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Mixture-of-Experts Approach for Enhanced Drug-Target Interaction Prediction and Confidence Assessment

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In recent years, numerous deep learning models have been developed for drug-target interaction (DTI) prediction. These DTI models specialize in handling data with distinct distributions and features, often yielding inconsistent predictions when applied to unseen data points. This inconsistency poses a challenge for researchers aiming to utilize these models in downstream drug development tasks. Particularly in screening potential active compounds, providing a ranked list of candidates that likely interact with the target protein can guide scientists in prioritizing their experimental efforts. However, achieving this is difficult as each current DTI model can provide a different list based on its learned feature space. To address these issues, we propose EnsDTI, a Mixture-of-Experts architecture designed to enhance the performance of existing DTI models for more reliable drug-target interaction predictions. We integrate an inductive conformal predictor to provide confidence scores for each prediction, enabling EnsDTI to offer a reliable list of candidates for a specific target. Empirical evaluations on four benchmark datasets demonstrate that EnsDTI not only improves DTI prediction performance with an average accuracy improvement of 2.7% compared to the best performing baseline, but also offers a reliable ranked list of candidate drugs with the highest confidence, showcasing its potential for ranking potential active compounds in future applications.