Biomedical Science: Translation of Machine Learning to Clinical Applications

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Abstract

In recent years, expanding uses of artificial intelligence (AI) and machine learning have revolutionized pharmaceutical research and development, allowing us to harness multi-dimensional biological and clinical data from experimental to real-world settings (ML). Precision medicine discovery and development, from target validation to medication optimization, is driven by patient-centered iterative forward and reverse translation. As evidenced by deep characterizations of the genome, transcriptome, proteome, metabolome, microbiome, and exposome, the integration of advanced analytics into the practise of Translational Medicine is now a critical enabler for fully exploiting information contained in diverse sources of big data sets such as "omics" data. In this article, we provide an overview of machine learning (ML) applications in drug discovery and development, aligned with the three strategic pillars of Translational Medicine (target, patient, and dose), and discuss how they can alter the science and practise of the discipline. Model-informed drug discovery and development will be revolutionised if ML approaches are integrated into the science of pharmacometrics. Finally, we believe that cross-functional team activities involving clinical pharmacology, bioinformatics, and biomarker technology experts are critical to realising the promise of AI/ML-enabled Translational and Precision Medicine.

Keywords

AI, ML, DL, Drug

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1. Introduction

Over the last decade, big data and technological innovation have changed medicine and healthcare. Today's modern technical solutions can generate real-time health and medical data at the individual level in a real-world setting. They are at the heart of a digital disruption that has the potential to shift medicine's practise to a more targeted and individualised model, aided by data-driven judgments based on real-world evidence, patient-participatory medication discovery, and healthcare democratisation. Pharmaceutical Research and Development (R&D) has evolved in recent years to become a highly dynamic process facilitated by patient-centered iterative forward and backward translation [1]. The Drug Discovery, Development, and Deployment Map depict a network view of the process and its accompanying cross-sector ecosystem, challenging the traditional chevron (linear, sequential, and left to right) image of the pharmaceutical R&D pipeline. A Bayesian learning mentality that takes into account all available data is critical in delivering new healthcare solutions on time and with the appropriate feeling of urgency to meet unmet medical needs. While advances in biology, biomedical engineering, and computational sciences have increased our ability to generate and store multi-dimensional data from a variety of sources (e.g., laboratory, clinical trial, real-world, literature), consistent real-time integration of this data for principled and timely decision making in pharmaceutical R&D and healthcare remains a pipe dream. Recognizing the necessity of effective knowledge management, the pharmaceutical sector has begun to develop digital capabilities and incorporate Data Science breakthroughs into their R&D departments [2].

This idea relies heavily on machine learning (ML), deep learning (DL), and artificial intelligence (AI) approaches in general. ML is a subset of AI that consists of a set of algorithms that analyse data, learn from them, and then use those learning's to make intelligent decisions. While AI refers to the output of a computer generated by emulating human behaviour, it does not specify how the problem was addressed. The classification of machine learning algorithms into supervised, unsupervised, deep learning, and reinforcement learning is a basic and commonly used classification. Supervised learning is task-driven, and it starts with datasets with known labels or outcomes to perform classification and prediction tasks on incoming data [3].

Unsupervised learning approaches, on the other hand, are data-driven and focus on identifying structures and patterns within the data. Discovering groupings and clusters, identifying item relationships, and finding a more compact representation of the data are just a few examples. Reinforcement learning focuses

on decision and policy making and employs algorithms to learn interactively how to react to an environment from mistakes [4]. Finally, DL uses NNs with multiple layers to handle the most difficult problems, inspired by the biological neural network (NN) of the human brain. Such a learning process is significantly more competent than typical machine learning models. While both ML and DL fall under the umbrella of AI, it is DL that is responsible for the most human-like artificial intelligence. Integration and application of AI/ML approaches throughout the translational to clinical drug development continuum has already had a significant influence on our capacity to optimize the value of data. Furthermore, these methodologies have improved knowledge management for both the investigated drug and the disease/patient population, allowing for R&D optimization across the three essential interdependent strategic pillars that make up Translational Medicine practise: target, patient, and dose [5].

2. Conclusion

Machine learning methods have demonstrated to be more competitive than traditional methods, particularly when it comes to the integration and analysis of huge, multi-dimensional, and heterogeneous data sets. Such methods can yield meaningful insights that can be used for hypothesis development and be supplemented by later assessments in more mechanistic MID3 frameworks without the need to explicitly make assumptions on the underlying data and system relationships. The goal is to create a highly interdependent and iterative interaction between the disciplines of Quantitative Systems Pharmacology and Pharmacometrics. Big data and advanced technologies, such as artificial intelligence (AI) and machine learning (ML), hold a lot of promise for enabling effective forward and reverse translational discovery of sources of variation in benefit-risk profiles, and ultimately bringing the right therapeutic solution to patients.

3. References

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