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Current concepts and future perspectives of artificial intelligence in the pharmaceutical industry. A scoping review.

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Abstract

Recent years have seen a meteoric rise in the pharmaceutical industry's digitalization of data. Yet the difficulty of gathering, analyzing, and applying such knowledge to tackle complicated clinical problems is a consequence of digitization. Because of its ability to process vast amounts of data with greater automation, AI is being used for this reason. Artificial intelligence (AI) refers to a technological system that uses a collection of sophisticated tools and networks to simulate human intelligence. Also, it doesn't pose a serious threat to supplant humans in every situation where they're physically present. Artificial intelligence (AI) makes use of computers and software that can analyze and learn from data on their own to choose the best course of action for achieving goals. This review explains how its applications are rapidly expanding in the pharmaceutical industry. Data extraction was done according to the standard Cochrane systematic review methodology. Pubmed, Web of Science, Scopus, and Embase databases were searched from the year 2000 to 2022, for r'andomized clinical trials (RCT)and observational studies.

Keywords: ‘pharmaceutical’, ‘AI’, ‘machine learning’, ‘Artificial intelligence’.

Introduction

Recent years have seen a meteoric rise in the pharmaceutical industry's digitalization of data. Yet the difficulty of gathering, analyzing, and applying such knowledge to tackle complicated clinical problems is a consequence of digitization (1). Because of its ability to process vast amounts of data with greater automation, AI is being used for this reason. Artificial intelligence (AI) refers to a technological system that uses a collection of sophisticated tools and networks to simulate human intelligence. Also, it doesn't pose a serious threat to supplant humans in every situation where they're physically present. Artificial intelligence (AI) makes use of computers and software that can analyze and learn from data on their own to choose the best course of action for achieving goals. (2) This review explains how its applications are rapidly expanding in

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the pharmaceutical industry. The McKinsey Global Institute predicts that the rapid development of AI-guided automation will drastically alter the way people work.
The pharmaceutical industry is thriving on innovative ways to develop new targeted drugs and combat diseases, thanks to advancements in biotechnology and artificial intelligence (AI) practice, as well as an increase in population consumption and demands. From a patient and business perspective, there is a demand to develop efficient drugs at a lower cost. (3)
Human intelligence is related to the ability of the human brain to observe, understand, and react to an ever-changing external environment. (4)

Materials and Method

Data sources

Data extraction was done according to the standard Cochrane systematic review methodology. Pubmed, Web of Science, Scopus, and Embase databases were searched from the year 2000 to 2022, for randomized clinical trials (RCT)and observational studies, with keywords 'pharmaceutical', 'AI', 'machine learning', 'Artificial intelligence'.
Screening of eligible studies, assessment of the methodological quality and data extraction were conducted independently and in duplicate. Two reviewers evaluated the references using the same search strategy

Components of artificial intelligence

Reasoning, knowledge representation, and solution search are all part of AI's toolkit, as is the core paradigm of machine learning (ML). Algorithms developed for ML are able to spot patterns in data that has been further sorted. Deep learning (DL) is a branch of machine learning that uses neural networks (ANNs). These are made up of a network of highly complex computing elements called "perceptons," which are meant to imitate the organic neurons in the human brain and the way in which electrical impulses are carried throughout it (5). Algorithmic Neural Networks (ANNs) are composed of a collection of nodes that take in data at various points and transform it into an output, either independently or in tandem. Multilayer perceptron (MLP) networks, recurrent neural networks (RNNs), and convolutional neural networks (CNNs) are all examples of ANNs that can be trained with supervised or unsupervised methods (6, 7).
MLP networks can be used as universal pattern classifiers [11] and are useful for a wide variety of tasks such as pattern recognition, optimization assistance, process identification, and control. Recurrent neural networks (RNNs) are closed-loop networks that can memorize and retain data, like Boltzmann constants and Hopfield networks. Image and video processing, modeling biological systems, processing complex brain functions, pattern recognition, and high-level signal processing are just some of the many applications of convolutional neural networks (CNNs), a series of dynamic systems with local connections characterized by their topology [13].

Artificial intelligence and machine learning

AI incorporates the human brain's physiology and function to build intelligent systems focusing on perception, learning, and reasoning. In the pharmaceutical industry, the implementation of artificial intelligence (AI) and machine learning (ML) will aid in the understanding of target-

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disease associations, drug candidate selection, protein structure predictions, molecular compound design, disease mechanisms, the development of new prognostic and predictive biomarkers, biometric data analysis from wearable devices, imaging, precision medicine, and, more recently, clinical trial design, conduct, and analysis. (3)

AlphaFold is an artificial intelligence network used to determine a protein’s 3D shape based on its amino acid sequence. In 2020, AlphaFold released the structure predictions of five understudied SARS-CoV-2 targets, which will help in understanding pathophysiology and targeting membrane proteins. (4)

Machine-learning predictive models were also used in clinical development. These predictive models test whether the models derived from cell line screen data could be used to predict patient response to erlotinib (treatment for non-small cell lung cancer and pancreatic cancer) and sorafenib (treatment for kidney, liver, and thyroid cancer), respectively. (5) The use of AI and MI-assisted tools aids in data quality review trials. These contribute to data monitoring, the implementation of predictive analytics, and visualization for cross-database checks and real-time "smart monitoring" of clinical data quality. (2) With modern-day data collection, the demand for AI and ML techniques will increase and provide more opportunities for different scientific and other related purposes. However, practitioners must be aware that the conclusions of AI and ML methods can be misleading if not interpreted correctly with confounding factors, reliable algorithms, and clinical questioning. (1)

Hiring activity related to artificial intelligence in pharmaceutical studies

According to a recent study that looked at the quarterly percentage change in job positions in the global pharmaceutical industry, "General and Operations Managers," with a 11% share, emerged as the top artificial intelligence-related job roles in the pharmaceutical industry in Q3 2022, with new job postings increasing by 12% quarter on quarter.

Software and Web developers, programmers, and testers came in second with a share of 8% in Q3 2022, with new job postings dropping by 2% over the previous quarter. "The other prominent artificial intelligence roles include data scientists, with an 8% share in Q3 2022, and biological scientists, with a 6% share of new job postings." (6)

The use of AI technology will help pharmaceutical companies work in a more efficient environment. Pharmaceutical studies are costly and unpredictable, despite initial clinical navigation and careful testing. The implementation of AI has the ability to analyze patient records through algorithms and processing methods, thereby saving time and money and enhancing clinical trial efficacy and success. (7)

Cyclica is a biotechnology company that combines biophysics and AI to discover small molecule drugs for screening against protein pharmacological targets. They have partnered with Bayer to create faster and cheaper drugs using an AI network of cloud-based technologies, known as the Ligand Express. (8) Patients with Parkinson's disease are remotely monitored using AI-powered Medopad technology developed in the United Kingdom in collaboration with Tencent Holdings.Motor function testing can be completed in three minutes, allowing doctors to assess the severity of symptoms and schedule an appointment if necessary. (9)

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Healx is a promising startup focused on examining existing drugs to repurpose them for curing rare diseases. Using AI and ML, gathering resources, clinical trials, drug designs, multiomics data, etc., to identify a new disease target (10), the company isn't directly focused on creating new drugs to cure these conditions. Instead, they use AI technology to examine existing drugs and repurpose them for curing rare diseases. (10)

Artificial intelligence also allows for following patients and assessing compliance. Adherence to medications can be tested using a mobile phone by videotaping the patient swallowing a pill. This was adopted by AiCure Company, a New York-based mobile SaaS platform. (11) With the rising prevalence of diabetes and cancer in China, AstraZeneca has partnered with Ali Health, an AliBaba subsidiary, to use AI technology to provide patients with faster and less expensive ambulance diagnosis pickups. (12)

When matching eligible patients to clinical trials, the use of IBM Watson Technology enables coordinators to assign trials more easily. Watson helps in processing and analyzing patients' medical records and allows quicker criteria to be established. (13) Novartis is currently implementing AI and ML techniques to target drug therapy. Machine learning enables companies to identify image cells and pathologies for algorithmic and experimental trials. This will help in establishing a quicker experimental analysis worth exploring. (14)

Verge Genomics is another manufacturer that develops drugs based on targeting disease genes for complex diseases such as ALS and Alzheimer's. Using AI, Verge is able to identify new drug treatments, mapping out hundreds of genes and reducing the cost of drug development. (15)

Bayer and Merck & Co. were granted the breakthrough device designation from the FDA for artificial intelligence software that aims to support clinical decision making in chronic thromboembolic pulmonary hypertension (CTEPH). This will help radiologists assist in quicker diagnosis and better outcomes. (16)

The state of artificial intelligence in business

The top companies, in terms of the number of new job postings tracked by GlobalData as of Q3 2022, were Johnson & Johnson, Evolent Health, GSK, and Intermountain Healthcare (accounting for a total of 14%). In the US pharmaceutical industry, on the other hand, the US had the highest share of artificial intelligence-related new job postings in Q3 2022, with 73%, followed by the UK (5%), and India (3%).

Another survey in partnership with GlobalData questioned the thoughts, plans, and practices of artificial intelligence in the future among business professionals. The survey covered the importance of different aspects of AI among professionals, including its importance, awareness, replacing existing jobs with automated ones, investment costs, and the risk of cyber security. (17)

The use of nanorobots in the pharmaceutical industry

The advent of micro- and nano-electromechanical systems has opened the door to the fabrication of implantable robots for use in a wide range of applications, such as the precise administration of medications or genetic material. Nanorobots with built-in or external power sources, sensors, and artificial intelligence are attracting a lot of attention because of the astonishing developments

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in nanotechnology. Information processing, signaling, sensing, actuation, communication, the performance of biological activities at cellular levels, and targeted drug administration are just some of the ways in which these smart structures improve upon the efficacy and safety of conventional therapies. (18) Nanorobots have a lot of potential in the areas of toxin detection and theranostics. Several novel types of controlled-release drug delivery systems have been proposed for targeted therapy in a wide range of disorders, especially the chronic ones that would be of great value in personalized medicine. These include swimming microrobots for controlled delivery of drugs; transient microrobot systems for targeted drug delivery using touch- or nano-communication frameworks; and wirelessly controlled and deeply penetrable microrobots. (19)

Challenges and future prospects

State-of-the-art and high-performance approaches and improvements in computer science have improved drug screening strategies and advanced drug delivery platforms such as feedback-controlled, programmable, and microchip-based devices. However, various problems remain. Size of the drug reservoir, distribution efficiency, biocompatibility, supplying optimum drug concentrations, long-term operability, or dangers associated with improper design are challenging concerns (20, 21). Safe biomaterials and drug delivery systems with predictable drug release profiles provide prolonged and homogeneous drug concentrations, increasing patient adherence. The use of a miniature actuator increases medication reservoir without increasing device volume (22); Fully functional nanorobots for theranostics and targeted medication delivery are challenging to make (23, 24). This requires a deeper understanding of biological processes, interactions of nanorobots within the body, their movement in liquid environments, the application of appropriate algorithms for controlling against environmental perturbations, the design of cores capable of recognizing cells and molecular cues, size reduction, an appropriate power supply, propulsion, actuation, sensing, system integration, navigation control, and relabeling. In designing nanorobots, tumor heterogeneity, noise, and uncertainty should be considered. Inappropriate nanorobot therapeutic activity does not eradicate tumors and can cause harm. Concerning capsule robots, suitable power backup, locomotion, space for drug reservoirs, anchoring mechanisms, control over drug release profiles, incorporation of bi-directional communication systems, telemetry, image sensing, capacity of drug storage, theranostic activity, controlled drug release, clinical efficiency of delivered drugs, safety issues, and high costs remain challenges. Successful AI-based techniques result in stable, functional, biocompatible drug delivery systems with accurate dosage, targeted distribution, and few safety concerns. ANNs as highly adaptive nonlinear optimization algorithms and other machine learning approaches such as genetic programming, fuzzy logic, or decision trees can be applied to current drug discovery (25). ANNs have gained popularity in many scientific fields, including the pharmaceutical industry, due to their ability to model nonlinear data, solve complex problems, analyze large and multivariate data sets, make predictions, model and optimize formulation processes, design-controlled drug delivery systems, and simulate protein-protein or small molecule-protein interactions. Despite the benefits of AI tools, such as rapid and continuous performance of a variety of tasks (e.g., designing bionanorobots and controlled drug delivery),

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AI strategies can be associated with several problems, such as high costs of maintenance and repair, frequent upgrading of software, lost code recovery, system reinstating, a lack of common sense, creativity, judgment, or an appropriate response to the changing environment, and a reflection of data inaccuracy in the ANN models that may not clarify variable correlation. Developing a reliable ANN model requires a vast amount of data and a large sample size. ANNs can model complicated datasets and predict clinical treatment response but selecting appropriate algorithms or datasets might be difficult. Despite machine learning-based models' ability to speed up drug discovery, rational drug design, target prediction, and the development of safer drugs, integrating experimental procedures and in silico simulations and developing interpretable machine learning models are necessary to reduce false negative or positive predictions (26).
The availability of high-quality, up-to-date data is another challenge associated with AI, since the two go hand in hand with large data collection and processing. As the foundation of AI is the creation of predictive models, the presence of noise in the training data can affect the accuracy of the models that are created from it. Drug manufacturers could take action by instituting strict policies on the quality and handling of data. Another is group work, which can increase the availability of high-quality shared data resources. For more precise forecasting, they should include both successful and unsuccessful drug development attempts. These massive datasets can also be combined to serve as feature data, training data, and validation data for the associated algorithms. Combining several data sources strengthens and refines these algorithms' results.

Conclusion

Drug development takes a long time and involves cost; therefore, new methods and approaches need to be used. Massive amounts of multivariate data present tremendous opportunities for AI technologies to analyze, solve, classify, model, accelerate, and discover biomarkers, drug targets, potential drug candidates, and their pharmacological properties, relationships between the formulation of drugs, and more. Application of AI-powered platforms for matching patients with the most appropriate clinical trials may greatly minimize errors and enhance cost-effectiveness, in addition to generating novel therapies with desired features. The development of more efficient medications or delivery systems is facilitated by the analysis of large-scale molecular information and data links, which reveal novel insights into the molecular mechanisms of diseases and variables impacting cell or tissue function. In this way, AI would play a significant role in both the drug discovery process and personalized treatment.

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