REVIEW ARTICLE

The Applicability of Artificial Intelligence to the Health-care Sector

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Abstract

Almost all sectors are seeing an increase in the use of artificial intelligence (AI). It can be applied in a variety of sectors, including research, technology, and health, and is not limited to any one area. Artificial intelligence (AI) focuses mostly on how computers simulate human brain processes through data analysis. AI can be a potential option to solve all the drawbacks of medication development, which include expensive research and development expenses and unknown time consumption. There is a possibility of overlooking some important information because so much data are available. Expert systems, deep learning, and machine learning algorithms are some of the methods being used to overcome these problems. Drug development delays and clinical and commercial failures can be minimized with the effective application of AI in the pharmaceutical industry. This evaluation includes details on AI's evolution, subfields, general implementation, and use in the pharmaceutical industry. It also offers insights into AI's shortcomings and obstacles.

Key words: Artificial intelligence, computer-aided system, data management, drug development, machine learning, pharmaceutical sciences

INTRODUCTION

The field of engineering science that studies the development of intelligent machines, especially intelligent computer programs, is known as artificial intelligence (AI). It is an electronic device's capability, or a robotic framework with laptop capability, to perform input and provide outcomes in a way that is similar to how humans pay attention when learning, making decisions, and solving issues.[1] The goal of AI is to create. Intelligent devices are becoming a necessary component of the technology sector. The pharmaceutical sectors have undergone a significant shift thanks to AI. It is largely being taken advantage of in the health-care sector across the board. The combination of computer processing and human intelligence has resulted in this technology.[2] It is a sophisticated form of computer-assisted methodology that involves gathering data from multiple sources, formulating rules to handle the needed data, and modeling potential outcomes to identify suitable outcomes and processes that can mimic human behavior. It is composed of components that make working with neural networks easier, such as machine learning (ML) and deep learning.[3]

At the first academic meeting on AI in 1956, John McCarthy presented the first case in favor of the technology. The possibility of building computers with independent thought and learning was put out by mathematician Alan Turing, and scientists quickly turned their attention to this theory.[4] In 2017, speech recognition is anticipated to grow by 28.5%. Global sales from big data and business analytics reached US$ 122 billion in 2015, and by 2020,[5] it is expected that this figure will have surpassed US$ 200 billion. AI has had a tumultuous history since the 1950s. That was always thought to be the domain of dreamers, but things began to change in 1997 when Garry Kasparov, the chess champion, was defeated by IBM's Deep Blue computer. The S1 million Jeopardy prize was successfully won by the brand-new IBM Watson supercomputer in 2011. Since then, Watson has expanded into the pharmaceutical and health-care sectors. To accelerate

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Received: 07-11-2023
Revised: 08-05-2024
Accepted: 27-05-2024

the creation of novel immuno-oncology medications, Watson partnered with Pfizer in 2016. IBM Watson, an online resource that enables investigators to find links throughout different setups utilizing dynamic visualizations, was presented by IBM and Pfizer in December 2016. Between 2017 and 2022, the AI market is predicted to bring in up to 10 times as much money.[6]

CLASSIFICATION OF AI[7]

AI could be separated into two groups.
- In light of caliber
- In light of the existence [Table 1]

The subsequent classifications pertain to AI methods based on their caliber
- Artificial narrow intelligence or weak intelligence: This setup is designed and instructed to perform a specific task, such operating a vehicle, directing traffic, playing chess, or recognizing faces. Tagging on social media and Apple SIRI's virtual assistant are two examples.[8]
- Strong AI, sometimes referred to as synthetic artificial general intelligence (AGI): Another name for it is human-level AI. It has the potential to simplify human intellect. Consequently, it may address issues when given new assignments. All human-capable tasks can be completed by AGI.[9]
- Artificial superintelligence: In fields ranging from science to art, brainpower outperforms intelligence in tasks such as arithmetic, sketching, space exploration, and other related domains. A computer can be a trillion times smarter than a human or merely marginally more intelligent.[10]

CATEGORY OF AI TECHNOLOGY[11]

AI scientists categorized the AI technology according to the existence depending on whether it was already in use or not.

Type 1: This kind of AI system is called a reactive machine. Think about the IBM chess program Deep Blue, which in the 1990s beat Garry Kasparov. It does not have the memory to rely on past experiences, but it can identify checkers and make predictions on a chessboard. It is ineffective in other situations and was designed with such applications in mind. One such illustration is Google's Alpha Go.

Type 2: This kind of AI program is referred to as a restricted system of memory. That technology can analyze historical data to address present-day and future problems. This is the only method used in the creation of some autonomous car decision-making procedures. The observations are used to record the observed actions, such as vehicle lane changes.

Type 3: The AI system in question is referred to as a "theory of mind." It suggests that everyone makes decisions based on thoughts, ideas, and desires. There is no such AI.

Type 4: These are called self-awareness traits. The AI systems are self-aware and sentient. Should the machine possess self-awareness, it would identify its circumstances and leverage the ideas that are stored in other people's minds. There is no such AI.[12]

Table 1: Classification of AI

According to the caliber	• Low intelligence • Restricted AI • AI in general • Super intelligence in AI
According to the existence	• Type 1 Superhuman AI • Type 2 limited memory system • The theory of mind is the cornerstone of Types 3. • Being conscious of type 4

AI: Artificial intelligence

OBJECTIVE OF AI IN THE PHARMACEUTICAL INDUSTRY

Objectives includes[3]

- Drug discovery: AI is able to forecast the potential effects of various chemicals on biological systems. This lowers the amount of time and money needed to discover possible new medications.
- Drug Development: AI has the ability to expedite the drug development process by optimizing clinical trial designs, identifying the most suitable patient groups for trials, and predicting patients' responses to medications.
- Personalized medicine: AI can assist in maximizing therapeutic efficacy and reducing adverse effects by evaluating patient data and customizing drug regimens for specific patients.
- Drug repurposing: By analyzing large, complicated datasets, AI can find new applications for already-approved medications, which may result in the development of disease-treating medications that do not need to be created from scratch.
- Manufacturing optimization: Pharmaceutical production processes can be predicted and optimized by AI, resulting in constant drug quality and decreased waste.
- Predictive analytics: AI can forecast disease outbreaks or patient-specific health concerns by evaluating patient data, allowing for early interventions.
- Natural language processing (NLP): used to analyze and extract useful information and data for research from vast amounts of scientific publications.
- Supply chain management: AI can optimize the pharmaceutical supply chain, predicting demand, and ensuring timely delivery of medicines to where they are needed.
- Safety monitoring: AI can uncover possible medication safety risks more quickly than traditional approaches by

continuously monitoring and analyzing adverse event reports.

- Cost efficiency: AI has the potential to reduce costs in a number of pharmaceutical business sectors by optimizing workflows and enhancing forecasting.

ADVANTAGES AND DISADVANTAGES OF AI IN PHARMACEUTICAL INDUSTRY[13]

Advantages

- The pharmaceutical sector can now employ AI to address problems that were previously outside the purview of simple data analysis.
- AI can do specific tasks more accurately, which reduces expenses while increasing output. AI offers insightful information that will greatly improve clinical study results. Comprehensive knowledge of customer behavior, market dynamics, and their interactions.
- It makes it easier for companies to select patients for clinical trials and helps them find issues with drugs' safety and efficacy much earlier.
- It promotes the creation of new AI algorithms and improves the functionality of antiviral detection systems. It is also beneficial for the industry's patient screening process for clinical trials. If AI was well constructed, it would make fewer errors. They would be lightning fast, precise, and accurate.
- Future robotic surgery will surpass humans in precision in performing a variety of surgical procedures.
- AI can now understand and analyze vast volumes of biological data thanks to deep learning and natural language processing, which is revolutionizing the drug discovery process.

Disadvantages[14]

- It can be altered to initially cause widespread destruction
- It is effective in corrupting the following generation
- Joblessness will arise if robots start to supplant people in all professions
- May be costly to build, maintain, and rebuild
- Machines can easily inflict destruction when handled improperly. Many people fear that, at the very least
- AI makes humans dependent on it, and as we have already seen in part with cell phones and other technologies, humans lose their mental faculties
- In addition, robots have the capacity to exceed people and subjugate them.

TECHNOLOGIES USED IN AI[15,16]

1. NLP: Give computers a lot of natural language data to digest and look at
2. Support vector machine: The method creates an optimal hyperplane that classifies new cases given a collection of labeled training samples
3. Heuristics: Escape routes in the mind that reduces the burden of making decisions. For example, applying common sense, profiling, estimation, well-informed estimate, or generalization
4. Artificial neural networks (ANN): The way that organic nerve systems, such as the brain, process information is the model for information processing that was initially created in the 1940s. An artificial neural network is a function of mathematics. A ANN employs samples of data instead of all datasets to obtain remedies and save money and time. ASNN (PYTHON) consists of trio interconnected layers. Neural networks use a feedback process called back-propagation, or back prop, to learn new information, just like the brain does. ANNs are used in picture compression, character identification, stock market predictions, and self-driving cars. The pattern-recognition capabilities of brain neural networks are mimicked by ANNs. The artificial neuron system takes information from several external sources, evaluates it, and makes decisions, just like a single neuron in the brain. It is interesting to note that ANN mimics both adaptive biological neurons and the biological nervous system. ANN is a helpful modeling method, particularly for non-linearly correlated datasets, which are frequently encountered in pharmaceutical operations

TOOLS OF AI

- Robot pharmacy: The UCSF Medical Center uses robotics to produce and monitor pharmaceuticals in an effort to improve patient security. Drug has been carefully manufactured in 3,50,000 dosages by the system; it is much smaller than a human and can administer precise doses of medication; one of the uses of robotics is the production of hazardous chemotherapy medications for injectable and oral use. This gives the UCSF nurses and pharmacists more time to concentrate on direct patient care and work in tandem with the doctors to maximize their expertise [Figure 1].[17]

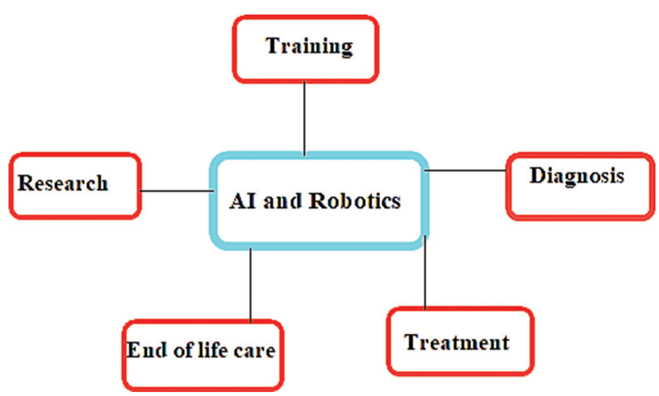

Figure 1: Flowchart of artificial intelligence robotics

- Medicine and engineering designing intelligence (MEDI) Robot: MEDI stands for medicine and engineering designing intelligence. The project manager for the development of the pain management robot was Tanya Beran is an Albertan professor of community health sciences at the University of Calgary. Her inspiration came from her experiences working in hospitals, where young patients cry throughout treatments. Even if the robot is incapable of thought, planning, or reasoning, it is possible to make it seem like AI by connecting with the children beforehand and then outlining what to expect during a medical procedure.[18]
- **Erica robot:** The new care robot Erica was developed in Japan by Hiroshi Ishiguro an Osaka University researcher. It was developed in collaboration with the Japan Science and Technology Agency (ATR), Kyoto University, and the Advanced Telecommunications Research Institute International. Its characteristics blend those of Europe and Asia, and it speaks Japanese.[19]
- **TUG robots:** Prescriptions, food, specimens, supplies, and big items such as trash and linen can all be transported by autonomous robots at the hospital called Aethon TUG. It comes in two varieties: An interchangeable base platform for transporting racks, bins, and carts and fixed and secured carts.[20]

APPLICATIONS FOR AI IN PHARMACEUTICAL INDUSTRY[21]

Manufacturing process improvement

- AI offers several chances to enhance processes in development and manufacturing.
- AI is capable of quality control, maintenance, material waste reduction, design time reduction, improved production reuse, and more.
- AI has a wide range of applications in increasing industrial efficiency, resulting in speedier output and reduced waste. For instance, computer numerical control can be used to handle process data, which is generally input by human participation.
- The AI ML algorithms look for areas where the process might be simplified in addition to ensuring that activities are completed extremely precisely.[3]

Drug discovery and design

- From developing new compounds to identifying novel biological targets, AI is assisting in the discovery and validation of pharmacological targets, as well as target-based, phenotypic, and multitarget drug discoveries, therapeutic repurposing, and biomarker identification.
- The potential for AI to expedite the approval and launch of drugs is the primary benefit for pharmaceutical companies, especially when used in clinical trials. This could result in large cost savings, enabling patients to access additional treatment alternatives and more reasonably priced pharmaceuticals.[3]

Rare diseases and personalized medicine[21]

- AI is being utilized in a number of ways to identify diseases such as cancer and even predict future health issues depending on an individual's genetic composition. It does this by combining data from analytics, patient biology, and body scans [Figure 2].
- IBM Watson for Oncology is one instance, which

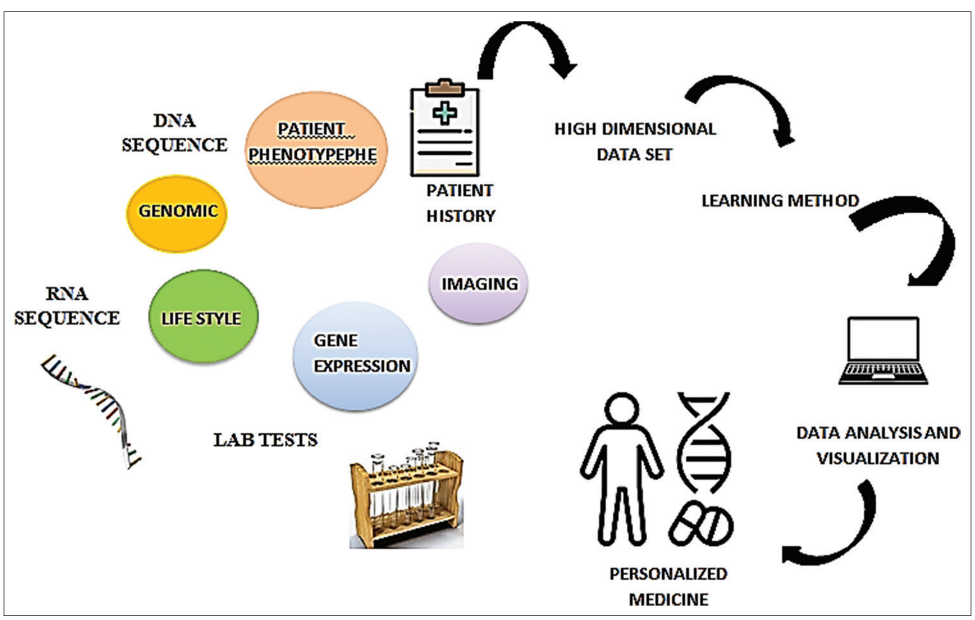

Figure 2: Artificial intelligence in acquiring and analyzing data of a patient in personalizing the treatment

suggests a customized treatment plan based on the medical background and data of each patient.
- AI is also being utilized to create customized medication regimens based on test outcomes, previous medication reactions, and patient history pertaining to drug reactions.

Drug repurposing

- One of the most apparent areas where AI-based solutions can provide significant value for pharmaceutical businesses on a tight budget is the repurposing of pharmaceuticals.
- Repurposing established medications or late-stage drug candidates for novel therapeutic applications is a preferred approach for numerous biopharmaceutical firms, as it minimizes the possibility of unforeseen toxicity or side effects in human trials and probably requires less research and development expenditure.
- Drug adherence and dosage
- Pharma companies have significant challenges in ensuring voluntary participants in clinical studies adhere to a drug research protocol.
- Patients in medication studies who disobey trial regulations face expulsion from the study or the possibility of tainting the study's findings.
- Taking the recommended dosage of the medicine under study at the designated periods is one of the key components of a successful drug trial. Having a mechanism to guarantee medication adherence is crucial for this reason.
- AI is able to separate the good from the bad using both algorithm test results and remote monitoring.

MOVING TOWARD AI IN PHARMA DEVELOPMENT[22]

- Although there are many opportunities to use AI in biotech and pharmaceutical development, implementing these technologies can be a slow process.
- The process of "training" AI in what functions for drug research can take longer than in other applications, and traditional drug development and discovery techniques also call for a more gradual adaptation.
- For instance, when social media uses AI to tag your photograph, it receives instant input from you regarding the accuracy of the results, enabling the AI to learn rapidly.
- It can take months or years for a new chemical to be proven as a drug candidate in the drug discovery process. However, it is indisputable that AI will revolutionize the pharmaceutical sector, and businesses who can quickly adopt new procedures would stand to gain a competitive edge.

Research and development

- Pharma firms all over the world are creating cutting-edge ML algorithms and AI-powered technologies to speed up the drug discovery process.
- These technological techniques can be utilized to address issues related to complicated biological networks because they are made to identify intricate patterns in sizable datasets.
- The R&D of such drugs, which have a higher chance of successfully treating a disease or medical condition, can be funded by pharmaceutical firms. This is an outstanding capacity to examine patterns of various diseases and determine which composite formulations are most appropriate for treating specific symptoms of a given ailment.

Future directions AI[23]

Companies such as Google and Uber are already using self-driving car technology. AI will have a big impact on automated transportation since it will help drivers with disabilities and cut down on accidents. More sophisticated AI systems could help in hazardous industrial jobs and replace human workers altogether. AI is the next frontier in the life sciences for pharma, as AI systems can foresee climate change using environmental technology and data sciences.

To control risk, pharmaceutical companies need to assemble portfolios. To do this, they have to ensure that R&D funds are distributed in a way that supports decision-making,

A. By raising the probability of effective medication discovery.
B. Yield a discernible rise in income.
C. To benefit from an ecosystem for manufacturing, sales, and marketing that incorporates R and
D. AI-powered bots: Just like with applications, pharmaceutical companies will soon be able to create bots for physicians.

FUTURE SCOPE OF AI[24]

- AI is utilized in research and science.
- AI concerns regarding online safety.
- AI when analyzing data.
- AI in medical services, etc.
- AI in transport, AI in home.
- AI in the workplace and academia.

AI in cyber security

Another area where AI is helpful is cyber security. The increasing migration of business data to cloud computing and IT networks is making hackers a more serious danger.

AI in data analysis

Data analysis is significantly impacted by AI and ML. Every algorithm has the capacity to improve with each iteration, gaining greater precision and accuracy in the process. AL can be useful for data analysts who handle large datasets.

AI in transport

AI has applications in the field of transportation. Aircraft has been using autopilots to navigate while in the air since 1912. An autopilot system manages an aircraft's course, however, it is not limited to aviation technology. Ships and spacecraft also utilize autopilot to help them stay on their desired course.

AI's importance in the pharmaceutical industry is profound. Here's a brief overview[3]

- Clinical trials: AI can improve the efficiency of trials by assisting with patient recruiting, monitoring, and retention.
- Personalized medicine: AI is able to evaluate patient data and make tailored medication recommendations.
- Drug repurposing: AI can find novel applications for current medications.
- Manufacturing: AI can streamline the pharmaceutical production process, guaranteeing quality while cutting expenses.
- Supply chain optimization: AI can control inventories, forecast demand, and cut down on waste.
- Drug adherence: AI-driven applications monitor medication adherence and remind users to take their prescriptions.
- Disease identification and prediction: AI is able to forecast the onset and course of diseases by examining medical records.
- Cost efficiency: AI has the potential to drastically lower the price of medication research and distribution through automation and optimization.
- Regulatory compliance: AI can assist in making sure pharmaceutical companies adhere to all legal and regulatory obligations.

CHALLENGES THAT PHARMA COMPANIES FACE WHILE TRYING TO ADOPOT[25]

- The unfamiliarity of the technology – due to its novelty and esoteric nature, AI still feels like a "black box" to many pharmaceutical companies.
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- Inadequate IT infrastructure is due to the fact that the majority of already in-use IT applications and infrastructure were not created or designed with AI in mind. Even worse, pharmaceutical companies have to upgrade their IT systems at great financial cost.
- Pharma businesses have to go above and beyond to compile and organize this data into a format that can be evaluated because a large portion of it is in free text format. Notwithstanding all of these restrictions, one thing is certain. AI has already redefined pharmaceuticals and biotech.

AI has been making significant inroads into the pharmaceutical industry. Here's a brief overview of its roles

- Drug discovery and development: Compared to conventional approaches, AI can uncover possible medication candidates much more quickly by analyzing large datasets. Algorithms using ML can forecast how certain substances could function as possible medications for particular illnesses.
- Personalized medicine: AI may evaluate patient data to customize therapies for specific patients, increasing the likelihood that a therapy will be successful.
- Clinical trials: By determining who would be the ideal trial participants, forecasting patient outcomes, and refining trial designs, AI can assist with patient recruitment.
- Drug repurposing: AI can assist in finding new applications for already-approved medications, which may be a more economical strategy than creating a brand-new medication from scratch.
- Production and supply chain optimization: Demand forecasting using predictive analytics can help to optimize manufacturing schedules and cut waste.
- Safety and pharmacovigilance: More quickly than with conventional monitoring techniques, AI systems can monitor social media and patient data to spot possible drug side effects.
- Sales and marketing: AI can be used to steer marketing tactics by analyzing patient preferences, physician prescribing habits, and market trends.
- Drug interactions: AI has the ability to forecast possible drug interactions, which is particularly useful for patients who are taking several medications.
- Disease prediction and prevention: AI can assist in forecasting disease outbreaks and identifying groups that are at risk by evaluating large datasets.
- Medical imaging: AI can assist in improving picture clarity or in the early detection of problems that the human eye might miss in diseases that require imaging.
- Molecular modeling: The ability of AI to model and forecast molecular activity is crucial for the development of new drugs.
- Chat bots and virtual health assistants: They help patients through treatment procedures, give them immediate

medical information, and remind them to take their medications.

The following domains see the application of AI[26]

- Diagnosing a disease

Digital therapy and customized care:
  - Radiation therapy
  - A retina
  - Cancer is
  - Additional chronic illnesses.
- Drug research
  - Bioactivity and toxicity prediction;
  - Clinical experiments:
  - Patient discovery, recruitment, and enrollment in clinical trials
  - Trial, patient compliance, and endpoint identification monitoring.

Forecasting of an epidemic/pandemic

AI in disease diagnosis[27]

Analysis of diseases becomes essential for planning a thoughtful course of care as well as ensuring patients' well-being. Human error leads to inaccuracies that impede precise diagnosis, and incorrect interpretation of the information produced makes the work complex and laborious. AI can provide appropriate assurance in accuracy and efficiency, which can have a variety of applications. The uses of various technologies and approaches for the aim of disease diagnosis have been presented following a vivid survey of the literature. Various environmental expressions indicate that as the human population grows, there is an ever-growing demand on the health-care system. Despite the existence of sensitive, conflicting, non-analyzing incongruities, a significant body of evidence has shown that innovative approaches can define their applicability by illustrating the as-yet-uncovered current reality. Patients should be categorized according to how severely their disorders have impacted them; this will help in diagnosis. A diagnosis is the state in which a person's condition is identified based on specific pre-existing issues.

AI in digital therapy/personalized treatment[27]

AI may be able to find a significant association in the raw datasheets that will help with the disease's diagnosis, management, and prevention. Numerous more recent methods utilized in this developing field of computational knowledge have the potential to be employed in nearly every area of medical study. The task of gathering, evaluating, and applying a wealth of knowledge must be met in order to solve the complicated clinical problems. The evolution medical AI has aided professionals in resolving challenging clinical issues. Health-care professionals can receive assistance in manipulating data from systems such as ANNs, evolutionary computing, fuzzy expert systems, and hybrid intelligent systems. The organic nervous system serves as the foundation for the artificial neural network. Neural networks are a type of interconnected computer processor network that can process input in parallel using computations. A binary threshold function was used to create the first artificial neuron. The most widely used model with many layers – input, middle, and output – was the multilayer feed-forward perceptron. Links with a numerical weight connect each neuron.

AI in radiotherapy

A relatively new technology that is very helpful in radiation treatment planning is automated treatment strategy. With treatment planning using automation, quality, consistency, and error rate of the plan are effectively improved. Three categories – multi-criteria optimization, automated rule implementation, and reasoning modeling of prior knowledge in clinical practice – can be used to group the treatment workflow. The clinical guidelines can be implemented with a basic automated computer software that has structures. The patient's anatomy and physiology can be examined by the treatment planning system, which can also simulate the thought process that manual treatment planning typically uses. Promising accuracy has been demonstrated using three-dimensional dosage distribution and dose models for spatial dose. Radionics uses a variety of imaging biomarkers to provide detailed information about malignancies. Radionics can be used to forecast the toxicity and results of radiation therapy for specific patients.

AI in retina

Retinal high-resolution imaging has made it possible to monitor human health in a remarkable way. A single retinal photograph can yield highly tailored data, and when combined with high-definition medications, an ophthalmologist or retinal specialist can create a personalized treatment plan and implement an ever-improving learning health-care system.

AI in cancer

AI has been more important in the realms of cancer diagnosis and treatment because to its wide range of applications. A multilayer perceptron (MLP) neural network was trained with gene expression data to predict the lymphoma subtypes of non-Hodgkin lymphoma. Lymphoma subtypes make up the output layer of the neural network, whereas 20,863 genes make up the input layer. Burkitt, mantle cell lymphoma (MCL), follicular lymphoma, marginal zone lymphoma, and diffuse large B-cell lymphoma (DLBCL) (MCL) are among the subtypes of lymphoma. High accuracy lymphoma subtype predictions have been made using an AI neural network. Using gene expression data, an artificial neural network was trained to find new prognostic markers for MCL. The results showed that 58 genes had high accuracy survival predictions, with 10 genes linked to bad survival and 5 genes to favorable survival. According to a multivariate analysis of gene expression using the MLP, three genes are correlated with poor survival and four genes with favorable survival for DLBCL patients.

AI in other chronic diseases

Based on computer programming skills, several computerized therapies are offered. Joysticks or multiple-choice questions are used in the behavioral and cognitive approach, which is the main focus of the therapies. Intelligent computer-assisted instruction is a new type of computer interaction that has recently been developed. It has the ability to employ additional AI technologies, such as expert systems and natural language understanding. Using AI, one can use n of-1-medication recommendations and develop a combination therapy based on the patient's own biopsy. Regular monitoring is necessary for chronic diseases, and with the use of AI, virtual medical assistants can help with this monitoring. Numerous businesses have set up this kind of support, which usually consists of text-based virtual coaching through mobile applications; AI can also be used to deliver dietary advice that are precisely focused on gut flora. An integrated system based on deep learning can be used to forecast arterial fibrillation. a smart watch, a single-lead electrocardiogram sensor, and data from an accelerometer tracking physical activity. Diabetes treatment makes considerable use of case-based reasoning, which is created using the AI method. The computerized system detects issues and retains the most efficient method for each patient.

AI in drug discovery

Lack of suitable technology makes it difficult to build many therapeutic compounds from a chemical space; however, this can be worked around by utilizing AI during the process of developing new drugs. The link between quantitative structure and activity has an impact on forecasting activities. The various metrics, like log P or log D, can be utilized to produce forecasts, anticipate the generation through calculations, and support the important molecule's pharmacokinetics as well as its biological safety, effectiveness, and adverse effects. The vast area necessitates the delocalization of molecules based on their three-dimensional distribution and attributes. To demonstrate the bioactivity, it is best to gather all previous data on the selectivity and molecular placement utilizing a variety of domains, such as PubChem, ChemBank, DrugBank, and ChemDB. Virtual screening is done using a variety of *in silico* techniques, which often yield better analysis, faster removal, and more variety. Drug design algorithms choose a lead compound to bind with and produce activities by taking into account the lead compound's physical, chemical, and toxicological properties. Various physicochemical characteristics can boost biological activity and efficacy. AI-based QSAR techniques are used in QSAR with an eye toward the possible use of the drug candidate. It can take 10 years to find and develop biological activity if the conventional methods for calculating statistical differences are followed.

AI in prediction of bioactivity and toxicity

The affinity for the receptor or protein of interest determines its effectiveness. When a medicine and the goal are considered comparable, it is assumed which they would converse with the same object. The drug-target interactions are predicted by Chem Mapper and the similarity ensemble technique. One may also take connection, the substructure, or both into account. Since deep learning is not dependent on the 3D structure of proteins, deep learning algorithms have demonstrated improved performance. The methods include deep affinity, protein, and drug molecule interaction prediction. Making the prediction is essential to avoid harmful consequences. Pre-clinical studies are often conducted after the *in vitro* assays, wherein timeliness can be distinguished and more opportunities for improvement exist. To cut costs, a number of Web-based technologies are available. The National Institutes of Health, the Environmental Protection Agency, and the US Food and Drug Administration (FDA) conduct the Tox21 data challenge, which evaluate computer methods for estimating the toxicity of medications. For identifying both static and dynamic elements inside the chemical descriptors, an algorithm called deep tox outperformed all other processes, whereas eToxPred was utilized to estimate the toxicity of tiny compounds. The guilt-by-association idea is applied by TargeTox, a biological target-based drug toxicity prediction system.

AI in prediction of bioactivity and toxicity

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Clinical trial design, patient identification

Hiring and enrollment according to the FDA, by lowering population heterogeneity, prognostic enrichment, and predictive enrichment, AI models can help improve the quality of trial design and patient selection. In addition to its many other uses, Bayesian non-parametric models (BNMs) have emerged as a very helpful tool for developing clinical trials. This model applies a non-parametric methodology and is adaptable. With a finite subset of restricted parameters, this paradigm enables the usage of infinite-dimensional parameter sets. This method reduces the amount of time needed for trial designing and clustering. Two well-liked BNMs are Markov Chain Monte Carlo techniques and Dirichlet Process Mixture Models. These BNMs have a wide range of uses in the design of clinical trials, including immuno-oncology, cell therapy, and dose selection in trials involving cancer patients. The variety of the patient group makes dose selection challenging and increases the risk of selecting the wrong dose and target population in the future. Because BNMs take into account all of the variables and heterogeneity of the research individuals, they are an efficient and useful method for dose selection in such patients. Multiple populations are subjected to adaptive dosage selection using Bayesian non-parametric design. In light of the communities' heterogeneity, this makes information sharing across many populations easier. These models reduce inaccuracies by assisting in the precise selection of the ideal dosage.

Monitoring trial, patient adherence, and endpoint detection

Another problem in the clinical experiment is keeping an eye on the trial participants, which may be done with wearable technology that supports AI. Such monitoring is personalized, power-efficient, and real-time. Recently, risk-based monitoring (RBM) has become a viable and affordable technique to replace traditional monitoring, thanks to AI's support. A more sophisticated RBM version might be able to save costs while improving the effectiveness and caliber of data monitoring at the trial site. Predictive analysis and data visualization are two tools that al-assisted "smart monitoring" might utilize to enhance trial site performance and data quality assessment. To collect accurate data and ensure the trial's success, patients must comply with the adherence criteria. The trial's ability to efficiently monitor patient adherence is enhanced by wearable sensors and video monitoring, which automatically and continuously gather patient data. AI-enabled makes medical image-based endpoint and disease detection significantly faster and more affordable than manual reading. According to recent improvements, AI may be able to replace the conventional clinical trial methodology with one that is safer, faster, and less expensive.

AI in forecasting of an epidemic/pandemic[28]

Pandemics have no boundaries and can result in both morbidity and death. Numerous pandemic outbreaks have occurred worldwide, including the COVID-19 outbreak, the Spanish flu, the black death, cholera, influenzas, and AID. These outbreaks have the potential to disrupt social and economic systems. Early diagnosis and effective treatment of the illness are critically dependent on each other, which lessens the toll that it has on people's health as well as on the political, social, and economic institutions. Surveillance is crucial to achieving early detection. Extensive resources, labor, and time are required for active surveillance. It is difficult to forecast epidemics and pandemics in real life. But because to recent developments, it is now possible to examine the spread of terrible diseases. AI is the greatest choice for achieving surveillance while making effective use of available resources. Many health-care sectors are implementing ML and deep learning, which is found to be more efficient than human resources. Because of their complexity, developing epidemiological models continues to be difficult. Models for predicting outbreaks have recently been created using ML. AI is utilized in pandemic and epidemic detection, prevention, response, and recovery. Prediction, surveillance, and information are starting to be widely employed in prevention, particularly in light of the most recent COVID-19 outbreak. Because of its fluctuating epidemic peak, periodic peaks, etc., influenza epidemic forecast is always difficult in Colorado. Even in regions with variable seasonal influenza, a reliable forecast is achievable with the integration of the self-adaptive AI model. For instance, ML and ensemble techniques have been employed in Taiwan to accurately anticipate seasonal influenza cases. The predictive accuracy of the ML feed-forward propagation neural network model (MSDII-FFNN) for influenza is 90%. Australia and the USA have used ML anonymized mobility map (AMM) to forecast influenza cases. By combining data from smartphones, AMM is able to forecast epidemics by taking into account people mobility across state lines. Ebola is still a problem in Africa. Numerous methods have been used to forecast Ebola, incorporating a neural network hybrid created by Umang *et al*. that exhibits 100% precision while using random forest for classification method. Reliable findings in predicting the propagation have been obtained by integrating ML with experimental models involving artificial societies. For instance, the consequence of studying the transmission of Ebola in a computer model of Beijing has been anticipated.

Lessons from COVID-19 on adopting AI[29]

In addition to highlighting many of the obstacles to success, the COVID-19 epidemic offered days after the first stay-at-home directives were issued, and contests to combat the virus were launched on Kaggle and other websites. Methods were created to forecast the virus's course, calculate the epidemiological spread and the impact of self-quarantines, identify the illness, search the literature, contrast state and federal efforts to stop the virus's spread, and more. Health-care and pharmaceutical companies searched for medications or combinations of already-approved treatments due to the lengthy development times for new pharmaceuticals – a well-known issue. These attempted to control the spread, lessen the cytokine storm, lessen the intensity of symptoms, and forecast which patients would improve with therapy or require ventilators or hospitalization. Additional AI applications ranged from enhancing the scalable manufacturing of current pharmacological therapies to virtual screening of molecules utilizing deep learning. AI's data-driven prioritizing and scientific expertise combined to assist find potential remedies.

CONCLUSION

In the pharmaceutical sector, AI has the potential to be revolutionary. AI can speed up drug discovery, enhance clinical trial designs, enable personalized treatment, and improve supply chain management by utilizing enormous datasets. However, incorporating AI necessitates large financial outlays, careful verification, and moral issues. Despite its difficulties, AI holds great promise for expedited and cost-effective medication discovery as well as patient-specific therapy.

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Source of Support: Nil. **Conflicts of Interest:** None declared.