An Iterative Transfer Learning Approach to Multiobjective de novo Drug Design with Recurrent Neural Networks and Nondominated Sorting

Yasonik, Jacob (School: Homestead High School)

A plummet in the research productivity of drug discovery has been observed in recent decades, with higher costs, longer timelines, and lower success rates of drug candidates in clinical trials. Current methods largely rely on trial and error, and are unable to consider multiple objectives (e.g., activity, toxicity, absorption, etc.) collectively. De novo drug design, a promising new method of drug discovery, has been used to generate molecules from scratch: making for a more scalable approach. In particular, recurrent neural networks have been shown to be able to generate novel molecules. By selecting the best of the molecules generated and fine-tuning the network on them, recurrent neural networks are able to optimize a certain trait. However, optimizing for multiple molecular properties all at once has proved challenging, and has impeded the use of de novo drug design in industry. In this work, a nondominated sorting algorithm was applied to select the best of the molecules generated by the recurrent neural network. The nondominated sorting algorithm is distinctive in its ability to account for multiple properties together. This approach was used to successfully optimize multiple molecular properties simultaneously in a proof of concept, showing its unique scalability and multiobjectivity as a method of drug discovery.

Awards Won:
Third Award of $1,000