CPQ Medicine (2018) 3:4
Perspective

Leading Edge Artificial Intelligence Empowering Therapeutics Discovery

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Received: 03 October 2018

Published: 29 November 2018

Keywords: *Artificial Intelligence; Drug Discovery; Structured Data; Unstructured Data; Machine Learning; Deep Learning; Robotics; Natural Language Processing; Image Processing; Speech Recognition; Big Data Analytics; Predictive Modeling; Statistical Analysis; Precision Medicine; Clinical Trials*

Foundational Perspective: Brief Overview of Artificial Intelligence-Driven Platforms

The Big Picture of AI-Driven Technology

First progresses in artificial intelligence (AI) start with the cybernetics era. The symbolic approach through rules-based techniques evolved later to the statistical framework as a result of the breakthrough in neural network design. This approach substantially increased accuracy in natural language processing (NLP) and computer vision, hence revolutionizing AI research.

In a few words, AI allows machines, including computer systems and robots, rendering intelligence through algorithms by creating cognitive systems. Machines acquire the capability to learn from deducing patterns on raw data by recognizing model variables entailing sample inputs. These cognitive systems can process, analyze, and scale data, and communicate seamlessly with other interconnected machines, while making actionable decisions independently, that is, no demanding human intercession. This process is known as machine learning. Deep learning is a machine learning technique that trains machines and software applications to unveil high-level information hidden among large amounts of data.

Like humans, machines learn from past own experiences, which suggests the concept of incremental intelligence, mimicking human intelligence, but at the speed of a computer! Such a disruptive synergy between human knowledge and computational performance has given place to a breakthrough, game changing technology, capable of empowering all the industries, including the pharmaceutical sector [1].

The Role of AI in the Drug Discovery Space

In particular, the drug discovery space is prone to be greatly benefitted from the empowerment of machines and applications with human-like cognitive capabilities. Most unresolved problems in the drug discovery space require machine learning, smart reasoning, problem solving, intelligent planning, and model self-correction. AI is dramatically exploiting automated decision making processes by using highly accurate and accelerated data driven, intelligent, self-learning models [2]. Indeed, many pharmaceutical and biopharmaceutical companies are carrying out the development of a varied number of potential cures for multiple diseases, including severely underserved areas such as rare and chronic diseases. New predictive and prognostic solutions obtained by deploying AI-driven platforms are helping life scientists and medical researchers to identify optimal therapeutic targets.

Early stage drug investments are multi-billionaire [3]. Therefore, AI-driven platforms focused on drug repurposing and drug combination therapies are becoming extraordinary relevant in the life-cycle planning and the portfolio growth agenda of most important market participants. In fact, clinical trials are demonstrating that combination therapies, usually from co-development, are resulting in better efficacy [4]. Hence, companies that internally develop combination therapies can leverage AI-driven platforms to maximize the potential synergy of drugs.

AI-driven platforms work with huge databases containing a plethora of information from genes, gene mutations, protein targets, molecules, signaling pathways, disease events, clinical records, clinical trials, allowing matching this information to find hidden drug-disease correlations.

AI-driven technology is inspiring companies to develop therapies for severely underserved therapeutic areas. Coordinated efforts between database holders, AI developers and drug manufacturers will facilitate early development and market access of much new therapeutics.

The Road Ahead: Groundbreaking AI-driven Precision Medicine

AI-driven Platform Technologies Paving the Way of Precision Medicine

A technology opportunity engine recently published by Frost & Sullivan [5] provides several insights from the investigation of AI-driven platforms energizing the pharmaceutical industry. The rise in the demand for deep learning solutions, the dominance of machine learning in the market, the increasing number of startup companies and research organizations for R&D, and the use of robotics in the treatment of chronic disease conditions and aging population are significantly driving the market.

The advent of new technologies coming from the technology synergy among bioinformatics, systems biology and structural cell biology tools, in addition to computer science, material sciences, and traditional medicinal chemistry constitutes a key factor of success of AI-driven solutions in drug discovery. The utilization of gene editing techniques is presently expanding fast across human therapeutics, leading to disruptive innovations, as it is evidenced in the forecasted growth rate for the coming years accelerated by the introduction of AI-driven genomics.

Although many challenges remain to be addressed to effectively provide real world solutions driven by AI-based technologies, a vibrant ecosystem is observed involving all the stakeholders in the space, from government authorities, regulatory bodies, venture holdings, academic centers, research hospitals, clinical institutions, healthcare payers, patients and care givers, to medium and large pharmaceutical companies, innovation labs, startups and spinoffs, data analytics and artificial intelligence companies, committed to deliver innovative precision medicine-based technology platforms [6,7].

According to Frost & Sullivan, AI, including machine learning and deep learning approaches, among many other branches of AI, is prone to lead a significant positive traction across the pharmaceutical industry, leaving behind years of trial-and-error, blockbuster drug development. AI-driven platforms are starting to become precision medicine a reality [8]. Optimally designed to identify new therapeutic targets and create novel molecules while minimizing drug screening time and enhancing patterns identification, AI-driven platforms are revolutionizing drug discovery. Precision medicine is facilitated by accessing the best suited drugs for each specific therapy and identifying therapeutic applications for repurposed drugs.

The path toward success involves six critical points for discussion [9]:

• **Opportunities:** Structured and unstructured data from multiple sources can be dramatically leveraged by establishing new correlations between molecular/biological entities and disease onset and progression.

• **Collaboration:** Strategic collaborations between AI-driven companies and large pharmaceutical companies is expected to generate a solid AI-based pipeline, thus addressing new therapeutic areas at reasonable and affordable costs.

• **Reimbursement:** Reimbursement challenges may be extraordinarily overcome by empowering drug discovery and development with AI-driven technologies.

• **Regulation:** AI-driven platforms leverage data from ongoing clinical trials, thus allowing illustrating the optimal pathways for further clinical validation planning and development.

• **Clinical Trials:** AI-driven platforms strongly facilitate patient recruitment for clinical trials thanks to the access to extremely large databases, so that eligibility may be instantaneously determined.

• **R&D Innovation:** AI-driven platforms help multiple companies to take advantage of machine and deep learning approaches for ground work on scientific literature, clinical outcomes, dissertations and proceedings, drug profiles, facilitating investigation, hence leaving truly creative tasks to scientists.

Clinical Translation: Technology Transfer and Innovation Ecosystem

Technology Adoption in the Development of New Therapeutics

Frost & Sullivan's intellectual property (IP) assessment on AI-driven platforms protection reveals that most patent fillings are associated with the following five trends [9,10]:

• **Data Mining:** results for the period 2012-2017, deliver a total of 6,528 granted patents deeply associated with data mining technology innovations, from which, approximately, 3,065 patents and patent publications mention their applicability into drug discovery applications.

• **Visual Maps:** A continuous increment in patenting activity during the past 5 years has been evidenced, totaling patents and patent publications in 17,690. Around 4,671 publications are applied to complex biology visualization.

• **Novel Algorithms:** patent protection related to the development of innovative algorithms is tersely knitted to clinical and therapeutic applications involving specific target applications such as drug discovery, totaling 7,836 patents.

• **Optimization:** the number of patents issued has increased substantially over the past five years. Simulation and optimization computational frameworks evaluating uncertainty are growing significantly fast, totaling 7,352 patents.

• **Numerical Models:** Numerical simulation techniques constantly adapt to novel challenges. A total of 13,012 patents that have been granted between 2012 and 2017 related to numerical simulation solutions for drug discovery models.

Final Remarks

AI is dramatically impacting the entire drug discovery and development landscape, from the very basic life science research to clinical trial and regulation approval steps leading to final commercialization.

AI-driven platforms have the ability to exploit enormous sets of multisource data to transform them into valuable, usable and actionable decisions. AI-driven platforms have the ability to empower both science and business, hence providing end users with the broadest spectrum of solutions conceivable.

Both large pharmaceutical companies and start-up companies are implementing AI-driven drug discovery platforms. This fact is heavily evidenced through the advent of new collaborative partnerships between leading pharmaceutical and biopharmaceutical companies and expert participants in the AI space, worldwide.

Acknowledgements

I would like to thank all contributors from industry involved with the development and delivery of this article from the TechVision Group at Frost & Sullivan.

Biolography

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