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Artificial intelligence in drug discovery

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AI has been an important driver for many new business innovations like web search, content references, product recommendations. Dr Amit Gangwal, Associate Professor, SVKMâ??s Institute of Pharmacy, Dhule, Maharashtra , gives an insight



Artificial intelligence (AI), particularly deep learning (DL) domain, has gained huge accomplishment in a wide range of uses like computer games, natural language processing, speech recognition, computer vision, driverless vehicles, automated interfaces for visual perception, decision making, translation between languages and others. None of the fields is untouched by AI. AI and robotics are no longer science fiction, they are transforming healthcare, though a bit late versus other fields for instance automobile, gaming, telecom, banking and financial markets, e-commerce, manufacturing, education, supply chains, marketing and others.

At present, there is no challenge to AI. For AI (actionable insights) one has to resort to AI (artificial intelligence) only. AI is getting progressively sophisticated at doing what human experts do, but more competently, more quickly and at a highly competitive cost. Within the technology industry, AI has been an important driver for many new business innovations like web search, content references, product recommendations etc.

According to a report published by Accenture, “Explainable AI won’t replace human workers; rather, it will complement and support people, so they can make better, faster, more accurate decisions”. AI technology can enhance business productivity by up to 40 per cent.

According to another assessment (by research firm PWC), “by 2030, the global GDP could rise by 14 per cent as a result of AI-enabled activities. That is equal to $15.7 trillion."

It is therefore not an exaggeration to say that AI is changing our everyday life. Lately, there is increasing interest in exploring AI, machine learning (ML and its subtype, DL) for discovering drug molecules for various diseases and in predicting reactions and retrosynthetic analysis besides other domain-specific applications. AI has its say in almost all the departments of health industries and institutions; may it be medical imaging (AI-driven interpretation of various medical scans), drug discovery (including clinical trials), drug repositioning, QA, marketing, sales, production, pharmaceutical analysis and others.

Current AI techniques include ML methods and DL models. The much talked about the term, ML, was coined by IBM’s Arthur Samuel in 1959. According to him, “Machine learning is the field of study that gives computers the ability to learn without being explicitly programmed.”

Professor Samuel was an AI pioneer and employee at IBM. Finally, DL is a subtype of ML that uses layers of artificial neurons, called neural networks, and has established improved performance versus standard computer vision algorithms.

The potential for both AI and robotics in healthcare is vast. Just like in our everyday lives, AI and robotics are gradually becoming a part of our healthcare system, very much like e-commerce websites or streaming platforms analysing our browsing and purchasing history before serving us highly customised data using various ML and DL models.

The ever-accruing data generated like never before, in clinics, pathologies permits and encourages more applications of AI, ML and DL. Similarly in pharmaceutical industries, a huge amount of data is generated from each and every step involved in drug discovery and development ranging from lead identification to post-marketing surveillance. High-speed Internet connectivity, lightning fast-parallel processing computing unit (that is graphics processing units-GPUs), collaborations with cross-functional teams (like AI, tech, pharma and medical) and decentralizsed data access (unlike data silos) through

federated machine learning (still widespread application is limited) are among the major catalysts behind widespread and faster acceptability of AI across the domains. These applications have changed and will continue to evolve the way both doctors and data scientists approach clinical problem-solving.

A sizable number of AI companies are developing and deploying their patented-inhouse developed tools like AI platforms and algorithms. These proprietary products are laced with such powerful functionalities (to assist, guide, empower and complement experts belonging to various health or medical fields) as drug discovery, insights in clinical trial studies, diagnosis through medical imaging. Interestingly few companies showed openness to collaborate with pharma majors (like Novartis, Pfizer, GSK, Roche, AstraZeneca and others) or health majors and few are using their proprietary products for generating insights for their own team, engaged in drug discovery, medical imaging and clinical trials.

Biopharmaceutical companies continue to make significant investments in AI and ML to both improve their decision making across R&D and commercialisation, and to deliver better outcomes for patients, physicians, and payers. Pharmaceutical industries are not an exception and though late or through some tie-ups, various organisations are hugging AI tools in various stages of drug discovery like lead identification, target study, clinical trials. Two major routes are being used by drug discovery scientists for AI-driven or mediated drug discovery: de novo drug design and drug repurposing.

Two major organisations which deserve a special mention here are Exscientia and Insilico Medicine. These are creating headlines the world over by leveraging AI in the drug discovery process (in target selection, ligand selection and Insilico Medicine in a clinical trial as well) through their in-house developed patented AI technologies. It is inevitable to study AI in drug discovery and not to discuss these two big, as these two are beacons not only for AI companies engaged in drug discovery but also for pharma giants. Their frequency of announcing breakthroughs is matchless. In two separate developments in January 2022, Insilico Medicine and Exscientia announced strategic alliances with Fosun Pharma and Sanofi respectively.

Yes, AI-driven drug discovery has a promising future but like other innovations or disruptive innovations, it has also some limitations or hiccups as the technology has gone far ahead in other fields but in the case of drug discovery it is pretty new and has to taste success through clinical trial routes and even after that also.