ROLE OF ARTIFICIAL INTELLIGENCE IN FIELD OF PHARMACY

Abstract

Artificial intelligence (AI) is a field within computer science that enables machines to operate efficiently and analyze intricate data. The realm of AI in healthcare and pharmaceutical research has experienced a significant surge in research and development. This comprehensive review delves into the opportunities and challenges presented by AI in these domains. A variety of databases, including Google PubMed, and Science Direct, Scholar, were searched with particular keywords and terms, such as "artificial intelligence," "pharmaceutical studies," "drug investigation," "medical trial," "disease detection," etc., in order to discover pertinent literature. The selection process was limited to research and review articles that had been released in the previous five years. The use of AI in disease diagnosis, digital therapy, individualized treatment, drug development, and pandemic or epidemic prediction is covered in detail in this article. While neural networks as well as deep learning have been the most widely used artificial intelligence (AI) methods, Bayesian nonparametric models have shown promise in the design of clinical trials. Wearable technology and natural language processing were used to monitor clinical trials and identify patients. Researchers should expect quick and affordable medicinal and healthcare research as artificial intelligence (AI) methods develop, which will eventually result in better services for the general population.

Keywords: Artificial Intelligence, Global Impact, Pharmaceutical Field

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I. INTRODUCTION

A collection of intelligent behaviors and processes created by computer models, algorithms, or rules is referred to as artificial intelligence (AI). Machines may now replicate human cognitive skills like learning and problem-solving because to these mechanisms. [1, 2] AI has revolutionized disease detection, automation, and therapeutic choices in the healthcare industry in recent years. In addition, there are significant chances for AI to further explore the worlds of pharmaceutical and healthcare research, thanks to its ability to evaluate enormous amounts of data from multiple sources. The application of AI in healthcare and other industries has been the subject of in-depth research in recent years. Automation of robotic processes, machine learning (ML), natural language processing (NLP), and physical robots are examples of AI technology used in the healthcare sector. [3] ML, for instance, utilizes neural network models and deep learning techniques to analyze imaging data and identify clinically significant elements, particularly in cancer-related diagnoses. [4] By mapping the crucial information from diverse imagery and textual data, machine learning (ML) techniques are being extensively integrated into natural language processing (NLP) to explore unstructured data in databases and records, such as lab reports, doctor's notes, and so forth. This helps in the medical care planning process. Patients now have access to customized treatment options and a quick, precise diagnosis because to constant disruptive technology. [5] Solutions based on artificial intelligence have been found, such as frameworks that can utilize a variety of data styles, like as imaging, markers, biometrics, and feelings that patients have reported. The ability to identify harmful illness early on is made possible by AI advancements, increasing the likelihood that avoidance will occur as a result of early detection. Many healthcare specialties, including the profession of nursing, telemedicine, cleaning, the field of radiography an operation, and rehabilitation, use mechanical robots. [6]

From medication discovery to product management, artificial intelligence has a big influence on every facet of pharmaceutical product development. Artificial intelligence (AI) tools such as data mining (ML), neural networks, and Intelligence-based quantitative structure-activity relationship (QSAR) are used in the drug development space. Drug screening and design heavily rely on these techniques, which include virtual testing (VS), supported vector machines (SVMs), deep artificial neural networks (DNNs), and recurrent neural networks (RNNs). Artificial intelligence (AI) neural networks are modeled after biological neural networks, which process input data and produce an output response. **ANNs, or artificial neural networks,** are made up of linked information-processing units, whereas DNNs handle feedback through multiple levels. RNNs, on the other hand, do sequential data analysis, use the results of one study as the starting point for another. SVMs are used for regression and classification of input data. The use of AI is utilized in the development of pharmaceutical products to identify suitable excipients, establish the process for development, and guarantee adherence to guidelines. ANNs and model systems for experts (MES) are used in this process. Artificial Intelligence (AI) is applied in manufacturing to identify and fix manufacturing problems, as well as to automate and customize manufacturing processes. To get the required quality in the finished result, artificial intelligence technologies such as tablet modifiers and meta classifiers are used. [7]

AI has been incorporated into clinical trials to aid in subject selection and trial monitoring, resulting in a decrease in dropouts due to the close monitoring. In addition, AI technologies like ML and NLP tools are utilized in market analysis, product positioning, and

product costing. The use of artificial intelligence in a variety of industries, including the fields of medicinal chemistry, medicine, medicinal products, and biological investigation, has been examined in recent articles. AI has particularly been used in the identification of illnesses, with a focus on identifying cancers and therapy, target protein finding out, computer-aided drug design, virtual testing, and in vitro pharmacokinetic assessment.[7]

This chapter discussed the role of artificial intelligence (AI) in the following areas:

a. Disease diagnosis;
b. Personalized care/digital therapy:
   - Retina;
   - Cancer;
   - Other persistent disorders.
c. Discovery of drug
   - Bioactivity and Toxicity Prediction
   - Human trials:
     - Patient identification, recruitment, and enrollment in clinical trials;
     - Monitoring trial, patient adherence and endpoint detection.

1. Artificial Intelligence in Healthcare Diagnosis

The analysis of diseases plays a crucial role in developing a compassionate treatment plan and ensuring the well-being of patients. However, the inaccuracies caused by human error pose a significant obstacle to achieving accurate diagnoses. Additionally, the misinterpretation of information further complicates the already challenging task. Artificial Intelligence (AI) offers a promising solution by enhancing accuracy and efficiency in disease analysis. Extensive research has been conducted to explore the applications of different technologies and methodologies in disease diagnosis. As the human population continues to evolve, the healthcare system faces a growing demand due to various environmental factors. [8]

Multiple diagnostic strategies are currently available, but their reliability has raised concerns. Therefore, it is crucial to prioritize the use of AI in identifying and determining the early predictive stage of diseases rather than focusing solely on treatment or diagnosis. By utilizing AI for diagnosis, early treatment can be initiated, leading to significant improvements in patients' conditions and enhanced efficiency in AI modules. [9, 10]

AI has gained significance in the field of **cancer and dementia**, [11, 12] It is crucial to remember that programs cannot display discrimination if they are not produced by themselves or connected to previous data. A pertinent and targeted dataset is required to ensure statistical surveillance. The importance of the found clusters will determine whether or not AI will be accepted in addition to user input. Learning without supervision can be applied for diagnosing hepatitis. [13] Generally, larger and diverse datasets contribute to the effectiveness of AI, although the outcome may be difficult to comprehend. Detection of atrial fibrillation and the classification of dermatological illnesses are two instances of deep learning in diagnostics [14]. [15] Data can be randomly divided into several sets for algorithm estimate by using cross-validation.[16] Accuracy, sensitivity, and specificity are three crucial aspects that AI commonly focuses on in terms of measurement.

Several studies have been conducted on predictive modeling, particularly in the field of early **Parkinson's disease prediction.** [17] To aid in the diagnosis of lung diseases, a rib segmentation algorithm was developed using chest **X-ray images.** [18] But rib-wise X-ray image segmentation is difficult for traditional methods. The authors of this study have developed a technique that makes use of chest X-ray pictures from pneumonia patients that have undergone unpaired sample augmentation. A numerous scales network then picks up the picture features. According to the study, this approach performs exceptionally well in rib segmentation, which may be helpful in determining the presence of cancer of the lungs and other lung conditions.. [19] Researchers have also recently employed algorithms and machine learning techniques to identify and classify cardiac arrhythmia by **analyzing electrocardiogram signals.** [20] Additionally, tuberculosis was categorized and identified using an optimization algorithm based on genetics (GA) along with a support vector machine (SVM) classifier in a separate investigation. [21]

2. AI in Personalized Care/Digital Therapy

AI can create a strong association in the unprocessed datasets, which can then be applied to disease prevention, diagnosis, and therapy. This new field of study offers the possibility to apply a variety of sophisticated computational understanding tools to nearly every facet of medical science. A great deal of knowledge must be acquired, analyzed, and applied to address the complicated clinical concerns. The advancement of artificial intelligence in medicine has helped physicians resolve complex clinical issues. Healthcare professionals can get help manipulating data from systems such as artificial neural networks (ANNs), evolutionary computational algorithms, fuzzy expert systems, and hybrid intelligence systems. Inspired by the workings of the biological nervous system, artificial neural networks (ANNs) are networks of interconnected computer processors called nerves that can process input in parallel.The first artificial neuron was created using a binary threshold function. [22] With its input, middle, and output layers, the multilayer feed-forward perceptron became the most often used model. Each neuron is linked to the others by linkages that have weights in numbers. In 1974, Paul Werbos developed a novel method known as "backpropagation learning," which includes an appropriate teaching algorithm.. [23]
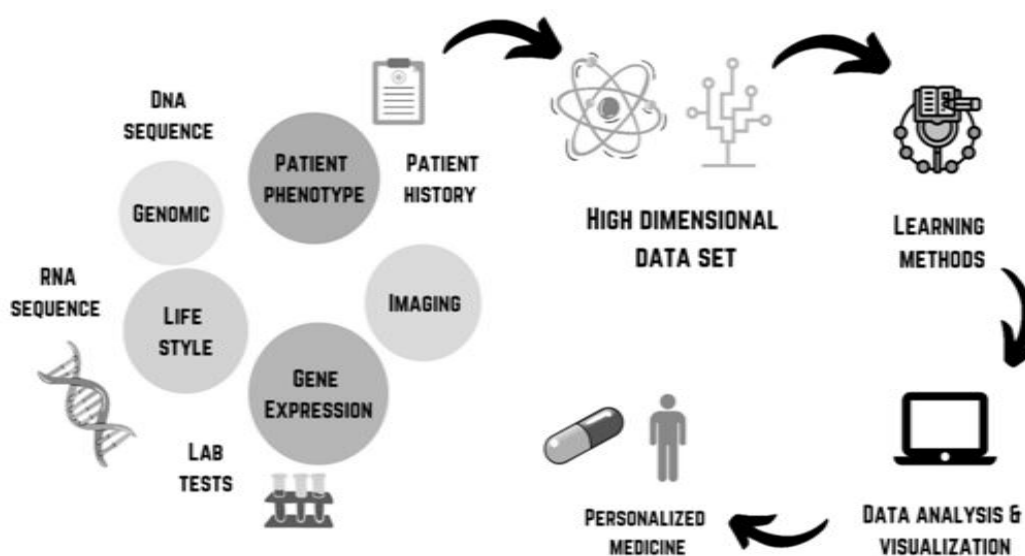

Figure: AI in Personalized care/digital therapy: [1]

- **Artificial Intelligence in Retina:** The assessment of human health has been greatly enhanced by the high-resolution imaging of the retina. Through a **single photograph** of the retina, personalized data can be extracted. With the use of high-definition medicines, ophthalmologists and retinologists are able to determine a personalized therapy and establish a healthcare system that continuously improves. [24]

- **AI in cancer:** Because AI has so many uses, it has grown more significant in the detection and treatment of cancer. In a study, gene expression data was utilized in a multilayer perceptron neural network to predict the lymphoma subtypes of non-Hodgkin lymphoma. The neuronal network's input layer comprised 20,863 genes, while the output layer included the cancer subtypes, which included Burkitt, lymphoma of the large B cells (DLBCL), follicular lymphoma, also known as marginal zone lymphoma, and mantle cell lymphoma (MCL). Remarkably, the AI neural network achieved a high level of accuracy in predicting the lymphoma subtypes. [25] AI is employed in the detection of cancer to reduce the time required while ensuring a high level of accuracy. The utilization of **AI-based PET imaging in lymphoma aids in the assessment of tumor burden,** which subsequently contributes to the characterization of the tumor, measurement of heterogeneity and prediction of treatment response. [26]

- **AI in Other Persistent Disorders:** Intelligent instruction using computers is a relatively new form of computer interaction. Expert systems and natural language comprehension are just two of the AI technologies that this creative method may include. [90] By using AI, a customized combination therapy can be created by evaluating the patient's individual biopsies and putting n-of-1 prescription recommendations into practice. With virtual medical assistants, artificially intelligent technology (AI) can streamline the process of routine monitoring, which is necessary for chronic illnesses. Many businesses have already started providing this kind of support; usually, they provide text-messaging-based instruction via mobile apps. Furthermore, AI can also provide tailored nutrition recommendations based on the individual's **gut microbiome**. Additionally, an integrated system utilizing deep learning can **predict arterial fibrillation.** [27]

3. AI in Discovery of Drug

If one follows traditional approaches to obtain statistical differences, it can take up to ten years to control the biological activity that has been discovered and developed . Target receptor binding is influenced by the drug's solubility, inherent permeability, degree of ionizing radiation and partition coefficient while developing an innovative medication. The Simplified Molecular Input Line Entry System (SMILES) algorithm is one example of an algorithm used to predict binding characteristics. [28] Six physicochemical properties are often determined using the Estimation Program Interface Suite via the method known as the quantitative structure-property relationship (QSPR). Deep learning and neural networks based on the ADMET predictor and ALGOPS program have been employed to predict the lipophilicity and solubility of various compounds. [29] Many undirected graphs are used to predict solubility [30]. A number of variables are taken into account when forecasting a new chemical entity, including the surface area, bulk, proton count, refractivity, volume, logarithm P, sum of the indexes dissolving index, and rotatable bonds. [31]

- **AI in Bioactivity and Toxicity Prediction: Chem Mapper** and the similarity ensemble approach are utilized to forecast the interactions between drugs and targets. [32] The consideration can also be given to the substructure, connectivity, or a combination of both. Deep learning techniques have demonstrated enhanced performance, as they are not reliant on the 3D protein structure. Approaches such as Deep Affinity, protein, and drug molecule interaction prediction are employed. [33]

  Deep Tox, an algorithm, surpassed all other methods by accurately identifying both static and dynamic characteristics in chemical descriptors. On the other hand, **eToxPred** was utilized to estimate the toxicity of small molecules. **TargeTox**, a drug toxicity prediction system based on biological targets, operates on the principle of guilt-by-association. [34]

  A scoring function is utilized to anticipate the characteristics of newly discovered molecules. **PrOCTOR** has the capability to accurately predict if a drug would be unsuccessful in clinical trials due to its toxicity. Additionally, it has the ability to identify adverse drug events. [35] By combining computer science, geometry, and assessment with drug discovery based on structure for predicting protein structure, AI can offer useful data. [36]

- **AI in Human Trials:** The exorbitant expenses linked to clinical studies therefore affect the costs of patient therapy. To stay profitable, biopharma companies therefore include in the expenses of unsuccessful trials' research and development when setting the price of authorized medications. Clinical trials must be carried out and conducted using a variety of procedures, including trial design, patient recruitment and selection, site selection, monitoring, data gathering, and analysis. Patient recruitment and selection are among the most difficult procedures to complete; 80% of trials take longer to enroll participants than expected, and enrollment issues cause 30% of phase-III trials to end early. A multi-centered worldwide experiment requires a lot of time and money to monitor. The time between the "last subject last visit" and the data reporting to regulatory organizations presents extra challenges because it necessitates laborious gathering and analyzing the data processes. Yet the advent of AI and digitization has significantly altered these difficulties with human studies.. [37]

- **Trial Design, Patient Identification, Recruitment and Enrolment:** In addition to its many other uses, Bayesian nonparametric models, or BNMs, have proven to be an invaluable tool in the field of clinical trial design. This particular model is adaptable because it uses a nonparametric methodology. This method efficiently minimizes clustering and shortens the trial design period by permitting the use of infinite-dimensional parameter sets with a restricted subset of parameters. Dirichlet's process combination models and Markov Chain Monte Carlo (MCMC) methods are two examples of BNMs that are often used. BNMs have many uses in the field of clinical trial design, including immuno-oncology, cell therapy, and dose selection in trials including cancer patients. Patient heterogeneity in these situations makes dose selection challenging and increases the risk of selecting the wrong dose and omitting future groups.. BNMs prove to be efficient and effective tools for dose selection in such scenarios, as they take into account the variability and heterogeneity of the study subjects. [37] Bayesian nonparametric design enables **adaptive dose selection in**

multiple populations, allowing for the exchange of information between populations while accounting for their heterogeneity. These models aid in the precise determination of the optimal dose, thereby minimizing any inaccuracies. [38]

- **Tracking Trial Progress, Patient Compliance, and Endpoint Identification:** The powered by AI method known as risk oriented monitoring (RBM) has just come to light as a more effective and economical replacement for traditional monitoring. Advanced RBM has the ability to save expenses while enhancing the effectiveness and caliber of data monitoring at research locations. Prediction analysis and data visualization, along with AI-assisted "smart monitoring," can improve trial site performance and data quality control. To get accurate data and complete the experiment successfully, it is crucial to make sure patients meet the adherence guidelines. Patient data can be automatically and continuously collected by using portable sensors and video monitoring, which improves the success of patient adherence monitoring. [39]

4. CONCLUSION

The pharmaceutical sector is continuously progressing with its technological advancements, and the integration of AI presents a valuable opportunity to reduce both the cost and time associated with drug development. The effectiveness of AI in disease diagnosis is clearly illustrated through the utilization of deep learning, neural networking, and unsupervised learning techniques. These advanced AI tools possess the capability to analyze unorganized data and establish connections with acquired knowledge to accurately forecast the outcome, thereby proving valuable in predicting specific disease diagnoses. AI has been useful in a number of contexts, such as case-based reasoning, intelligent computer-assisted instruction (ICAI), vector regression evaluation, and clinical decision support for tracking the progression of chronic diseases and maximizing treatment. In automated education, the vector regression technique helps find relationships between variables, and information-based answer extraction (ICAI) helps give patients useful information. Healthcare teams can monitor and treat patients using specific patient information because of clinical decision support and case-based reasoning, which both use past experiences to solve challenges. The ongoing challenge to develop customized medicines has been rendered possible in large part by these technologies. Furthermore, methods such as high-resolution retinal imaging and Radiomics, which forecast radiation treatment results and toxicity for particular individuals, advance our understanding of human health. Finding and introducing novel medications to the market is the primary objective of pharmaceutical research and development, but this is an arduous and expensive procedure. From target selection to clinical trials, AI offers the ability to expedite this process. Finding biological molecules with the power to alter the disease is the first step in the drug discovery process. The physicochemical and pharmacokinetic properties of thousands of synthetic compounds created to target specific illnesses are ascertained using computer-assisted drug and quantitative structure-activity relationship (QSAR) or quantitative structure-property relation (QSPR). To forecast the degree of lipophilicity and solubility of new chemical entities (NCEs), deep learning and neural networks are used. These models are based on the ADMET predictor and ALGOPS computer software. Chem Mapper and similarity combination method are two examples of AI technologies that are used to predict drug-target interactions. In terms of toxicity testing, AI plays a key role. As a result, the application of AI-powered techniques will open up a

wide range of opportunities in various fields of medical and health care research, which could influence future research.

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