An ensemble method for drug-target interaction prediction

Lu Yijingxiu

Abstract:

The prediction of drug-target interaction (DTI) is an important step in the process of drug discovery to identify putative new drugs or novel targets for existing drugs. DTI prediction methods are generally categorized into two groups: docking simulation and machine learning methods. Using machine learning methods to predict DTI has become popular given its great performance. However, it is hard to make consensus over different computational methods as they provide different opinions on ambiguous data points. In our work, we present a DTI prediction ensemble model to aggregate model architectures with different encoding schemes, achieve better performance on diverse datasets.