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The Role of Machine Learning in Drug Design and Delivery

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Editorial

Over roughly the past twenty years, machine learning algorithms such as artificial neural networks, support-vector machines, decision trees and decision forests, and Bayesian learning have seen extensive use in many aspects of drug design and delivery. In this article we will discuss some of these uses.

Definition of Machine Learning

In machine learning, one uses algorithms to make computers "learn;" i.e. to create decision functions from representative samples of data [1]. It is generally used when a purpose-specific algorithm to perform a task is unavailable or infeasible.

The applications discussed in this article typically use learning machines to perform supervised classification; i.e., the construction of algorithms to determine of the presence or absence of an exemplar in a class based on the values of the data comprising said exemplar. For example, a pharmacologist who wished to predict whether potential drug compounds were neurotoxic or not might use machine learning to construct a decision function from a set of drugs of known neurotoxicity or lack-thereof, and the function thus created would classify other drug compounds as belonging to the mutually exclusive classes of "neurotoxic" or "non-neurotoxic."

Applications

Machine learning has several advantages over conventional statistical methods in drug design. The vast majority of commonly-used learning machines are nonlinear, and thus potentially able to model relationships that may not be adequately represented by linear quantitative structure-activity relationship models. Further, learning machines are designed to generalize from incomplete data, and the scientist need not assume a particular model when using them.

Machine learning is often used to enhance the effectiveness of conventional methods of drug discovery; for example, by using chemical data to construct functions to rank the probability that a chemical compound will have activity against a known target. Similarly, machine learning is often used in ligand-based drug design to create ligand-receptor scoring functions and binary predictions of ligand-receptor affinity, among other uses. Additionally, machine learning is widely used in target screening, such as by interpreting machine vision data to detect and identify target locations on cells, and in hit evaluation; e.g., to predict the side-effects of new drugs.

Learning machines also see numerous uses in ADMET evaluation, being used to predict such diverse characteristics as intestinal absorption, albumin binding, metabolic stability, and clearance time. With respect to toxicity, machine learning is used in a wide variety of aspects of toxicity detection and prediction, with a notable example being the generation of mandated toxicological data for drugs marketed in the European Union [2]. More prosaically, machine learning is used in detecting toxicities such as hepatotoxicity, nephrotoxicity, and ototoxicity. Little work, though, has been done on the applications of machine learning to drug-related cardiotoxicity and neurotoxicity, suggesting opportunities for investigators who wish to explore these fields.

Finally, machine learning has application to multiple aspects of drug delivery system design. Broadly speaking, machine learning finds the most use in the design and optimization of the preformulation and formulation of drug delivery systems (e.g., predicting the drug release profiles for individual components and for delivery systems as a whole, respectively), as well as applications in *in-vivo - in-vitro* correlation and quantitative structure-property relationship modeling. Machine learning has also seen use in the prediction of drug stability, being used for such tasks as predicting the shelf lives of drugs and the stability of drug delivery systems.

In summary, machine learning algorithms have application to numerous aspects of drug design and delivery [3-8], and it is reasonable to expect that their role will continue to increase in the future.

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