Novel Evolutionary Artificial Intelligence Methods for De Novo Drug Design

Goswami, Anish (School: West Linn High School)

The current methods for drug development against a target disease are not cost-effective. The process is not efficient and has a high failure rate. It can take up to 12 years to design, create, and test a drug. This process also has a failure rate of 86%. The research and development phase of drug design takes a long time, second only to clinical trials. One major issue with the current process is that it uses handwritten rules and human expertise which are both prone to error. In this project, we propose a novel method based on evolutionary artificial intelligence. This method involves 3 steps. The first step uses a deep recurrent neural network to generate molecules. Second, a non dominated sorting algorithm to optimize molecules for drug-like properties. The third and final step uses a convolutional neural network to predict binding scores between a target and a molecule indicating whether or not the molecule is active against the target. This is a fully automated method. It does not need human intervention or handwritten rules. In this project, we developed a recurrent neural network program and a non dominated sorting algorithm. We also trained a convolutional neural network from the DeepPurpose library. We targeted malaria as it is still a deadly disease in the developing world. We were able to create hundreds of molecules that could possibly be active against malaria.

Awards Won:

Oracle Academy: Award of $5,000 for outstanding project in the systems software category.