

Using Artificial Intelligence Neural Networks to Repurpose Pre-Existing Drugs and Analyze Drug Relationships, Year 3

Seela, Krithik (School: Lake Highland Preparatory School)

As burgeoning crises have exposed failures of the drug discovery cycle - an inability to quickly and effectively develop new drugs - artificial intelligence-based drug repositioning models are emerging as an effective, less capital-intensive way to repurpose pre-existing drugs to treat new conditions. Two computational models were developed using data from DrugBank, SuperTarget, and deepSNAP libraries. The first model takes in user input regarding the effects of a condition and successfully provides suitable drug candidates, developing novel relationships by analyzing which drugs treat similar effects to the condition being researched. The second model consists of two artificial intelligence graph neural networks (GNNs). The GNNs consist of tens of thousands of nodes, representing drugs, and edges, representing relationships between drugs. This model can penalize and train itself to become more accurate. These models were supplemented with data from different databases which has improved accuracy, with the GNNs being able to predict FDA approval and drug compatibility with a 2-4% increase in accuracy and the repositioning model being able to provide a larger number of drug candidates. In addition to this, the GNNs were modified to predict relationships using different features and combinations of drugs to uncover new connections and improve both accuracy and efficiency. The user interface was also expanded to include a larger series of questions and to integrate the GNNs instead of only the repositioning model. This scales up the opportunities for concrete applications as well since it means users can now utilize both the repositioning model and the GNNs in combination with each other.

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