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Opinion Article

Predicting Drug-Drug Interactions Using Multimodal Graph Representations

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DESCRIPTION

The prediction of Drug-Drug Interactions (DDIs) has always been a central concern in drug development and clinical pharmacology. With the rise in polypharmacy, especially among the elderly and patients with chronic illnesses, accurately predicting harmful DDIs is essential for patient safety. Traditional experimental methods are resource-intensive and often unable to keep pace with the fast-growing number of possible drug combinations. In this context, computational methods, especially those using artificial intelligence, have emerged as potential alternatives. Among them, Graph Contrastive Learning (GCL) combined with dual-view fusion has recently gained attention for its potential to model complex biomedical relationships and enhance the strongness of DDI prediction.

Graph-based models have a unique advantage in representing the rich relational structure between drugs, targets, enzymes and pathways. Unlike linear models or matrix factorization, Graph Neural Networks (GNNs) capture high-order dependencies and nonlinear associations. However, a key limitation of many graph-based models is their sensitivity to noisy data and overfitting when labeled data are scarce. This is where contrastive learning, which has demonstrated remarkable success in vision and language models, becomes an important tool. By maximizing the agreement between different views or augmentations of the same node (drug) while minimizing similarity with other nodes, GCL encourages the model to learn more generalizable and discriminative representations.

The incorporation of dual-view fusion further elevates this framework by capturing complementary information from heterogeneous sources. Typically, one view is derived from the molecular structure or SMILES representation of a drug, while the other is constructed from drug interaction networks, pharmacological profiles, or biological annotations. The fusion of these distinct perspectives enables the model to learn a more holistic embedding of drug properties, which is essential for accurate DDI prediction. It reduces the dependence on any single modality and enhances robustness against missing or noisy data.

The most compelling aspect of this approach is its capacity to address the cold-start problem, a common issue in DDI prediction where new or less-studied drugs lack sufficient interaction data. Through contrastive pre-training and leveraging structural similarity, the model can infer potential interactions based on shared latent features with well-characterized drugs. This greatly increases the model's applicability in drug discovery pipelines and early-phase clinical trials, where experimental interaction data may be limited or unavailable.

Nevertheless, there are challenges that must be acknowledged. The quality of predictions still heavily depends on the coverage and accuracy of the input data is it structural, pharmacological, or relational. Data biases in existing drug interaction databases can propagate through the model, resulting in spurious associations. Additionally, contrastive learning frameworks often require careful design of positive and negative pairs, which is non-trivial in biomedical settings where relationships are complex and context-dependent. Improper sampling strategies could degrade the performance and mislead model training.

Another consideration is scalability and generalizability. While dual-view GCL models perform well on benchmark datasets, real-world deployment demands scalability across large, dynamic drug libraries and continuous updates as new data becomes available. Maintaining performance consistency while integrating new drugs or interaction types remains a critical hurdle. Combination with real-time electronic health records or pharmacovigilance systems will require further optimization, validation and regulation.

Despite these challenges, the direction is potential. As biomedical data becomes increasingly rich and diverse, fusion-based models that intelligently combine multiple sources of information will become essential. Graph contrastive learning, with its ability to extract meaningful structure from high-

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dimensional, relational data, is well-suited for such applications. Combined with advanced fusion techniques, this framework represents a next-generation solution for DDI prediction.

In conclusion, drug–drug interaction prediction based on graph contrastive learning and dual-view fusion is not merely a methodological advancement it is a change toward more intelligent, data-driven drug safety evaluation. Its potential to enhance drug development efficiency, minimize adverse effects and guide personalized medicine is significant. With continued innovation, validation and cross-disciplinary collaboration, this approach could redefine how we identify and manage DDIs in clinical and pharmaceutical contexts.