creation and assessment must become increasingly automated as we transition to more hypotheses than can be evaluated.[24]

AI's speed and scalability provide answers, notably in the reinforcement learning domain, where AI learns how to learn. A machine learning technique, for example, generated 15 000 iterations for a new Callaway golf driver club, compared to the typical human 8–10 iterations.[25] BERG's latest approach to cancer screening illustrates the possible advantage of moving away from the scientific method. The confluence of AI data-driven techniques and scientific hypothesis-driven skills will start to give R&D process advances as AI approaches acquire trust within pharma.

Absence of investment: - Pharma firms have been reluctant to invest in AI, despite their habit of embracing new technology. Some companies may be strategically awaiting the field's stabilization. However, with new AI–pharma hybrid paradigms developing in firms like as BenevolentAI and Insilico Medicine, as well as a talent scarcity, companies who postpone their AI strategy risk trailing behind.[26] Articles in Forbes and the Wall Street Journal frequently laud the competitive benefits of AI, and pharma firms have nervously turned to external partners in a wave of high-profile alliances — including Novartis and Pfizer with IBM Watson, AbbVie and Merck with Atomwise, Amgen with GNS Healthcare, GSK and Sanofi with Exscientia, and Takeda with Numeratexii.[27] Despite this, AI has barely penetrated 16 percent of healthcare firms compared to >30% of high-tech enterprises. According to the press releases, these agreements are worth $100 million, compared to $34 billion in worldwide AI investment in 2016. With pharma's multitude of AI-ready challenges, isolated external collaborations may address technical gaps, but they don't help the industry's AI skills or tackle pressing issues. Furthermore, customizing off-the-shelf AI systems outperforms third-party solutions in many cases.

Reliability and Safety: - When AI is used to manage equipment, provide therapy, or make decisions in healthcare; reliability and safety are important concerns. AI might make mistakes, which could have significant consequences if the error is difficult to identify or has knock-on effects.[28] For example, in a 2015 clinical experiment an AI app was used to identify which individuals were likely to suffer problems after pneumonia and so should be admitted to the hospital. Due to its failure to take contextual information into account, this app incorrectly directed clinicians to send asthmatic patients home.[29]

Transparency and Accountability: - It can be difficult or impossible to discover the underlying logic that creates AI results. Some AI is private and purposefully kept hidden, while others are simply too complex for humans to understand.[30] Because machine learning systems constantly modify their own settings and rules as they learn, they may be extremely opaque. This complicates the process of validating AI system outputs and detecting data mistakes or biases.

Data bias, Fairness and Equity: - Although AI applications have the potential to minimize human bias and mistake; the data used to train them might reflect and reinforce biases.[31] Concerns have been expressed regarding the possibility of AI causing discrimination in ways that are concealed or do not correspond with legally protected criteria including gender, race, disability, and age. The House of Lords Select Committee on AI has warned that datasets used to train AI systems are frequently underrepresented in the general population, and as a result, AI systems may make biased decisions that reflect societal prejudices.[32] The advantages of AI in healthcare may not be dispersed equitably. Where data is limited or difficult to acquire or render digitally, AI may perform less well. People with uncommon medical diseases, as well as those who are underrepresented in clinical trials and research data, such as Black, Asian, and minority ethnic communities, may be affected.

Trust: - DeepMind's collaboration with the Royal Free Hospital in London sparked a public discussion regarding commercial firms having access to patient data. Pundits have cautioned that if people don't believe that AI is being created in the public interest, there may be a backlash against the technology.[33] On a practical level, if AI systems are to be successfully implemented in healthcare, both patients and healthcare professionals must be able to trust them. Clinical trials of IBM's Watson Oncology, a cancer diagnosis tool, were reportedly halted in some clinics because doctors outside the United States did not trust the model's recommendations and believed it reflected an American-specific approach to cancer treatment.[34]

7. CONCLUSION

Human beings are the most advanced machine that have ever been created. Healthcare and Pharmaceutical industry is actually one of the areas where the impact of artificial intelligence could be extraordinarily positive in the future. However, the transformation will not happen overnight. Rather, it will happen gradually over the next 10 to 20 years. The benefits of machine learning, AI, Big data, and data science in healthcare are enormous; they have an incredible chance to address both very rare diseases and diseases that impact various parts of the population in very diverse situations. If we're going to cure cancer it's probably going to come through data science. Disease identification, radiology and radiotherapy, clinical trial research, drug development, personalized medicine, and rare disease identification and treatment will be the most significant topics of study in pharma and healthcare. It will also change many areas of the pharmaceutical industry, although it cannot guarantee disease cures and may eventually replace people with machines. It is unrealistic to expect AI to develop solutions on a humanitarian basis. It has the ability to assist healthcare researchers in gaining a better knowledge of diseases, improving clinical decision-making and empowering research. But there is potentially a darker side to this technological revolution one which could profoundly change the world way we work and way we live today and this technological revolution will challenge us like never before.

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