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Artificial Intelligence (AI) in Drug Discovery and Medicine

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Abstract

Artificial intelligence (AI) is a branch of computer science that deals with the development of algorithms that seek to simulate human intelligence. The phrase "artificial intelligence" was likely coined during a conference at Dartmouth College in 1956. The earliest work of medical AI dates back to the early 1970s. Over years, AI has found implications in various fields. In this article, we summarize its applications in drug discovery and medicine.

Keywords: ***Artificial intelligence; Drug discovery; Medicine; Machine learning; Deep learning***

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Introduction

Artificial intelligence (AI) means simulation of human intelligence process using computers. The process comprises acquiring information, developing rules for using the information, drawing approximate or definite conclusions and self-correction. AI comprehends a subfield called machine learning (ML) which involves use of statistical methods with the ability to learn with or without being explicitly programmed [1]. A further subfield of ML called deep learning (DL) which incorporates artificial neural networks that adapt and learn from the vast amount of experimental data. The remarkable difference that makes DL a subfield of AI is the flexibility in the architecture of neural networks such as convolutional neural network (CNNs), recurrent neural networks (RNNs) and fully connected feed-forward networks [2].

AI is and umbrella term that encompasses multiple components, our focus in this article is to highlight its applications in drug discovery and medicine in brief.

Drug discovery

Technologies incorporating AI have become versatile tools which can be applied universally in various stages of drug development, including identification and validation of drug targets, designing of new drugs, drug repurposing, aggregating and analyzing biomedicine information and refining decision-making process to recruit patients for clinical trials [3]. Other uses of AI in drug development include prediction of feasible synthetic routes for drug-like molecules [4], pharmacological

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properties [5], protein characteristics as well as efficacy [6], drug combination and drug-target association [7] and drug repurposing [8]. Also, identification of new pathways and targets using omics analysis has become possible via the generation of novel biomarkers and therapeutic targets, personalized medicine based on omics markers and discovering connections between drugs and diseases has progressed rapidly [9]. DL has proved outstanding success in proposing potent drug candidates and accurately predicting their properties and possible toxicity risks [10].

AI platforms which can predict on- and off-target effects and in vivo safety profile of compounds before they are synthesized include DeepTox (predicts toxicity of new compounds) and PrOCTOR (predicts the probability of toxicity in clinical trials) [11,12]. Another AI tool, Read-Across Structure-Activity Relationships (RASAR) [13], which links molecular structures and toxic properties by mining a large database of chemicals could accurately predict toxicity of unknown compounds.

A novel AI platform called AiCure is a mobile application to measure medication adherence in a Phase II trial of subjects suffering from schizophrenia. It was reported that AiCure increased adherence 25% compared with the traditional 'modified directly observed therapy' [14]. AI predictive modelling in selection of a patient population would increase success rate in clinical trials [15].

Medicine

Oncology

For classification of skin cancer, researchers used convoluted neural networks (CNNs) to classify tumours in an automated manner. They confirmed that classification of tumours is possible based on generated images because of variability in appearance of skin lesions [16]. Skin cancers are usually detected using clinical screening and dermascopic analysis, followed by biopsies and histopathological analysis. However, using pixels and disease labels as inputs, CNNs are able to effectively identify and classify cancers in a much less time-consuming approach [17].

Once cancer has been diagnosed, analysis of tumour volume is crucial for deciding the treatment protocol. Tumour segmentation was traditionally time-consuming, CNNs make the process of tumour segmentation much simpler and more accurate. CNNs were used for segmentation of brain tumours, inputs for CNN being patches extracted from images to form a hierarchy of complex features using trained networks [18].

Radiology

A CNN to assess bone age based on pediatric hand radiographs was able to estimate age with accuracy similar to that of a radiologist [19]. AI based computer aided detection (CAD) is regularly used in breast cancer screening programs in the USA, providing a second opinion to radiologist's initial read of mammograms [20]. Combination of CAD with radiologist has reliably been found to improve nodule detection rates in both chest radiography [21] and CT [22] compared with either CAD or radiologist alone.

Ophthalmology

A CNN was trained to screen diabetic retinopathy (DR) and its performance was comparable to that of a panel of certified ophthalmologists [23]. A CNN applied to Optical Coherence Tomography (OCT) could successfully differentiate cases with advanced age-related macular degeneration (AMD) or diabetic macular edema, which require timely treatment, from less severe cases [24]. A CNN has been trained on retinal fundus images to predict cardiovascular health risk factors such as high blood pressure and performed as well as the methods that require invasive blood tests to measure cholesterol levels [25].

Cardiology

A CNN to map a sequence of electrocardiogram samples to a sequence of rhythm classes and its performance in detecting a wide range of heart arrhythmias was reported to be superior to board-certified cardiologists [26]. Deep learning models were able to accurately predict pathological events using representation of patients entire original electronic health records. The records were effectively used to predict the need for palliative care, in-hospital mortality and unplanned readmission [27].

Internal medicine

Several studies have emphasized growing role of AI in internal medicine and care of patients in intensive care unit [28]. Sepsis is a common cause of morbidly and mortality in critically ill patients. The Artificial Intelligence Sepsis Expert algorithm was developed to precisely predict onset of sepsis in ICU patients 4-12 hours before clinic recognition [29]. InSight uses AI algorithms to predict onset of sepsis before clinical recognition [30].

Neurology

AI was found advantageous in identifying multiple sclerosis with optical coherence tomography (OCT). A study demonstrated that measurements of the retinal nerve fiber layer thickness obtained via OCT is able to detect patients with multiple sclerosis using an artificial neural network better than any single OCT parameter [31]. A potential application of AI is in assessment of brain tumors through automatic and reliable segmentation methods of large amount data produced by patient's magnetic resonance imaging [32].

Pulmonology

A machine learning program designed for early detection of chronic obstructive pulmonary disease (COPD) exacerbations and subsequent triage, the model's accuracy and safety indicators surpassed that of individual pulmonologists in identifying exacerbations and predicting triage in 101 cases [33]. AI has potential to play a significant role in diagnosis of tuberculosis [34].

Conclusion

Experts strongly believe that AI will permanently change the pharmaceutical industry and the approach to discover new drugs. With AI, the possibility of linking regenerative medicine with pharmacology and gene therapy emerges. AI has the potential in medicine to improve quality of care for specialties and rare diseases through screening, evaluation, and treatment suggestions. Developing a deeper understanding of underlying theories in AI will allow us to provide best possible patient care in the near future.

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