

Advanced Artificial Intelligence in Pharmaceutical Industry and Drug Discovery & Development

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ABSTRACT

AI Technology that pharmacy profession can be more efficient. Artificial Intelligence advantage in reduced of time required & cost for drug development. AI plays an important role in pharmacy in drug discovery and development, drug delivery and formulation development, poly-pharmacology, Hospital pharmacy, etc. AI enhances drug formulation and manufacturing, improves pharmacovigilance and drug safety, and supports drug pricing and market access strategies. AI stands poised in reshape are pharma industry and way for more efficient, and personalised in impactful approach to drug development & healthcare. Artificial Intelligence is field of pharmacy by enhancing drug discovery, optimize clinical trials, improve patient care, streamlining pharmaceutical operations. AI algorithm Analyse vast data sets to the identify potential drug candidates predict drug interactions, personal treatment based on individual patient data. This review aims to provide be overview of AI impact on pharmacy in drug discovery & development and pharmaceutical industry. The balance between technological advancement and responsible for the implementation.

KEYWORDS: Artificial Intelligence in pharmacy, Drug Discovery & Development, Pharmaceutical Industry, AI History, Future scope AI, Application Of AI, etc.

I. INTRODUCTION

Artificial Intelligence machine learning, particularly intelligent computer learning, is a field of study known as artificial intelligence (AI). Programs that deliver outcomes in the comparable to how human attention is processed [1]. Artificial intelligence (AI) is computer science area. It helps computers solve problem. AI used symbolic programming (symbol & rules) for problem solving. It has greatly evolved into a science of problem

solving with huge application in business, healthcare, engineering [2].

The main objective of these artificial intelligence to identify useful information processing problems and give the abstract account of how to solve it. The account is known the method & correspond to the theorem in mathematics. Artificial intelligence in field that deals with the design and application of their algorithms for analysis the learning from and interpreting data. AI in compasses many branches of noted statistical and machine learning, pattern recognition, clustering, similarly based method [3]. (AI) Artificial Intelligence technology which finds application in multiple aspects of life and industry in resent time the pharma industry discovers novel and innovative ways to use the powerful technology to help solve some of biggest problem facing pharma product today. Artificial intelligence in pharma referred use of automatic algorithm to perform task which traditionally in human intelligence. Over the last five years, the use of artificial intelligence in pharma industry has redefined how scantiest develop new drug track disease and more [4].

AI algorithms can analyse vast amounts of data from various sources, including clinical trials, scientific literature, and genetic data bases, to identify potential drug candidate, dear significant accelerate due to process [5]. AI can also optimize drug design by analyse the chemical structure of compounds the predict their properties. These can help to identify potential modifications to improve their efficacy and safety, consider reduce the time and cost associated with traditional drug design methods [6]. AI can analyse large data sets from clinical trials, identified patterns, predict outcomes. These help researchers to identify potential safety issue and optimize dose regimens, leading to better patient outcomes [7]. AI can also significantly contribute to drug discovery by identifying new drug targets AI algorithms can analyse vast amount of biological data, such as genomic and proteomic data,

to identified potential targets for drug intervention [8].

By understanding the underlying molecular mechanism of diseases, AI can help researchers identify novel targets that were previously unknown or overlooked. This opens up new avenues for drug development and allows researchers to explore innovative therapeutic approaches [9]. In drug discovery, AI technology is used in both drug screening and design; the algorithm includes, to name a few, ML, DL, AI based quantitative structure activity relationship (QSAR) technology, QSARML, virtual screening (VS), support vector machine (SVMs) deep virtual screening, deep neural networks (DNNs), recurrent neural networks (RNNs), etc. neural networks in AI are inspired by biological neural networks where they input & output response after processing the information received. Artificial neural networks (ANN) have several connected units for processing the information. DNNs are similar to ANN there are several layers of data process units. RNNs process the data in sequence by the output data of previous analysis is process as input data for next phase analysis. SVMs are used for classification and regression of input data [10].

In pharmaceutical product development, AI is used to choose the appropriate excipients, selecting the development process, and ensure the specification are achieved as per compliance during the process. The model expert system (MES), ANNs, etc. used in pharmaceutical product development. In manufacturing, AI is used in automated and personalized manufacturing, matching manufacture errors to set limit. Their AI technology such as meta classifier and tablet classifier used to achieve the desired quality of final product. the incorporation AI in clinical trials helps in selecting subjects and monitoring the trial, the drop outs are reduced because of close monitoring. Mostly concerning safety and dangers that may be potentiated by creation of machines that could match human cognitive capabilities. One of five predictions that made by Forbes for AI in 2019 is that may become an issue of national politics [11].

Innovation with the pharma sector is driven by extensive research & development, efforts across the diverse domains, including advanced manufacturing technology, innovative packaging solutions, and the customer centric marketing strategy [12]. From the development of small drug molecules to biologics, that is consistent emphasis on enhancing stability and potency to meet unmet medical needs. However, the evaluation of the potential toxicity associated with new drug remains

a significant concern, necessary on-going research and exploration. A primary objective is to deliver drug molecules that offer optimal benefits & suitability for use in Health care industry. Despite advancements, a pharmaceutical industry encounters various challenges that require further technological advancements to meet global medical & health care demands [13].

II. NEED OF ARTIFICIAL INTELLIGENCE (AI) IN PHARMACY

Pharmaceutical company access to a large number of compounds that have the potential to combat a wide range of specific diseases. However, the companies do not have any tools to identify them. Such Drug development & production are difficult task that can cost of pharmaceutical company up to \$2.6 billion and take up to 12-14 years to complete. This is where artificial intelligence can help pharmaceutical companies [14,15].

AI reduced the time required for drug development, which reduced the costs associated with drug development, improves the return on investment, and may even result in decrease in cost. Moreover, in pharmacists are the 13th best paid professionals, according to poll of 150 professionals conducted by U.S. news. A pharmacist's job to ensure the prescriptions received by pharmacy are filled with right medicine in right amount & medicine do not show any ADR (adverse drug reactions). However, scenario has changed in since last 5 years with robots are becoming more intelligent as result of the emergence of big data & AI. the Robots are now becoming more trust worthy for doctors & large number of institutions are now employing robots along with human supervision to carry out activity that were previously done by humans [16,17].

III. THE HISTORY OF ARTIFICIAL INTELLIGENCE

John McCarthy (September 4, 1927 – October 24, 2011) These is an American Computer Scientist & Cognitive Scientist. He was one of the **Founder & Father** of Artificial Intelligence (AI) [18].

He co-authored the document that **Coined the term Artificial Intelligence** (AI) Developed the Programming Language Family Lisp, significantly that influenced the design of the language ALGOL, popularised time-sharing & invented garbage collection.



FIG 2.1: JOHN MC CARTHY

McCarthy spent most of his carrier at the **Stanford University** [19]. John McCarthy together with Alan Turing, Marvin Minsky, Allen Newell & the Herbert A. Simon. McCarthy, Minsky, Nathaniel Rochester & Claude E. Shannon coined the term 'Artificial Intelligence' in a proposal the wrote for famous Dartmouth Conference in Summer 1956. This conference started AI (Artificial Intelligence) As field [20].

➤ The Development of Artificial Intelligence (1943-1952)

Year 1943: The first work which is now recognised as AI was done by Warren McCulloch and Walter pits in1943. They proposed model of artificial neurons.

Year 1949: Donald Hebb demonstrate & updating rule for the modifying the connection strength between neurons. His rule is now called Hebbian learning.

Year 1950: The Alan Turing who was the English Mathematician & pioneered machine learning in 1950. Alan Turing publishes **Computing Machinery & Intelligence** in which he proposed at test. The test check machine ability to exhibit intelligent behaviour equivalent to human intelligence, known Turing test.

➤ The Birth of the Artificial Intelligence (1952-1956)

Year 1955: An Allen Newell and Herbert A. created the first artificial intelligence programme which was **Named as Logic Theorist**. This program had proved 38 of 52 mathematics theorems, & find new & more elegant proofs for some theorems.
Year 1956: The word AI first selected by American Computer Scientist John McCarthy in Dartmouth conference. For the first time Artificial Intelligence **Chased the Academic field** [21,22].

➤ The Golden years-early Enthusiasm [1956-1974]

Year 1966: The Re-searchers stressed developing algorithms which can be solve mathematical problems. Joseph created the first chatbot in 1966, which named as **ELIZA**. He starts the role of psychotherapist. A user would type a message on an electric type writer connected to a main frame.

Year 1972: The first intelligent humanoid robot was boost in Japan which named as (**WABOT-1**).

The First AI Winer (1974-1980): The duration between years 1974 to 1980 was the first AI winer duration. AI winer refers to time period place computer scientist deals with the acute short of fund from there government for AI research. During AI winer, an interest of publicity on AI was decreased [23].

➤ The Boom of AI (1980-1987)

Year 1980: After AI winter duration AI come back with **expert system**. Expert system was programme they copy the decision make ability of human expert. The first national conference of American association of Artificial Intelligence on Stanford University.

➤ The Second AI Winer (1987-1993)

The period between the years 1987 to 1993 live the second AI winer time. Again, investors & the government stopped funding for AI research due to high cost but not efficient result. The expert system such as **XCON** was very cost-effective.

➤ The Emergence of Intelligence Agents (1993-2011)

Year 1997: In the year, IBM deep blue beats world chess champion, Gary Kasparov, & became the first computer to beat world chess champion.

Year 2002: For the first time, AI entered the home in form of Roomba, a vacuum cleaner.

Year 2006: AI come in the Business world up to the year 2006. Also start using AI [24,25].

➤ Deep Learning, Big data & Artificial General Intelligence (2011-2020)

Year 2011: In year 2011, IBM's Watson won jeopardy, to solve complex questions as well riddles. Watson had Demonstrate it could understand natural language can solved tricky questions fast.

Year 2012: **Google launched** which able to provide information to user as prediction.

Year 2014: In year 2014, Chatbot "**Eugene Goostman**" won competition in the infamous "**Turing Test**".

Year 2016: They are can AlphaGo Defeated human go champions.

Year 2018: The project Debater from IBM debated on complex topics with two master debates & perform extremely well. Google has demonstrated the AI program Duplex which virtual assistant was & has hair dresser appointment on people on person in other side didn't notice that was talking with machine [26].

➤ The Present Learning of AI (2020-2025)

Year 2020: They go on GPT-3 Showed powerful language generation. **Year 2022:** They also learn in AI which can Chat-GPT brought AI Conversation to the public. **Present:** present state of AI in Advanced Foundation Model like GPT-5, Claude, Gemini, & Mistral offer advanced reasoning. AI now used in Education, Medical coding, Health care, drug discovery & Development & clinical Research etc.

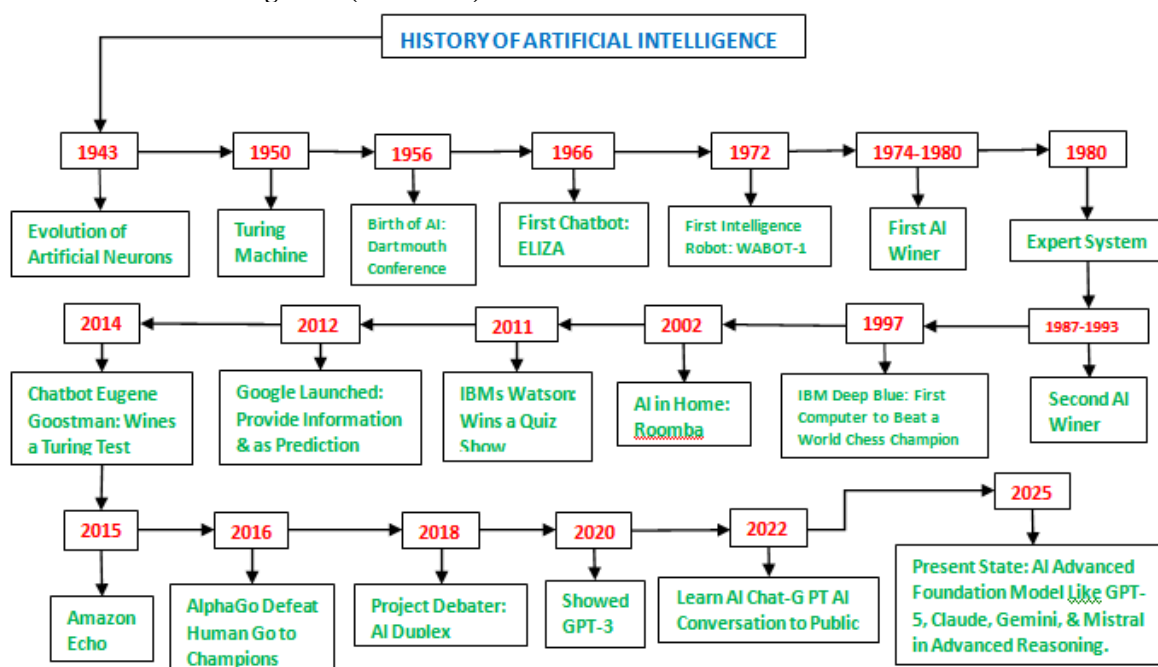
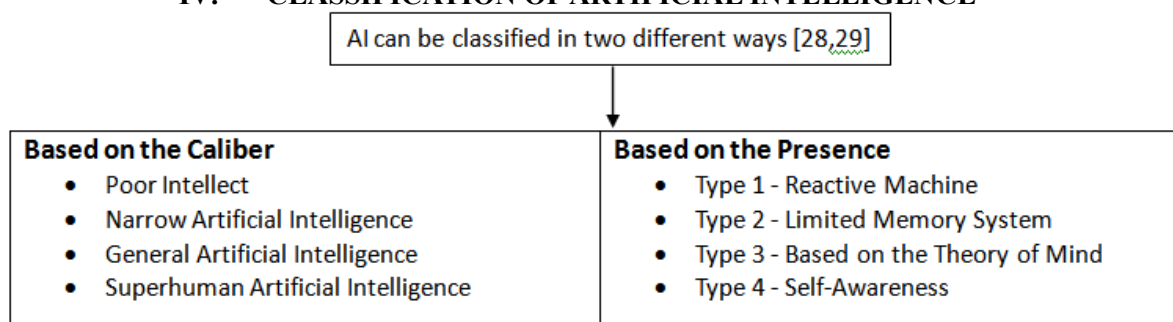


FIG 2.2: HISTORY OF ARTIFICIAL INTELLIGENCE [27]

IV. CLASSIFICATION OF ARTIFICIAL INTELLIGENCE



[A] Based on the Caliber

1. Narrow Artificial Intelligence or Weak Intelligence: This System is created and trained to carry out a certain activity, such as traffic signal, driving a car, playing chess. EX: Apple SIRI Virtual personal assistance, tagging in social media [30].

2. Strong AI, Famous as general AI: It processed by the name Human-Level AI. it can make intellectual capacity in humans simple. As result, can solve problem presented with new tasks.

3. ASI (Artificial Superhuman Intelligence): They Brain power more active than intelligent people in areas as the sketching, mathematics, space

exploration, etc. in discipline ranging from science to art. The spectrum from computer being only more intelligent than person to trillion times smarter. A. Hintze [31].

[B] Based on the Presence

AI Scientists Categorized the AI Technology depending on whether it was already in use or not. These are, what they are:

Type 1 - Reactive Machine: A Reactive Machine is the name given to sort of AI system. Consider the IBM chess program deep blue, which defeated Garry Kasparov in 1990s. on chess board can recognize checkers & make predictions, but it lacks memory to draw on previous experience. It made specifically use & useless in other circumstances. It specific single-purpose applications & lacks the ability to draw from past experiences to absence of memory system. This category is referred as reactive machine. Notable instances of system include IBMs chess program, which can identify chess board pieces & make predictions.

Type 2 - Limited Memory System: A Limited Memory System is the name given to this kind of AI system. This technology can analyse prior data to solve current & upcoming issues. Some of the decision-making processes in self-governing cars only created use this path. They observed not permanently put away in the remembrance. It possesses constrained memory system that leverages past experiences to address various issues. In context of autonomous vehicles, this system is adept at making decisions based on recorded observations, which can used for subsequent actions, but these records are not retained permanently.

Type 3 - Based on the Theory of Mind: The term “theory of mind” is used to describe this kind of AI system. It implies that everyone has thoughts, ideas, & wants that influence their decision-making. This AI doesn’t exist. It relies on the concept of “theory of mind” which implies that human decision-making is influenced by their unique thoughts, intentions, & desires. This kind of AI system does not currently exist.

Type 4 - Self-Awareness: These are referred to Self-Awareness. The AI system the sentient & have feeling of self. If the machine has self-awareness, it recognizes its situation & makes use of the concepts stored in other people’s minds. This AI does not exist. It own’s self-awareness including sense of self-consciousness. However, type of AI system does not exit at this time [32].

V. ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL INDUSTRIES

Each phase of the medicament design process uses AI Technology which significant lowest the cost & health risks associated with preclinical trials. Based on the vast amount of pharmaceutical data & machine learning process. Artificial Intelligence is useful implement for data mining [33].

➤ AI mainly used in pharmaceutical industries for:

1. Drug Discovery
2. Clinical Research or Clinical Trials
3. Disease Diagnosis
4. Novel Medication
5. Data Analysis
6. Drug Development
7. AI For the Detection of Tablet Defects
8. AI In Drug Manufacturing & Regulatory Compliance

[1] Drug Discovery

Pharmaceutical businesses have been able to accelerate their drug discovery process with use of AI technology in healthcare. On other hand, it automates the process of identifying targets. In addition, AI in healthcare 2021 supports medication repurposing by analysing off-target chemicals [34]. As consequence, AI drug development accelerates the procedure & minimises repetitive work in the AI & healthcare industries [35]. They several treatments that top biopharmaceutical firms have developed. Pfizer using IBM Watson, a system found on machine learning to support finding immuno-oncology therapy [36]. It has utilised specifically for signal & image processing, as well as for making predictions about changes in function, including bladder control, epileptic seizures, and strokes [37]. Klopman introduced a new program to study the structure activity relationship (SAR) of organic molecules [38].

Drug Discovery regularly takes a long time to test compounds opposed to samples of diseased cells. Finding compounds that are biologically active & worth investigating further requires even more analysis. To rapid up the screening process, Novartis research teams use images from machine learning algorithms to Prediction which non tested compound possibility be worth explore in more details. As computer in rapid compare to classical human analysis and laboratory experiments in un-covering new data set new and effective drugs can made available soon,

while reducing the operational cost associated with the manual in investigation of each compound [39].

Artificial Intelligence is playing the critical role in drug discovery specify in identified novel target drug. By these analyse intricate biological systems and sifting through vast data sets of genetic

& these are proteomic information, Machine-Learning Algorithms can be trained to detect patterns and predict potential targets for treatments. This process holds the promise of uncovering new & effective drug targets for various Diseases [40].

➤ Drug Discovery Cycle

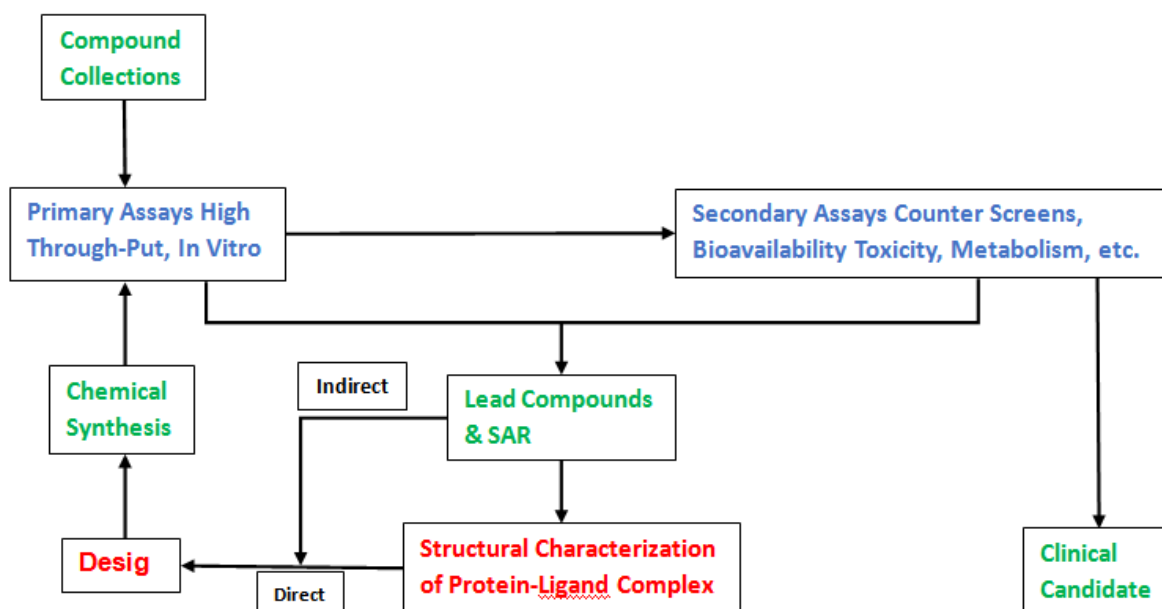


FIGURE 4.1: DRUG DISCOVERY CYCLE [41]

[2] Clinical Research or Clinical Trials

In Recent Years, the healthcare industry has been undergoing a revolution due to AI. Clinical Trials are one of areas where AI can have a significant impact. The trials are critical for testing the safety of new drugs & treatments. However, conducting clinical trials can be insufficient & the expensive and time consuming. Under are some ways in which AI support in clinical trials. Clinical trials analytics is crucial for advancing health care outcomes globally. The used of machine learning in clinical trials analytical holds promise for accelerating processes, enhancing patient stratification, & advancing precision medicine. Challengers remain such as need for high-quality, non-based training data, which can unleash the potential of machine learning, while balancing privacy concerns. Addressing these challenges in a thoughtful & ethical manner will pave the way for more effective & inclusive clinical trials analytics, ultimately benefiting diverse patient populations and advancing the field of medical research. AI helps optimize clinical trials design by predicting patient recruitment rates, patient responses, and potential

adverse events. This aids by the improving trial efficiency & reducing costs [42,43]. By using generative AI models built on data from medical imaging techniques such as X-rays, CAT scans, & MRIs, scientists could identify new biomarkers, deeply hidden visual signatures of disease activity & severity they Lead to unforeseen new treatments. The cumulative result will be shorter & more efficient trials with a greater likelihood of success [44].

[3] Disease Diagnosis

Doctors can use advanced machine learning system to collect, process, and analyse vast volumes of patient's health care data. Health-care provides around the world are using ML technology to store sensitive patient data securely in the cloud or a centralized storage system. This is known as electronic medical record's (EMRs) [45]. AI is used in hospital-based health care systems in a variety of ways, including arranging dose forms for particular patients and choosing appropriate or available administration methods or treatments plans [46,47].

[4] Novel Medication

Artificially intelligence computer systems are used broad or vast in medical sciences. Common applications include diagnosis patient's end-to-end drug discovery & development, improving communication between physician and patient, transcribing medical documents, such as prescriptions, and remotely treating patients [48,49]. The 1970 AI applications stayed first used to help with biomedical problem. From there AI-powered applications have expanded and adapted to transform the healthcare industry by reducing spend, improving patient outcomes, and increasing efficiencies overall.

[5] Data Analysis

AI-Driven data analysis also supports pharmacovigilance by mining vast data sources for signals of drug safety issues, enabling faster and more accurate reporting overall, AI enhances the efficiency, accuracy, and effectiveness of pharmaceutical research and healthcare delivery [50].

[6] Drug Development

AI can play significant role in drug development. by analysing big amounts of data, AI algorithms can identify possibility drug targets and predict their efficacy. This can help re-researchers develop new drugs. Faster & more efficiently [51,52].

AI holds the possibilities to improve the R&D process. From design and identify new molecules to target based drug validation and discoveries AI can do it all [53]. AI play the crucial role in drug development by enhancing the properties of potential compounds, forecasting their effectiveness and safety, and streamlining clinical trial design. Machine learning models can pharmacokinetic characteristics be on employed & drug to anticipate pharmacodynamic candidates, including absorption, distribution, metabolism & excretion (ADME). The potential side effect & interactions with other drugs. This integration of AI enables a more efficient and effective approach to drug development and evaluation [54,55]. AI in help accelerate the drug discovery process by enabling high-throughput screening of large chemical libraries and predicting the properties of new compounds before they are synthesized & tested in vitro or in-vivo [56,57].

[7] AI for the Detection of Tablet Defects

AI Detect the Tablet Defects has quality control process in pharmaceutical Manufacturing.

AI algorithms in computer vision technique are employed to analyse images of tablets, enable automatic & efficient detection of imperfection as cracks, chips, discolouration, shape & size. AI models on big data sets of labelled images the system learns to correctly identify different of defects. Using conventional method, x-ray computed tomography in analyse internal structure of tablets. Deep Learning is executed with x-ray tomography to detect tablet imperfection. Three difference model used the same research, including UNETA, which is apply for diagnosis of different characteristics of tablet from bottles. The internal cracks in internal structure of tablet were analyze with the help of UNetB. they UNet network used to check tablet imperfection with better accuracy & provide ease of identification of defects with significant reduced in time & financial costs & workload. This AI Powered detection not only improves the speed & accuracy of flaw identification but also reduced the dependence on manual inspection, minimize human errors & subjective judgment. [63,64].

[8] Artificial in Drug Manufacture & Regulatory Observation

AI being employed in drug formulation to predict optimal drug delivery system & improve manufacturing process. Leading to enhance drug stability & bioavailability [65]. AI can assist in analysis of complex regulatory data, expediting the drug approval process and ensuring compliance with regulatory standards [66]. AI algorithms analyse adverse drug reaction or effect data from various sources, such electronic health records to improve pharmacovigilance & drug safety surveillance [67].

VI. APPLICATION OF ARTIFICIAL INTELLIGENCE IN PHARMACY

1. Research & Development
2. Drug Development
3. Disease Diagnosis
4. Disease Prevention
5. Epidermic Prediction
6. Remote Monitoring
7. Manufacturing
8. Marketing
9. Rare Diseases & Personalized Medicine
10. Processing Biomedical & Clinical Data
11. Identifying Clinical Trial Candidates
12. Dosage Form
13. Medical Devices
14. Biological Product Development

[1] Research & Development: Pharma Companies around the world are leveraging advanced in ML Algorithms & AI-powered tools to streamline the drug discovery process. These intelligent tools are designed to identify complicated patterns in big datasets. They can be used to solve challenges associated with complicated biological networks [58].

[2] Disease Prevention: Pharma industry used AI to develop treat or heals for both known disease like Alzheimer's & Parkinson's in rare diseases. Generally, pharmaceutical companies do not spend their time and resources on finding treatments for rare diseases since the ROI is very low compared to time and cost it takes to develop drugs for treating rare diseases [59].

[3] Epidemic Prediction: AI & ML are already used by many pharma company & health care provide to monitor & forecast epidemic outbreaks across the global. These technology feed on data gathered from the

Different sources in web study the connection of various geological, environmental and biological factors on health of population of different geographical location, try to connected the dots between these factors & previous epidemic outbreaks. Such AI or ML models become particularly useful for under developed economics

that insufficient the medical infrastructure & financial framework to deal with an epidemic outbreak.

[4] Remote Monitoring: The breaks through in the pharma & health care sectors. Many pharma industries already developed variables powered by AI algorithms that remote monitor patients suffering from life threatening diseases.

[5] Manufacturing: Pharma company can apply AI in manufacturing process for higher production, improved efficiency & faster production of life saving drugs. AI used to manage & improve all aspects of the manufacturing process, including:

- Quality Control
- Predictive Maintenance
- Waste Reduction
- Design Optimization
- Process Automation

[6] Marketing: Given the reality pharmaceutical industry is sales-driven sector, AI can be helpful tool in pharma marketing. With AI pharma companies explore & develop unique marketing strategy that promise high revenues and brand awareness [60].

➤ **OTHERS APPLICATION IN AI**
Following some sectors of applications in AI:

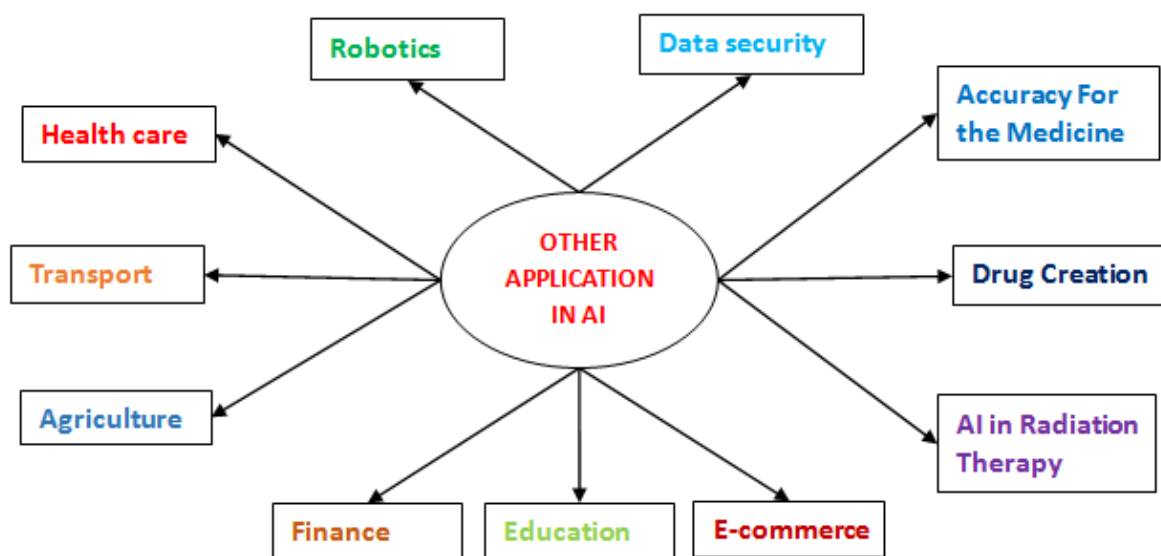


Figure 5.1: Other Application of AI [61]

VII. FUTURE SCOPE OF ARTIFICIAL INTELLIGENCE

1. AI in Science & Research
2. AI in Cyber Security
3. AI in Data Analysis

4. AI in Transport
5. AI in Health Care

[1] AI in Science & Research

AI is making many of progress in the scientific sector. Artificial intelligence can handle large quantity of a data & process it quicker than human minds. They make it perfect research where the sources contain the high data volumes. AI is already making breakthrough in this field [60].

[2] AI in Cyber Security

Cyber Security is another field that benefit from AI. As organization are transferring their data to it the networks & cloud, the threat of hacker's is becoming more significant.

[3] AI in Data Analysis

Data Analysis can benefit largely from AI & ML. AI algorithms are capable of improving with iteration & this way their accuracy & precision increase according. AI can help data analysis with handling & processing large datasets.

[4] AI in Transport

The transporter sector has been using AI for decennary. Airplanes have been using autopilot they in air since 1912. An autopilot system controls the trajectory of plane but it isn't restricted to aircraft alone. Ships & spacecraft also use autopilot to help them maintain the correct course.

[5] AI In Health care

The medical sector is using this technology for its advantages. AI is helping medical researchers & these professionals in numerous way [62].

VIII. CONCLUSION

During previous no many years the considers amount of increasing interest towards the uses of AI technology has been identify for analyze as well as analyze some important fields of pharmacy like drug discovery & dosage form designing, hospital pharmacy & Pharmaceutical industry etc. the AI technological approaches believe like human beings imaging knowledge, cracking problems & decision making. The uses of automated work flows & databases for the effective analyses employing AI approaches have been proved useful. As a result of the uses of AI approaches the designing of the new hypothesis, strategies, prediction & analysis of various associated factors can easily be done with the facility of less time consumption & inexpensiveness.

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