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Disrupting drug discovery

How artificial intelligence is transforming drug research

IBM Institute for Business Value

The impact of drug discovery

Scientific breakthroughs, such as the discovery of antibiotics and development of vaccines, have saved countless lives. However, the process of bringing a drug to market can now take up to 15 years at costs approaching USD 2.6 billion.[1] To help accelerate drug discovery, leading organizations and researchers are turning to artificial intelligence (AI) because of its ability to reveal hidden patterns and predict novel connections in biomedical data at a scale no human or traditional computing methods could possibly achieve.

Separating hope from hype

The process of drug discovery is difficult for many reasons, including the complexity of biology, the interconnectedness of biological systems and the internal and external factors that influence them. One approach to simplifying complexity is specialization. Scientists focus by system or therapeutic area, sometimes favoring depth of knowledge at the expense of breadth. However, accumulating evidence now suggests that various diseases, such as diabetes, heart failure, inflammation and cancer, are in fact interconnected, blurring established categorizations.[2] This issue highlights the need for capabilities beyond human expertise to holistically discover and analyze biological systems at scale. Working in concert with researchers, AI has the potential to both dramatically reduce costs and accelerate the speed of new discoveries.

AI use cases and data sources

AI platforms are especially powerful across the following domains:

- Predictions of new relationships between biological entities, such as drug-target, gene-disease, drug-adverse event, gene-pathway predictions for use cases – such as target identification, indication expansion of a drug or toxicity predictions.
- Clinical trial design, including optimizing clinical trial patient selection and stratification, biomarker measurements, duration and recruitment.
- Increasing confidence in existing knowledge and information, such as evaluating the certainty of biomedical knowledge.
- Personalized medicine, including patient stratification and designing and delivering the right treatment to the right patient.

AI platforms also can help researchers integrate and create value from a multiplicity of data sources:

- Unstructured data or knowledge sources, such as biomedical literature, text books and patents.
- Structured databases with classification based on features or biological concepts, such as drugs, chemicals, diseases, genomic, metabolomic, proteomic and biomarker data.
- Clinical data from unstructured and structured data sources, such as prescription claims, electronic health record data, clinical trial data and toxicology reports.
- Imaging, such as radiologic images, computed tomography (CT), magnetic resonance imaging, positron emission tomography (PET), PET-CT, ultrasound, x-ray and histologic images of cells and tissues.
- Data derived from computing devices embedded in everyday objects, including from the Internet of Things.

Repurposing drugs to treat Parkinson's disease

Parkinson's disease was first described more than 200 years ago, and a large volume of literature and knowledge exists regarding the disease. However, current treatments only manage symptoms and can't slow the disease progression. Thanks to AI, researchers are now looking at drugs already approved and used for other indications as potential options for treating Parkinson's and related conditions.[8] Because AI can decrease bias, hypotheses can be generated that might otherwise seem unlikely. Testing these hypotheses has the potential to reveal new solutions to old problems. For example, unwanted movements, or dyskinesia, are a debilitating side effect of medications typically used to treat Parkinson's, affecting up to 90 percent of patients. Canadian Researchers at University Health Network fed approximately 40 years of research and about 3,500 candidate drugs into an AI system. The top 5 percent of ranked candidate drugs resulted in the discovery of six candidates with novel yet plausible antidyskinetic mechanisms of action.[9]

Years of applying AI to biomedical challenges have helped researchers see orthogonal connections that traditional approaches would have missed.[3] For example, in 2014, biologists and data scientists at the Baylor College of Medicine used AI to identify an important protein related to many cancers. The AI system analyzed more than 70,000 papers in a matter of weeks. Researchers reading five papers per day would have taken nearly 38 years to achieve the same result.[4]

Although AI approaches can have a powerful impact, they do have limitations. Machine learning can prioritize and improve decision-making, but it doesn't replace laboratory and clinical validation. At this point, no AI-inspired, FDA-approved drugs are available, although preclinical experiments are underway.[5]

Creating value from mountains of data

Scientific advancement relies on data, but large volumes of data pose challenges to researchers. According to a recent study by the IBM Institute for Business Value, 84 percent of life science organizations realize value from both structured and unstructured data.[6] Researchers struggle to keep up with the literature, patents and other unstructured data in their own fields, and they often overlook other scientific areas that might enhance or inform their efforts. Nearly 80 percent of the data in the 1.2 billion clinical care documents that the US produces annually is unstructured.[7] Most medical breakthroughs aren't made in isolation, so it's prudent to integrate knowledge from distinct organizations and fields of study.

AI can parse and analyze large volumes of data and supports robust capabilities for data harmonization. In drug discovery, scientists can use AI to help with activities such as target identification, drug design and drug repurposing. The role of AI in this process is to augment scientists' abilities rather than replace them. Scientists play a crucial role in determining the data to use in AI analyses and provide expert evaluation and due diligence on the results. Traditional drug discovery can assess only a finite set of experiments or evidence at one time, which increases the potential for bias. But AI methodologies can help researchers avoid the implicit bias that arises when only limited, local data is used to draw a conclusion. AI in drug discovery also supports adoption of new types of analyses that aren't possible with traditional methods.

Collaborating to uncover insights

Isolating causative factors in ALS research

Amyotrophic lateral sclerosis (ALS) researchers have discovered certain genetic mutations that can be causative or risk factors for the disease. However, researchers don't know all of the genetic associations that might increase the likelihood of someone developing ALS. With AI, researchers can gain insights into not only genetic associations, but also the complexity of how the genome interacts with other factors, such as where a person resides or his or her occupation. Over time, AI systems improve as more data is brought in and as the reasoning approaches become richer and more accurate. In this way, AI systems can help discover new insights and capture them in a way that readily transfers to other problems.[10]

AI is able to bring together data sets using information from different patient cohorts and across a broad base of literature. With AI, it's possible to look at questions that have never been considered before. Taking advantage of technology to track and evaluate a broader spectrum of scientific publications can encourage collaboration among specialists and increases the likelihood of identifying unlikely connections across various fields.

New collaborations can be facilitated in several ways. One possibility is the creation of AI "institutes" with a particular focus, such as neurodegenerative diseases. An institute could act as a central hub that connects researchers to experts focused on AI in their fields in addition to researchers and organizations outside their typical networks, such as patient advocacy groups or specialized research organizations. Methods for discovering unique connections between fields can be developed in addition to a network of connections to researchers interested in forging those connections with AI.

Looking ahead

A variety of AI tools are available to help researchers today. Many of these tools are still in their first iteration and will continue to evolve. But as AI reaches more consumer markets, it will be incorporated into the workflow of more researchers and offer intelligent and enriched alternatives to traditional literature searches and painstaking analysis of isolated data.[11] The goal is to make AI available directly to scientists, so new use cases can be found and new problems solved. The potential rewards might be profound, including the expansion of knowledge and new medical and drug breakthroughs.

As you consider incorporating AI into your discovery research, consider these questions:

- What are you doing to focus on the most important information and filter out extraneous or irrelevant data?
- How holistic is your research approach? Are you looking broadly and deeply?
- Could your research be limited by your own biases? How can you increase the speed and efficiency of your research?

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Notes and sources

1 "Biopharmaceutical Research Industry 2018 Profile." Pharmaceutical Research and Manufacturers of America. April 2018. http://phrma-docs.phrma.org/industryprofile/2018/pdfs/2018_IndustryProfile_DynamicResearchandDevEcosystem.pdf

2 "Cardiovascular Diseases and Diabetes." American Heart Association. January 29, 2018. http://www.heart.org/HEARTORG/Conditions/More/Diabetes/WhyDiabetesMatters/Cardiovascular-Disease-Diabetes_UCM_313865_Article.jsp#.WyKmXVMvyRs; Coussens, Lisa M. and Werb, Zena. "Inflammation and cancer." Nature. December 19, 2002. Abstract U.S. National Library of Medicine. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2803035/

3 Bakkar, N., Kovalik, T., Lorenzini, I. et al. "Artificial intelligence in neurodegenerative disease research: use of IBM Watson to identify additional RNA-binding proteins altered in amyotrophic lateral sclerosis." Acta Neuropathol. 2018. Abstract. https://link.springer.com/article/10.1007/s00401-017-1785-8

4 "IBM Watson Ushers in a New Era of Data-Driven Discoveries." IBM. August 28, 2014. https://www-03.ibm.com/press/us/en/pressrelease/44697.wss

5 Buvailo,Andrii. "Artificial Intelligence In Drug Discovery: A Bubble Or A Revolutionary Transformation?" Forbes Technology Council. August 3, 2017. https://www.forbes.com/sites/forbestechcouncil/2017/08/03/artificial-intelligence-in-drug-discovery-a-bubble-or-a-revolutionary-transformation/

6 IBM Institute for Business Value. "Fast start in cognitive innovation: Top performers share how they are moving quickly." Unpublished data. https://www-935.ibm.com/services/us/gbs/thoughtleadership/cognitiveinnovation/

7 Schneider, John. "More than meets the eye: Unstructured data's untapped potential." Health Care Dive. https://www.healthcaredive.com/news/more-than-meets-the-eye-unstructured-datas-untapped-potential/435352/

8 Johnston, T., Lacoste, A., Visanji, N. et al. "Repurposing drugs to treat l-DOPA-induced dyskinesia in Parkinson's disease." Neuropharmacology. June 1, 2018. https://www.sciencedirect.com/science/article/pii/S0028390818302703

9 "How one Parkinson's patient drove a groundbreaking research effort." IBM. https://www.ibm.com/thought-leadership/passion-projects/parkinsons-watson-drug-discovery/

10 "Artificial Intelligence: The Next Frontier in Drug Discovery." Fortune Knowledge Group. 2018. https://fortunefkg.com/wp-content/uploads/2018/04/FKG_IBM_WATSON_DISCOVERY_WP_4_23.1813.pdf

11 Buvailo,Andrii. "Artificial Intelligence In Drug Discovery: A Bubble Or A Revolutionary Transformation?" Forbes Technology Council. August 3, 2017. https://www.forbes.com/sites/forbestechcouncil/2017/08/03/artificial-intelligence-in-drug-discovery-a-bubble-or-a-revolutionary-transformation/