**Abstract:**

Drug-target affinity prediction is a crucial step in the drug discovery process, as it can help to identify and optimize potential drug candidates to target specific protein(s). Drug-target affinity measures how strongly a drug binds to a protein. However, experimental methods are costly and slow, and existing computational methods have some limitations which could not replace properly lab experiments. For example, some approaches rely on 3D structural information of targets, which is not widely available, or use simple string representations of drugs, which may not capture their complex molecular properties

We propose an improved version of GraphDTA, a state-of-the-art model that predicts drug-target binding affinity using graph neural networks (GNNs) for drugs and convolutional neural networks (CNNs) for proteins. We use a stack of GAT layers and concatenate features from different layers to increase the expressiveness and complexity of our model. GATs calculate weights for different nodes and edges in the drug graphs based on their importance for the task.

We evaluate our model on the Davis dataset, which contains 68 drugs and 442 targets with 30056 interactions. We compare our model with five existing methods using mean squared error (MSE) and concordance index (CI) as metrics. Our model achieves MSE:0.249 and CI:0.881. Our experimental results show that our model achieves competitive performance on a benchmark dataset compared to the state-of-the-art methods.

CPS can improve the DD process and the healthcare outcomes by using DTA. DTA prediction can have applications in CPS scenarios, such as smart healthcare, personalized medicine, or drug repositioning.

* DTA prediction can use the latest and most advanced CPS technologies to improve its performance and efficiency. For example, smart healthcare can monitor, diagnose, treat, or prevent diseases with IoT devices. IoT devices can connect physical objects to the internet and enable data collection and transmission.
* Personalized medicine can use DTA prediction to avoid bad drug effects or combinations by selecting drugs that have high affinity with target proteins and low affinity with other proteins.
* CPS technologies can support the data and computation needs of DTA prediction by providing high-quality and diverse data sets, as well as fast and powerful computation models.

**Keywords**: Drug-target affinity prediction, Graph attention network, Smart healthcare, Personalized medicine, Drug repositioning