The Utilization of Deep Learning Based Universal Gene Function Prediction to Identify Gene Synergy to Further Predict Drug Synergy

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Drug-drug synergy is crucial for developing effective combination therapies, and gene function relationships play an important role in identifying these synergies. However, due to the complexity of gene function interactions and the limitations of existing methods (which often rely on incomplete annotations or narrow data sources), predicting drug-drug synergy remains a source of challenge. This study introduces the first framework to predict drug-drug synergy using universal gene function embeddings. Using GoBERT, a deep learning based gene function prediction algorithm, gene function embeddings can be generated, where each dimension represents the probability that a gene has a specific function, with values ranging from 0 to 1. The corresponding value is set to 1 if a function is experimentally confirmed to be possessed by a gene and 0 if confirmed not. For functions without experimental evidence, GoBERT assigns the probability value. Then, the cosine similarity between two gene function embeddings is calculated to quantify their predicted level of synergy, which can then be aligned with experimental drug data. The experimental results demonstrate strong performance, highlighting the potential of this framework for systematic and interpretable drug synergy prediction.

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