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Archives of Pharmacology and Therapeutics Commentary

Artificial Intelligence in Pharma: Positive Trends but More Investment Needed to Drive a Transformation

Peter Henstock*

Pfizer Inc., New York City, USA

*Correspondence should be addressed to Peter Henstock; peter.v.henstock@pfizer.com

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Abstract

Pharmaceutical companies have been actively adopting artificial intelligence (AI) approaches for drug discovery and are starting to focus this technology on clinical trials. The shift from large-scale collaborations to smaller strategic partnerships and recently to internal teams has led to increased headcounts that are being organized to deliver AI across the enterprise. Although the urgency of the COVID-19 could have been a perfect test case for leveraging AI, it drew awareness to the obstacles of data access. As data pipelines have already started to overcome these limitations, the next step to adoption will be to embrace the opportunity for AI to serve as a data-driven complement to scientific processes. Although pharma's AI investments remain tepid, the improving rates for funding AI initiatives are encouraging. With further investment and the increase in new AI techniques directed at pharma R&D challenges, AI has the potential to be a transforming force across the industry.

Keywords: Artificial intelligence (AI), Machine learning, Pharma, MLOps, COVID-19

Introduction

Over the past few years, pharmaceutical R&D has become aware of the potential benefits of leveraging artificial intelligence and its collective subfields including machine learning, deep learning, data science and advanced analytics. These technologies are being embraced across industries to provide enhanced automation, gain insights into data, and improve data-driven decision making. The evangelization from lower level technical experts has now been echoed by the top levels of many organizations, as exemplified by Vas Narasimhan's (Novartis CEO) goal to evolve AI to place it at the "heart of the company" [1] and Alex Bourla's (Pfizer CEO) aim to win the digital race in pharma using machine learning and AI to expedite R&D [2]. Although its value compared to pure science continues to be questioned, machine learning and particularly deep learning have introduced many compelling use cases.

A few short years ago, AI approaches were making waves across industries. Pharmaceutical companies were scrambling to identify ways of applying this new technology to its industry problems [3]. During this time, most major pharma engaged in large-scale top-down collaborations with AI giants such as IBM Watson and others [4,5] since internal AI capability was perceived as scarce. The BenchSci blog has tracked the various pharma AI partnerships including academic partnerships and various consortia memberships [6]. This phase was followed shortly by a bottom-up phase that engaged a sea of smaller companies that offered some form of general or industry-specific AI solution. Since AI became a crucial selling factor, existing companies also shifted or tweaked their product lines to include AI capabilities. With low start-up costs for cloud computing and AI, this rapidly developing industry posed a challenge to pharma in differentiating the offerings and evaluating the merits of the various AI solutions with limited internal resources. The collaborations and partnerships have become so abundant that the BenchSci blog announced in April 2020 that it "can no longer keep up with the growing number of startups using AI" that have partnered with pharma.

The initial partnering and excitement around AI has led to an increased awareness of the potential opportunities. New cutting-edge AI solutions for scientific workflows are periodically met with both excitement and skepticism requiring results be re-proven for every problem variation.

However, the IT/informatics and innovation groups are moving quickly toward AI through the corporate Digital transformations. Statistics and computational scientists are also paying more interest, shifting toward Leo Breiman's dual cultures [7] of model- and data-driven methodologies.

Evolving AI Organization

As the number of AI practitioners has increased across pharma, one challenge has been how to build and organize these new teams. In the pharma and life sciences fields, AI experts need to have not only the computer science scripting skills and math/statistics skills for machine learning, but also need subject matter expertise due to the nature of the work [14]. Finding those talented individuals with this combination of skills is still equated to chasing unicorns, despite the proliferation of academic and industry training programs in data science. The initial generic guidance of choosing diverse teams [8] has given way to a more specialized structure.

In the pharmaceutical space, the deep scientific focus impacts the organization of teams. Pharma doesn't have the equivalent of an Amazon recommendation engine division that tailors ads to users and brings in 35% [9] of its overall $114 billion retail market share [10]. Instead, divisions focused on particular therapeutic areas or aspects of R&D have initiated small AI teams to focus on their specific scientific priorities. This often leads to multiple disparate groups performing similar types of analyses such as natural language processing, image processing and predictive modeling, often with different approaches and tools. To standardize these approaches, many organizations have shifted to a centralized model that can focus on data and tool standards, and reuse code across applications. With the centralized model, it is much easier to keep up with the rapid pace of AI advancements--particularly in deep learning. However, each pharma division requires such specialized knowledge that the centralized model of general AI experts struggle to meet such a need. The trend is moving toward a hybrid model [10] with both central standardization and shared AI knowledge, but experience in dedicated application areas.

New internal groups in the AI enterprise landscape have also appeared in pharma that focus on deploying products. The top technology companies (Google, Facebook, etc.) have made continued investments in AI. Their research has advanced a set of AI products and services for object recognition, human language translation, chatbots for question-answering, robotic process automation (RPA), and many others. Most of these state-of-the-art products have been released as open-source tools that are now packaged and offered through cloud providers such as AWS, Azure and Google. Traditional IT and DevOps groups are now centrally hosting and offering these services through the available cloud and other infrastructures with new role titles [10,11]. These "MLOps" groups manage the machine learning and AI solutions and support of deployment and maintenance of internally developed AI tools.

Lessons from COVID-19 on adopting AI

The COVID-19 pandemic presented many opportunities for AI wins, but also highlighted many of the barriers to success [11]. Within days of the initial stay-at-home orders, Kaggle and other sites began competitions to tackle the virus. Approaches were developed to predict the virus' progression, estimate epidemiological spread and effect of self-quarantines, detect the disease [12], mine the literature [13], compare state and national responses in limiting the spread of the virus, etc. With the long timelines to develop new drugs, healthcare and pharma worked to identify drugs or combinations of existing treatments—a well-established AI problem [5-7]. These aimed to limit the spread, reduce the cytokine storm, reduce the severity of the symptoms and predict which patients would respond to treatment or would need hospitalization or ventilators [14]. Other AI applications focused on everything from virtual screening of compounds using deep learning [15] to improving the scalable synthesis of existing drug treatments [16]. The combination of the science and data-driven prioritization provided by AI helped identify candidate treatments [17].

While the urgent need to process complex data and propose solutions to the pandemic seemed the perfect opportunity for AI, the data limitations hampered efforts. Data for AI models and predictions did not cross borders for months, which delayed efforts. Public health results were not aggregated at city or regional levels for weeks. Access to health records was limited, biased and incomplete, but the workflows have subsequently improved. Daily reports are now expected as a top priority.

As the data workflows improve, several AI challenges still limit its widespread adoption in pharma. AI methods can help form hypotheses, analyze data, and optimize processes. In pharma organizations led by scientists, changing the research culture and creating an appropriate mindset to embrace the opportunity for AI remains difficult. A scientific culture aiming to make the best decisions must be willing to accept multi-disciplinary computational approaches such as AI. The utility of AI comes from a combination of the technology and the maturity of the organization to utilize it effectively. Leveraging techniques that provide insight and augment existing processes is an ideal starting point, and using approaches that provide interpretable reasons makes the case easier. However, the change management aspect remains a hindrance to wider adoption, which is not unique to pharma [18].

AI Focus Areas in Pharma

A glance at the literature on AI in pharma will reveal that most of the work is focused on the research or drug discovery aspects [19,20]. With open data sources and academic collaborations, the data and problems are more accessible. However, according to DiMasi et al. [21], the average out-of-pocket costs of research are only 31% versus 69% for the development (clinical trials), so industry conferences recently have been exploring how AI can impact clinical trials. A Tufts Center for the Study of Drug Development suggests AI in development is already underway but faces the lack of expertise, data organization, strategy and management--common issues in the early adoption of AI [22].

Opportunities in the clinical space include wearable sensors, operations such as recruitment, and more general tasks. The wearable sensor industry is expected to reach $2.86 billion by 2025 [23] and is certainly one of the largest opportunities for AI. The available sensors from pedometers to Fitbit® and Apple® watches provide many commercial opportunities for improved monitoring and fitness, but these and more advanced sensors can capture vast quantities of data which can be aggregated and leveraged to revolutionize clinical trials [24]. For example, to measure the effectiveness of a Parkinson's drug, patients must follow a 60 minute UPDRS protocol with a trained physician in the clinic while off medicine, take the medicine and, after it becomes effective, undergo a second 60 minute UPDRS protocol to produce a single measurement of UPDRS change. In contrast, a wrist sensor or the 3D accelerometer and gyroscope in an iPhone® can passively take measurements at 100 Hz [25,26]. The same 2-3 hour time period that yielded one number in the clinic can be used to record up to 100,000 measurements. Using AI, the sensor data can identify and characterize falling or balance issues along with patterns of walking, sleeping, sitting and standing. Though the use of such sensors for Parkinson's have demonstrated technical success [27-29], they still need regulatory approvals to transform clinical trials.

AI has the potential to impact almost every aspect of clinical trials including patient stratification, monitoring drug adherence, medical record sharing and utilization, analysis, operations and design [30]. Many believe that AI's best use case may be in the recruitment of patients for clinical trials since it is both expensive and the most likely cause of delays [31]. Chatbots and other technologies are being evaluated for patient retention. Even after recent improvements, 23% of studies fail to meet enrollment deadlines and studies still exceed 19% dropout rates [32].

In terms of technologies, deep learning has only recently started to tackle pharma's specific problems. Deep learning has been used for several years for high content screening and Google's recent use of BERT is changing natural language processing crossing across industries. A Nature Methods review by Moen et al. suggests that deep learning methodologies for cellular image analysis have the power to make complex analyses routine and enable previously impossible experiments [33]. Topics unique to pharma are now the focus of new research in deep learning. Ensemble methods using deep learning are now being used as an additional analysis tool in bioinformatics [34]. Generative Adversarial Networks (GANs) are being used for *de novo* designs and the optimization of small molecules for drug candidates [35]. Deep learning methods are also being used for drug repositioning [36]. These are exciting advances and suggest that AI will impact the field for many years through continually developing approaches such as deep learning. In fact, pharms is considered to be only in the 'early mature' phase of leveraging AI [20].

Potential Gains from Increased Investment

Given the opportunities that still exist and the relatively small investments that large pharmaceuticals have made to date in the AI area, there is still significant room for greater impact if not a transformation. The five largest pharma (Roche, Johnson & Johnson, Merck, Novartis and Pfizer) invest over $6 billion in overall R&D, ranking in the top 20 companies [37]. As a sector, pharma has the highest overall investment; the only companies with higher R&D are the familiar tech giants such as Google Alphabet, Microsoft, Facebook with dozens of AI products, and several car companies advancing self-driving car technology. Pharma's AI investments, consisting of cooperative arrangements, alliances, joint ventures along with internal efforts, remain unknown.

McKinsey predicts a sizable return from investments in AI. It believes pharma have started the AI journey by funding enterprise platforms for capturing data and have made short-term investments in some analytics core, but currently lack the organization and business will to replace the legacy systems to transform at scale. The 2018 US expenditure on AI by pharma and healthcare companies is increasing at a 26.9% compound annual growth rate and now totals $301 million, but still small compared with pharma's R&D $164 billion spending increasing at 3% [38]. This is consistent with McKinsey's 25% year-over-year increases in the use of AI reported elsewhere [18]. ESI ThoughtLab's recent survey of AI across industry sectors also found the pharma/life sciences investment is several fold lower than the average 0.75% of revenue that firms are spending on AI [39]. Analyzing use cases across industries, McKinsey estimates that pharmaceutical industry could gain 39% incremental value from AI investments as compared with other analytics techniques such as statistics and visualization [40]. Such an investment in AI would translate to a 45-75% increase in EBITDA with double digit gains in research, clinical trials, and commercial areas [41].

Conclusion

Pharmaceutical companies are now starting to capture the potential benefits of AI. The limitations in data workflows revealed by the 2020 pandemic impeded the progress of AI, but investments are already improving the data and analytics infrastructure. The increase in AI positions has changed organizations but a key remaining challenge is the recognition of AI data-driven approaches within the scientific processes. This will likely be overcome through the continued successes from pharma-focused deep learning and other evolving AI approaches. With the increased investments to drive AI throughout drug discovery and across clinical trials, AI offers the potential to transform the pharmaceutical industry.

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