REVIEW ARTICLE

Role of Artificial Intelligence in Pharmaceutical Sciences: Recent Advances, Applications, Challenges, and Future Perspectives

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ABSTRACT

Background

The global expansion of COVID-19 has made the development of pharmacological drugs a more pressing and important area of study. The expensive and time-consuming process of developing new drug molecules to treat any disease continues unabated. Over the past 20 years, artificial intelligence has substantially improved the performance of industrial and service systems. Expert systems, a rapidly developing technology, are a product of artificial intelligence research.

Applications

Today, it is commonly used to solve complex problems in a range of fields, including science, engineering, business, medicine, and weather forecasting. Sectors utilizing artificial intelligence technology have seen improvements in quality and efficiency. Utilizing existing data resources and discovering fresh and innovative leads is a crucial aspect of drug design. Following identification of the pharmacological target, numerous multidisciplinary fields collaborate using artificial intelligence (AI) and machine learning (ML) techniques to produce enhanced pharmaceuticals.

Scope

Artificial intelligence-powered medical technology is swiftly evolving into practical clinical practice-related solutions. This review article illustrates the application of artificial intelligence (AI) to a variety of medical specialties from the perspectives of seven different fields: machine learning, intelligent robotics, image recognition technology, expert systems, artificial neural networks, and evolutionary computation, followed by the potential and existing uses of AI in medicine.

Keywords: Artificial Intelligence (AI), Machine Learning, Pharmaceutical Industry, Generative AI.

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1.1 Introduction

Research in AI focuses on intelligent machine learning, primarily using intelligent computer programs, to achieve results that are similar to how people pay attention [1]. In general, this process includes acquiring data, developing efficient ways to use that data, presenting exact or approximate conclusions, and making self-monitored adjustments [2]. The most prevalent uses of AI are to examine machine learning and mimic human intellectual processes [2, 3]. AI is applied to do more precise evaluations and generate useful outcomes [3].

According to this viewpoint, AI technology combines computer intelligence with a variety of practical statistical models. The pharmaceutical business is thought to spend billions of dollars annually on the research and development of new drugs and chemicals. Pharmaceutical companies increasingly depend on big data to create clinical trials that are less likely to be unsuccessful, lowering the overall cost of Research and Development [4]. Human-like skills demonstrated by robots are regarded as the definition of artificial intelligence. This expression is used when a computer displays mental behavior that is comparable to that of humans, such as learning or problem-solving [5]. AI includes techniques like machine learning, which are widely recognized for identifying and predicting distinctive characteristics. Artificial neural networks, such as deep learning networks (DNN) or recurrent neural networks (RNN), are largely responsible for the rapid development of artificial intelligence.

AI in healthcare will help with a variety of jobs, such as retaining medical records along with additional data, automating repetitive tasks, creating treatment plans, using virtual nurses and digital assessments, providing medications, discovering novel therapies, and carrying out system audits. Software that can reason, plan, learn, and observe on its own is referred to as having artificial intelligence. Artificial intelligence has a branch known as "symbolic AI" to overcome its limitations. Sub-symbolic techniques such as neural networks, fuzzy systems, evolutionary computation, and other computational models, known as "computational intelligence," started to gain popularity and develop into a field of AI [6].

1.2 AI and ML: Key concepts and terminology

AI is a method used to build computers with behavior that resembles that of humans. AI is used in Machine Learning (ML), where AI is accomplished by employing algorithms that have been taught using data. Artificial neural networks (ANNs), also known as deep learning (DL), are a category of machine learning (ML) that draws motivation from the overall structure of the human brain. One of the most significant elements of human intelligence is the capacity of the brain to recognize, comprehend, and respond to a constantly evolving external world.

In addition to attempting to understand how the human brain operates, artificial intelligence (AI) strives to develop intelligent systems that can react rapidly and safely to an outside world that is persistently changing. By emphasizing either faithfulness to human behavior or rationality (doing the right thing in both cognition and action), researchers have developed various types of AI. AI subfields can either be broad, focused on perception, learning, and reasoning, or narrow, like chess.

Several academic disciplines have made contributions to the advancement of AI technology, including the field of neuroscience, the subject of mathematics, and philosophy. Machine learning powered by artificial intelligence (AI) uses statistical approaches to find patterns in data, which can be text, images, or just about anything else that has been electronically preserved. Three kinds of machine learning techniques are reinforcement learning, unsupervised learning, and supervised learning [7].

1.2.1 AI classification

AI can be classified in two different ways [8,9].

a) According to caliber

b) According to the presence

According to caliber, AI is categorized as;

1. Weak intelligence (ANI): sometimes referred to as artificially constrained intelligence (AI): This system was developed and taught to do a certain task, such as reading traffic signs, operating a vehicle, playing chess, or recognizing faces. Tags on social media and Apple SIRI's virtual personal assistant are two examples.
2. Artificial universal intelligence or powerful artificial intelligence (AI). It is also known as human-level AI. It can make human intelligence more understandable. As a result, it can handle challenges when given new responsibilities. AGI is able to do all human-level tasks.
3. Artificial Super Intelligence (ASI) is a cognitive ability that excels in whatever smart humans do, including arithmetic, drawing, and space exploration. This includes science and the arts. The range of intelligence for a machine spans from being only marginally smarter than a person to being a trillion-fold brighter.

AI researcher Arend Hintze [10], divided the AI technologies into those that were already in use and those that were not. They are:

- This type of artificial intelligence system is known as a reactive machine. Consider the IBM Deep Blue (IBM) gaming program, which in the 1990s defeated Garry Kasparov. It can identify the game of checkers and forecast moves on a chessboard, but it lacks the memory to draw on prior knowledge. It is worthless in other situations and has been developed only for those applications. Another example is Google's AlphaGo.
- This type of AI system is known as a restricted memory system. To address problems that exist now and in the future, this technology can evaluate historical data. This is the sole method used to generate some of the decision-making processes in autonomous vehicles. The observations are used to document the observed actions, such as lane changes for cars. The findings are not kept in mind for all time.
- The term "theory of mind" refers to this class of AI system. It implies that everyone has thoughts, ideas, and wants that influence their decision-making. This AI does not exist.
- This category is referred to as self-awareness. The AI systems have a sense of self and are sentient. If the machine possesses self-awareness, it will be aware of its surroundings and make use of the ideas that have been pre-programmed into other people's minds. There is no such AI.

1.3 Concept of Artificial Intelligence in the pharmaceutical industry

Computational power and algorithms for generating novel leads with therapeutic efficacy are essential in the modern drug discovery process [11]. Through a variety of research techniques, deep atomic insights are now accessible, and they often point out the root causes of malfunction, illness, or inhibitions. Based on it, the algorithms are updated in order to respond to the accurate mechanical action of the atom, which is essential for the process of creating new medications.

1.3.1 Artificial neural networks

Artificial neural networks (ANNs), popular models for computing, were developed using the human mind and its networking patterns as a foundation [12]. The simplest instance [13], shapes the mathematical chart with a network that is completely interconnected or feed-forward and has three distinct levels (input level, hidden level, and output level). The incoming input is transformed nonlinearly by neurons, a single processing unit that works layer by layer. The output of the layer preceding it is fed into this information as it is sent layer by layer. Molecular modeling and drug design both make extensive use of ANNs. The complexity associated with QSAR (quantitative structure-activity relationships), HTVS (high-throughput virtual screening), and statistical models utilized in pharmacokinetic and pharmacodynamic studies is removed [14]. For the numerical values driving the output, ANNs excel at understanding nonlinear connections and forecasting the results of the drug development process [15].

1.3.2 Deep learning methods

The DL method, which mimics a neural network and includes numerous hidden layers, is extensively used because it can be tailored to learn any complex function. It can learn as much as it can and produce incredibly reliable findings with enough data and computation time. It is possible to learn arbitrarily complex modules that directly offer appropriate neurons and trained sets thanks to the different layers that are hidden in DL sequences. The DL's use of a back-propagation method and a gradient-based optimization methodology allows for end-to-end differentiation [16].

1.3.3 Machine learning method

The fundamental paradigm for finding patterns in data is known as machine learning (ML), and it uses a number of method-based domains and algorithms to accomplish so. Every automation-based approach makes use of DL and ML but keeps the distinction. A branch of machine learning called deep learning (DL) focuses on artificial networks that link computing nodes. More categorization of machine learning is provided [17]. This simulates the propagation of electrical impulses and is comparable to human biological neurons.

1.3.4 Image recognition technology

Photo recognition is the process of using computers to decipher and evaluate photographs. It is a fundamental component of artificial intelligence systems based on deep learning methods. The three stages of photo recognition advancement are recognition of text, digital picture recognition, and object identification [18]. The five stages of recognition include input processing, preprocessing of images, picture extraction, classifier development, and output generation [19].

1.3.5 Expert system

Expert systems are a sort of computer program that helps people make decisions. It is one of the first effective AI systems that uses the corpus of knowledge that already exists to reason and resolve a wide range of complex problems [20, 21]. The expert system exhibits advantages in the recognition and identification of illnesses in addition to a strong capacity for clinical judgment. It is necessary to simultaneously consider the framework, the patient's medical background, and the doctor's educational and professional experience. Medical discoveries and information must frequently be updated in order to provide practitioners with the most recent diagnoses and treatments [22].

1.3.6 Intelligent robots

Robots with intelligence were employed in surgery in the 1980s. For instance, in 1988, prostate surgery and neurosurgical biopsies both employed PUMA 560. The US Food and Drug Administration (FDA) originally recognized ROBODOC, which was developed in 1992, as an intelligent robot. It was mostly utilized for hip replacement procedures in orthopedic surgery [23,24]. Three different robotic surgical systems, including ZUES and Da Vinci, a system that places robots automatically via endoscopes, are now approved by the FDA. Due to their accuracy, sophistication, and safety, intelligent machines are often utilized in orthopedics, urological medicine, stomatology, and other fields [25].

1.3.7 Fuzzy expert system

Fuzzy logic is an approach to reasoning, behavior, and thought that acknowledges and makes use of the fact that all that occurs in reality is a question of degree. Fuzzy reasoning understands that most circumstances would really fall into one of numerous shades of gray, as opposed to classical logic, which maintains that everything is either black or white. It gained popularity in 1965 [26], thanks to engineer Lofti Zadeh of the University of California.

1.4 Artificial Intelligence in Pharmaceutical and Healthcare Research

1.4.1 Research and Development

Pharmaceutical companies all around the world are utilizing cutting-edge ML Models driven by artificial intelligence to hasten the drug development process. Since these artificial intelligence technologies are designed to uncover nuanced patterns in vast datasets, they may be used to solve issues relating to complex biological networks [27].

1.4.2 Drug development

The application of AI has the potential to advance R&D. AI is capable of anything, from creating and finding novel compounds to target-based medication validation and discoveries [28].

1.4.3 Diagnosis

Modern machine learning algorithms may be used by doctors to collect, process, and evaluate large amounts of medical data. To securely store sensitive patient data on the cloud or other centralized storage systems, medical professionals all around the world are resorting to machine learning (ML) technology.

This acts as a representation of an EMR, or electronic medical record [29].

1.4.4 Disease prevention

Pharmaceutical companies may use AI to develop medicines for uncommon ailments as well as widespread illnesses like Parkinson's and Alzheimer's. Pharmaceutical firms normally do not devote their time and resources to this field since the return on investment (ROI) for finding solutions for rare diseases is typically rather low compared to the time and money needed to create medications to treat uncommon disorders.

1.4.5 Epidemic prediction

Today, a lot of pharmaceutical companies and healthcare organizations use AI and machine learning to monitor and forecast disease outbreaks globally. These tools gather data from a range of internet resources, examine the effects of various geological, environmental, and biological aspects on population health in various locales, and make an effort to make associations between these elements and earlier epidemic outbreaks. Such models based on machine learning and AI are especially beneficial for nations with low incomes that lack the financial and medical infrastructure necessary to tackle an epidemic outbreak.

1.4.6 Remote monitoring

It represents a milestone in the pharmaceutical and healthcare industries. Many pharmaceutical companies have already developed technologies that track patients with critical diseases using AI algorithms.

1.4.7 Manufacturing

Pharmaceutical companies may incorporate AI into their production procedures to improve output, raise efficiency, and speed up the development of life-saving drugs. AI has the potential to monitor and improve every stage of the manufacturing process, including:

- Quality control
- Tasks for predictive maintenance
- Reducing waste
- The design's optimization
- Process automation

Marketing

Artificial intelligence (AI) can be a helpful tool in pharma marketing since the pharmaceutical industry is a sales-driven sector. Pharmaceutical companies use AI to research and develop unique marketing strategies that ensure excellent revenue and company recognition [30].

1.4.8 Artificial Intelligence in COVID-19

Pyrexia (fever), a nonproductive cough (dry cough), shortness of breath, or trouble breathing are some of the signs of COVID-19. Ageusia (loss of taste), anosmia (loss of smell), bodily aches, and weariness are some possible symptoms. There have also been a few reports of episodes of diarrhea [31]. Machine learning, combined with artificial intelligence, has been the key framework in science and technology for the COVID-19 pandemic.

1.4.9 AI in Diagnosis by the Use of Radiology Images

Patients' COVID-19 infections were identified using computer tomography (CT) scans. The presentation of lesions and severity signals was controlled using the CT scan's capabilities. It looked at the terrain of imaging with radiographic structures and AI techniques. For AI data training and testing, radiological characteristics like PET, CXR, and CT were included in the study [32].

The fuzzy-based decision-making approach has been looked at in order to gauge the severity of COVID-19 in the Kingdom of Saudi Arabia (KSA). To stop the COVID-19 pandemic from spreading, a more accurate computer model for determining the severity utilizing social impact has been established [33].

An X-ray technique with an automatic system identifier for COVID-19 identification on chest images has been built using the intricate CNN architecture. In order to identify whether COVID-19 is present or not, the technique extracts feature descriptors from the chest X-ray image using a speed-up feature robust methodology and an integrated k-means clustering algorithm. The dataset for the study contained 340 X-ray radiographs and 170 photographs of COVID-19 classes that were both healthy and positive. Chest X-ray (CXR) has suggested the dilated CNN, branching design model, and VGG-16 approaches to identify the coronavirus infection. The VGG-16 used the model's front end's first ten layers to extract and apply the high-level merits [34, 35].

1.4.10 AI in Disease Tracking

Computer modeling, mathematical simulation, and information analysis are often referred to as computational biology for the progress of biology [36]. Disease dynamics modeling has helped to improve our understanding of the influence of certain traits that facilitate the spread of diseases and the role of mediation in preventing infections [37]. As a patient succumbs to their condition, their lungs start to look like glass and start to permeate. Various data-aided medication transposition approaches have been developed to locate diseases, individuals, or circumstances that might be treated with the medications used to treat various disorders [38].

One of the best strategies for improving classification performance is ensemble learning (EL). EL combines the results of several distinct deep learning algorithms that could possess special and distinctive skills. The various models are expected to act in a complementary manner when combined, producing an ensemble that performs better than the sum of its individual components and is more resilient to unreliable data [39].

Rajaraman et al [40]. pooled the predicted outcomes of nine unique DL-based models for two- and three-group classification tasks using a variety of well-known ensemble approaches. They are max voting, averaging, weighted averaging, and stacking. To enhance the model, they also recommended a repeated filtering strategy. In order to reduce model complexity without compromising model performance, the repeated filtering strategy was effective in identifying the appropriate number of layers for a given network. With no pruning and 99% with pruning, the accuracy for the three-group classification task was found to be 98%.

Additional CNN-based models for COVID-19 identification include CoroNet, CNN, COVID-CAPS, and Convolutional Capsnet, which employ the Xception26 architecture and the ResNet and MobileNet architectures, respectively [41–47].

2. AI in Pharmacovigilance

Artificial intelligence (AI) is increasingly transforming pharmacovigilance by enabling automated, scalable, and more accurate drug safety monitoring. Through the integration of machine learning (ML), deep learning, and natural language processing (NLP), AI systems can efficiently analyze large volumes of structured and unstructured healthcare data. These technologies enhance adverse drug reaction (ADR) detection, signal identification and risk assessment, thereby overcoming many limitations of traditional pharmacovigilance systems such as underreporting and delayed detection [48,49].

2.1 Adverse Drug Reaction Detection

AI-driven approaches have significantly improved ADR detection by leveraging diverse data sources such as electronic health records (EHRs), clinical trial datasets and spontaneous reporting systems. Machine learning and deep learning models can identify hidden patterns and relationships within large datasets, enabling early prediction and detection of ADRs [50].

Recent evidence suggests that ML-based models demonstrate strong predictive performance in ADR detection, with reported average area under the curve (AUC) values of approximately 0.76, indicating reliable classification capability [51].

Furthermore, integrating structured clinical data with unstructured textual information enhances detection accuracy and sensitivity. AI models can continuously monitor data streams, reducing delays in identifying potential safety issues and addressing the limitations of conventional pharmacovigilance systems [52,53].

2.2 Natural Language Processing in Pharmacovigilance

Natural Language Processing (NLP) plays a crucial role in pharmacovigilance by extracting meaningful information from unstructured data sources such as clinical narratives, biomedical literature and social media. NLP techniques including named entity recognition, relation extraction and text classification enable automated identification of drug-event associations [54,55].

Studies have demonstrated that NLP-based systems can effectively detect ADRs from EHRs and free-text clinical notes, uncovering safety signals that may not be captured in structured databases [54].

Additionally, NLP allows real-time monitoring of patient-reported data from online platforms, providing valuable insights into drug safety from a real-world perspective [56]. Advanced deep learning-based NLP models further improve performance by capturing contextual and semantic relationships in medical text [53].

2.3 Signal Detection and Risk Assessment

Signal detection is a fundamental component of pharmacovigilance, involving the identification of potential associations between drugs and adverse events. AI has enhanced this process by enabling automated analysis of large-scale pharmacovigilance databases and real-world data sources [55,56].

Traditional statistical methods are increasingly complemented by machine learning techniques that can identify complex, non-linear relationships and detect subtle safety signals [57]. AI-based models also facilitate real-time signal monitoring and prioritization, improving the efficiency of risk assessment processes [48].

Moreover, predictive analytics supports proactive risk assessment by identifying potential drug interactions and patient-specific risk factors, thereby enabling more personalized pharmacovigilance strategies [58].

2.4 Real-World Data Analysis

The use of real-world data (RWD), including EHRs, insurance claims and patient-generated data, has expanded significantly with the application of AI in pharmacovigilance. AI algorithms can analyze large and complex datasets to generate real-world evidence (RWE) on drug safety and effectiveness [48,57].

RWD provides insights into drug performance across diverse populations and clinical settings, allowing detection of rare or long-term adverse effects that may not be observed in clinical trials [57].

Additionally, AI facilitates continuous monitoring of drug safety by integrating multiple data sources, thereby improving the detection of emerging risks and supporting regulatory decision-making [49].

2.5 Challenges and Limitations

Despite its advantages, the implementation of AI in pharmacovigilance presents several challenges. One major limitation is data quality and heterogeneity, as inconsistent and incomplete data can affect model performance and reliability [54].

Another critical issue is lack of transparency and interpretability of AI models, which poses challenges for regulatory acceptance and clinical decision-making [50].

Bias in training datasets can also lead to inaccurate predictions and reduced generalizability across populations [53].

Furthermore, integration of AI systems with existing pharmacovigilance workflows and regulatory frameworks remains complex [49]. Ethical concerns, including data privacy, security and governance, must also be addressed to ensure responsible use of AI technologies [52].

Therefore, while AI has the potential to revolutionize pharmacovigilance, human expertise remains essential for validation, interpretation and regulatory compliance.

3. AI in drug discovery

3.1 Role of AI in Modern Drug Discovery

Artificial Intelligence (AI) is transforming the drug discovery process via efficient analysis of large-scale biomedical data. It helps in reducing the time and cost required to develop new medicines while improving decision-making across the development pipeline. AI supports the analysis of genomics, proteomics, cheminformatics, and patient datasets to accelerate drug discovery.By increasing success rates and reducing attrition, AI is becoming an essential part of modern pharmaceutical research [59].

3.2 AI in Target Identification

Target identification involves finding genes, proteins, or biological pathways associated with disease development. AI integrates genomics, proteomics, transcriptomics, and literature data to identify potential therapeutic targets. Machine learning models can expose hidden disease mechanisms and target relationships that may not be evident through conventional approaches [60]. This improves the selection of clinically relevant targets and increases the probability of therapeutic success.

3.3 AI in Target Validation

AI helps determine whether a biological target is suitable for drug development by predicting its action. Machine learning models identify binding pockets, including hidden allosteric sites, within protein structures. AI also evaluates biological relevance by integrating genomic, proteomic, and network-based evidence [61,62]. Furthermore, it predicts off-target interactions and possible toxicity risks, reducing late-stage failures [63].

3.4 AI in Hit Identification and Virtual Screening

AI-powered virtual screening enables rapid evaluation of millions of chemical compounds. Machine learning and deep learning models forecast ligand–target interactions and binding affinities. Compounds can be prioritized based on potency, selectivity, novelty, and ADMET properties This greatly reduces laboratory screening costs and accelerates hit discovery.

3.5 AI in Lead Optimization

Lead optimization focuses on improving the biological and physicochemical properties of drug candidates .AI predicts the effects of structural modifications on potency and selectivity [64]. Machine learning models detect possible toxicity issues such as hepatotoxicity and cardiotoxicity. AI also predicts pharmacokinetic properties, including solubility, bioavailability, metabolism, and clearance.

- **AI for De Novo Drug Design**

AI generative models can design entirely new molecules with desired characteristics.

Technologies such as Autoencoders, Generative Adversarial Networks, and diffusion models are commonly used. These approaches generate compounds optimized for target affinity and drug-likeness In silico optimization before synthesis reduces both development time and research costs [64].

3.6 AI in Drug Repurposing

Drug repurposing aims to identify new therapeutic applications for approved drugs. AI analyzes biomedical literature, omics datasets, and clinical records to identify novel indications. Because repurposed drugs already have known safety profiles, development timelines are shorter. Successful examples include AI-assisted identification of treatments for COVID-19 and several cancer-related applications [64].

3.7 AI in ADMET Prediction

ADMET prediction is necessary for assessing drug safety and efficacy during development. AI models forecast absorption, distribution, metabolism, excretion, and toxicity profiles early in the pipeline. Possible risks such as hepatotoxicity, cardiotoxicity, nephrotoxicity, and drug–drug interactions can be identified computationally. Early ADMET assessment helps reduce costly failures during clinical trials [64].

3.8 AI in Biomarker Discovery

AI facilitates the discovery of biomarkers associated with disease progression and treatment response. It integrates multi-omics, imaging, and clinical data to identify predictive signatures. Machine learning algorithms support patient stratification into molecularly distinct groups. These capabilities are fundamental to precision medicine and to the development of companion diagnostics [64].

3.9 AI in Clinical Candidate Selection

AI integrates efficacy, safety, pharmacokinetic, and biomarker information to support candidate selection [65]. Machine learning models select compounds most likely to succeed in clinical testing. Predictive analytics enables risk–benefit assessment and the estimation of clinical success probabilities. This supports productive resource allocation and portfolio management decisions.

3.9.1 Successful AI-Driven Drug Discovery Case Studies

AI-based drug discovery has produced several notable success stories.

In silco Medicine developed INS018_055 for idiopathic pulmonary fibrosis using an AI-driven discovery platform. Exscientia designed DSP-1181, among the first AI-generated drug candidates to enter clinical trials. Benevolent AI correctly identified baricitinib as a potential treatment for COVID-19 through knowledge graph analysis [65].

3.9.2 Challenges and Limitations of AI-Based Drug Discovery

The effectiveness of AI depends heavily on the availability of high-quality and unbiased datasets. Limited data, poor annotation, and algorithmic bias can affect model effectiveness and generalizability. Many advanced AI systems remain difficult to interpret, creating challenges for validation and regulatory acceptance. Adoption into pharmaceutical workflows and the shortage of interdisciplinary expertise remain major barriers [65].

4 Artificial Intelligence in Clinical Trials

4.1 Patient Recruitment

Patient recruitment is one of the most time-consuming and costly phases of clinical trials, often bringing about significant delays in study initiation. Artificial Intelligence (AI) improves this process through leveraging Machine Learning (ML) and Natural Language Processing (NLP) to analyze electronic health records (EHRs), clinical notes, laboratory reports, and patient databases to quickly and accurately identify eligible participants. AI-driven recruitment systems can greatly reduce screening time, improve eligibility prediction, increase enrollment rates, and enhance participant retention. Additionally, AI supports decentralized clinical trials through wearable devices and mobile applications, enabling remote participation and improving access to multiple patient populations. These advancements help accelerate recruitment while cutting operational costs [66,67].

4.2 Clinical Trial Design

AI is transforming clinical trial design through analyzing large volumes of historical trial data, patient demographics, disease characteristics, and biomarker information to optimize study protocols. Machine learning models can predict enrollment rates, determine appropriate sample sizes, identify relevant endpoints, and simulate multiple trial scenarios before study initiation. This allows researchers to design more efficient and statistically robust trials while reducing protocol amendments and operational risks. By enabling data-driven planning and predictive modeling, AI improves trial efficiency, shortens development timelines, and increases the likelihood of regulatory and clinical success [68].

4.3 Patient Monitoring and Safety Assessment

AI advances patient monitoring by persistently analyzing data collected from wearable devices, mobile health applications, telemedicine platforms, and electronic reporting systems. These technologies support live monitoring of physiological parameters, medication adherence, and patient-reported outcomes. Machine learning algorithms can detect early signs of adverse events and spot subtle safety concerns before they become clinically significant, allowing prompt intervention and enhanced patient safety. AI also supports patient engagement via personalized reminders, automated alerts, and compliance tracking, leading to higher adherence rates and better data quality throughout the trial [69].

4.4 Predictive Analytics and Trial Outcomes

Predictive analytics is one of the most valuable applications of AI in clinical trials. Through integrating genomic data, biomarker profiles, clinical characteristics, imaging results, and historical trial outcomes, AI models can predict treatment responses, identify high-risk patients, and estimate the probability of trial success. These data support precision medicine approaches, improve patient stratification, and enable more well-informed decision-making regarding trial continuation, modification, or termination. AI-driven predictions help refine resource allocation, reduce the costs of failed trials, and accelerate successful drug development programs [70].

5 Generative AI

Generative artificial intelligence (GenAI) marks a shift from systems that mainly recognize patterns to systems that generate new content—text, images, audio, video, code, and even scientific hypotheses using deep generative models such as GANs, VAEs, diffusion models, and transformers [71]. Recent surveys show GenAI now supports diverse domains: healthcare (medical imaging, drug discovery, synthetic clinical data) [72], education and language learning (personalized tutoring, resource creation, assessment, and writing support) [73]. Business and innovation management (new product design, marketing content, and process automation) and visualization and design tasks from data enhancement to interactive graphics [74]. Large language models and emerging multimodal models integrate text, images, and structured data, enabling powerful conversational and diagnostic tools but raising concerns over bias, misinformation, privacy, intellectual property, and accountability [75].

Across reviews, key research directions converge on improving explainability, robustness, cross-modal and multimodal generation, human–AI co-creation, ethical governance, and rigorous evaluation of real-world impact, especially in high-stakes fields like medicine and education [76].

5.1 Comparison of Generative AI and Traditional AI

Traditional AI systems (including conventional machine learning) are typically built to perform classification, regression, and decision-making tasks such as object recognition, sentiment analysis, or forecasting. Operate within predefined rules and models, mapping inputs to outputs in a relatively straightforward, interpretable way [77]. Rely heavily on task-specific training and labeled data for supervised learning [78]. Whereas generative AI systems Use deep generative models (GANs, VAEs, diffusion models, transformers) to synthesize new data that resemble training data, such as text, images, audio, and designs [79]. Aim at content creation and innovation, excelling at generating essays, images, music, product designs, and simulations, often for more open-ended problems [80]. Demand extensive data and computation, and their outputs can be novel but sometimes biased, inaccurate, or hard to predict and evaluate [81]. In summary, both share machine-learning foundations, but traditional AI is optimized for well-defined analytic tasks and efficiency, whereas generative AI emphasizes creativity, variability, and complex content generation, with greater power but also higher complexity and uncertainty [78].

5.2 Recent Advances and Applications of generative AI

Recent advances in large language models (LLMs) have rapidly accelerated the adoption of generative AI across healthcare and pharmaceutical sciences, enabling human-like text generation for tasks such as clinical documentation, medical question answering, and literature summarization [82]. Modern LLMs like GPT-3.5/GPT-4 and domain-specific medical models can pass or approach passing thresholds on medical licensing exams and match or surpass average graduate medical student performance, highlighting their potential as decision-support and educational tools [83]. In clinical practice, LLM-based systems are being piloted within electronic health records for drafting notes, discharge summaries, and insurance pre-authorization letters, as well as powering chatbots for patient communication and triage [84]. In pharmaceutical and drug R&D, generative AI and LLMs are used for mining biomedical literature, hypothesis generation, target–disease linkage, molecule and combination design, and for streamlining regulatory and clinical trial documentation, signaling a paradigm shift in drug discovery and development workflows [85]. At the same time, these advances raise critical concerns about hallucinated or obsolete medical content, bias, privacy, security, and accountability, prompting strong calls for regulatory oversight, ethical frameworks, and rigorous, domain-specific evaluation before large-scale deployment in high-stakes settings.

Future Perspective

5.3 Explainable AI

Explainable Artificial Intelligence (XAI) is expected to evolve from merely providing model interpretations to enabling transparent, trustworthy, and human-centered AI systems. Future research will focus on developing explanation methods that are more faithful, robust, interactive, and tailored to different user groups, ensuring that AI decisions can be understood and validated by domain experts, regulators, and end users. The transition from XAI 1.0 to XAI 2.0 will emphasize human–AI collaboration, adaptive explanations, and improved decision-making rather than only model transparency. Advances in explainability for large language models, foundation models, and multimodal AI systems will address challenges related to scalability, reasoning transparency, and cross-modal interactions. Additionally, integrating explainability with privacy preservation, fairness assessment, regulatory compliance, and adversarial robustness will be essential for deploying AI in high-stakes domains such as healthcare, finance, cybersecurity, and drug discovery. As AI systems become increasingly complex, XAI will play a critical role in fostering trust, accountability, ethical governance, and responsible adoption of artificial intelligence across diverse applications [71].

5.4 Precision Medicine

Artificial intelligence (AI) is expected to be a major driving force in the advancement of precision medicine by enabling the integration and analysis of vast amounts of genomic, clinical, imaging, and multi-omics data to support individualized healthcare decisions. Future AI systems will improve disease prediction, patient stratification, biomarker discovery, treatment selection, and therapeutic response monitoring through advanced machine learning and deep learning algorithms. AI-powered natural language processing and automated literature mining will facilitate rapid extraction of clinically relevant knowledge, while predictive models will enhance the identification of genetic variants and their clinical significance. The integration of real-world patient data, wearable technologies, and digital health platforms will further enable dynamic and personalized treatment strategies. Additionally, advances in explainable AI, data sharing frameworks, and ethical governance will improve transparency, trust, and clinical adoption. As these technologies mature, AI is expected to accelerate the realization of truly personalized, preventive, predictive, and participatory healthcare, ultimately improving patient outcomes and healthcare efficiency [72].

5.5 Digital Twins

Digital Twin (DT) technology is expected to revolutionize future power systems by enabling real-time monitoring, predictive analytics, intelligent decision-making, and coordinated control across grid, plant, unit, and component levels. DTs can improve economic dispatch through accurate forecasting and optimized energy scheduling, enhance wind farm performance by considering wake effects, equipment loading, and battery degradation, and support fault-tolerant operation through rapid fault detection, diagnosis, and corrective control actions. Furthermore, DTs facilitate predictive maintenance, asset lifetime estimation, and improved integration of renewable energy sources, leading to higher efficiency, reliability, resilience, and sustainability. As power systems become increasingly complex and decentralized, Digital Twins will play a key role in developing smart, self-adaptive, and economically optimized energy networks VV [73].

5.6 AI-Driven Drug Development

Artificial intelligence (AI) is expected to transform drug development by accelerating target identification, lead optimization, de novo molecular design, and predictive modeling while reducing time, cost, and failure rates. Future advancements will focus on deep learning architectures such as graph neural networks, message-passing networks, and three-dimensional symmetry-aware models for more accurate prediction of drug–target interactions and molecular properties. AI-driven generative models will enable the design of novel, biologically active, and synthetically feasible molecules through the integration of rule-based and rule-free approaches. The adoption of explainable AI, uncertainty estimation, transfer learning, multitask learning, and meta-learning will improve model interpretability and performance, particularly in low-data scenarios. Furthermore, AI-powered synthesis planning, robotics, and automated laboratories are expected to facilitate autonomous drug discovery pipelines, while the integration of multi-omics, real-world clinical data, and personalized medicine approaches will support the development of safer and more effective therapies. Overall, AI is poised to revolutionize drug development by creating faster, more efficient, and patient-centric pharmaceutical innovation [74].

5.7 Human-AI Collaboration

Human–AI collaboration is expected to evolve from simple human-in-the-loop systems to highly adaptive, intelligent partnerships where humans and AI jointly learn, communicate, and make decisions. Future systems will emphasize human-centered design, enabling users to actively participate in AI learning, reasoning, and decision-making processes rather than serving as passive observers. Advances in interactive machine learning, hybrid intelligence, explainable AI, and generative AI will foster greater transparency, trust, and adaptability, allowing AI systems to better understand human preferences, context, and goals. Collaborative environments will increasingly support continuous feedback, personalized interactions, shared decision-making, and consensus-building between humans and AI agents. Furthermore, the integration of multimodal communication, emotional intelligence, and ethical AI frameworks will enhance cooperation across healthcare, education, industry, and creative domains. Ultimately, the future of Human AI collaboration lies in creating synergistic partnerships that combine human creativity, contextual understanding, and ethical reasoning with AI's computational power, scalability, and analytical capabilities to achieve outcomes beyond the capabilities of either working alone [75].

6 Conclusion

The pharmaceutical sector has greatly benefited from the multidimensional system known as artificial intelligence. Scientists are fascinated by recent developments in AI, particularly when it comes to how it is being used in services and research in medicine and pharmaceuticals. Smart healthcare organizations and hospitals integrating AI, ML, and Big Data will determine the future of healthcare. The pharmaceutical sector, which is continually advancing technologically, will have an opportunity to lower the cost and time taken for drug development thanks to artificial intelligence (AI). Various concepts of AI are used to successfully explain how AI might be used to diagnose illnesses. In order to precisely predict a result, these AI technologies scan unstructured data and compare it to learned data, which is useful in establishing the diagnosis of a certain ailment. A few examples of how AI has been demonstrated to be an essential tool for chronic illness monitoring and therapy optimization are intelligent computer-assisted instruction (ICAI), case-specific reasoning, the vector regression method, and clinical decision support. Case-based reasoning assists in problem solving by helping in the discovery of links between variables, In order to acquire thoughtful responses from patients.

Scientists are researching every potential viral cure, and contemporary technology is always hunting for a potential treatment. It is important that technology is a part of our daily lives and that it is now being utilized to combat the coronavirus. This essay explains certain algorithms that are really employed in hospitals while highlighting the coronavirus problem. The desire to create a yardstick framework to evaluate the current approaches is also covered in the study.

The present approaches may reliably predict COVID-19 symptoms linked to various types of pneumonia using X-rays, but they are difficult to comprehend. Thus, we might infer that a variety of technological solutions are available to deal with the social and medical problems that the COVID-19 epidemic has caused. Few of these complex abilities are adequate to demonstrate any effect. A key component of COVID-19 mitigation is the CT investigation. Specifically, highly susceptible, asymptomatic patients with negative PCR data were utilized to make the initial COVID-19 viral identification. CT may be used for patient triage, deterioration evaluation, great cure estimation, and issue handling. Artificial Intelligence is remolding clinical research by boosting patient recruitment, optimizing trial design, strengthening safety monitoring, and facilitating predictive decision-making. Through advanced data analysis and machine learning, AI reduces costs, shortens development timelines, improves clinical results, and increases the probability of clinical trial success. Even though challenges related to data quality, privacy, bias, and regulatory acceptance remain, AI is expected to serve as an integral component of future clinical trials, supporting a more efficient, patient-centric, and data-centric approach to drug development.

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