

Structured Multi-View Representations for Drug Combinations

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Drug Combinations

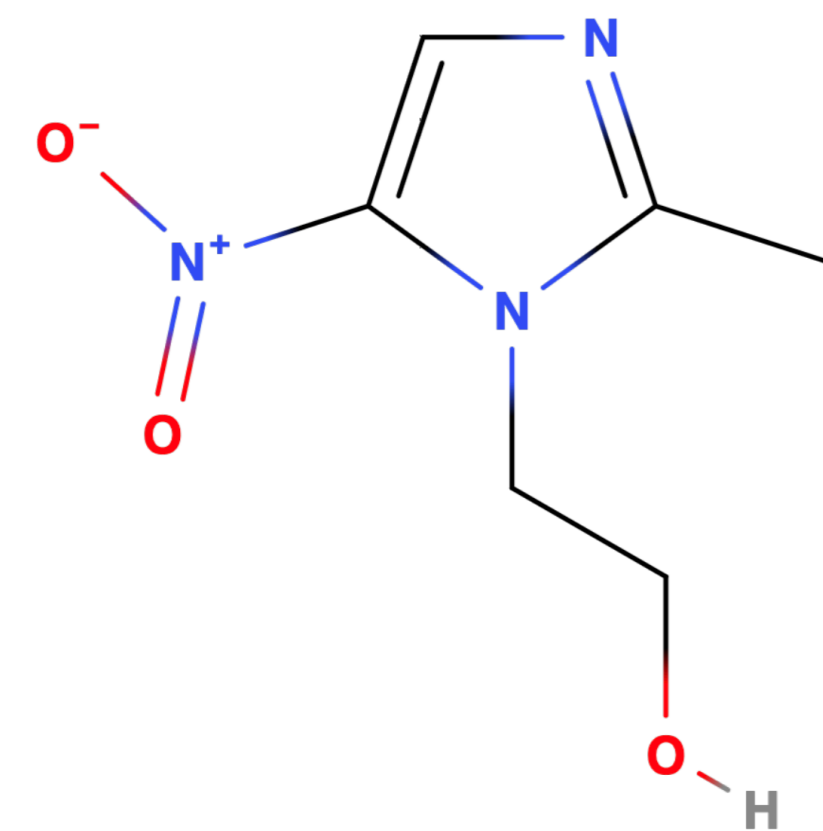
From data: prediction on pair of drugs

From domain: treating co-existing conditions

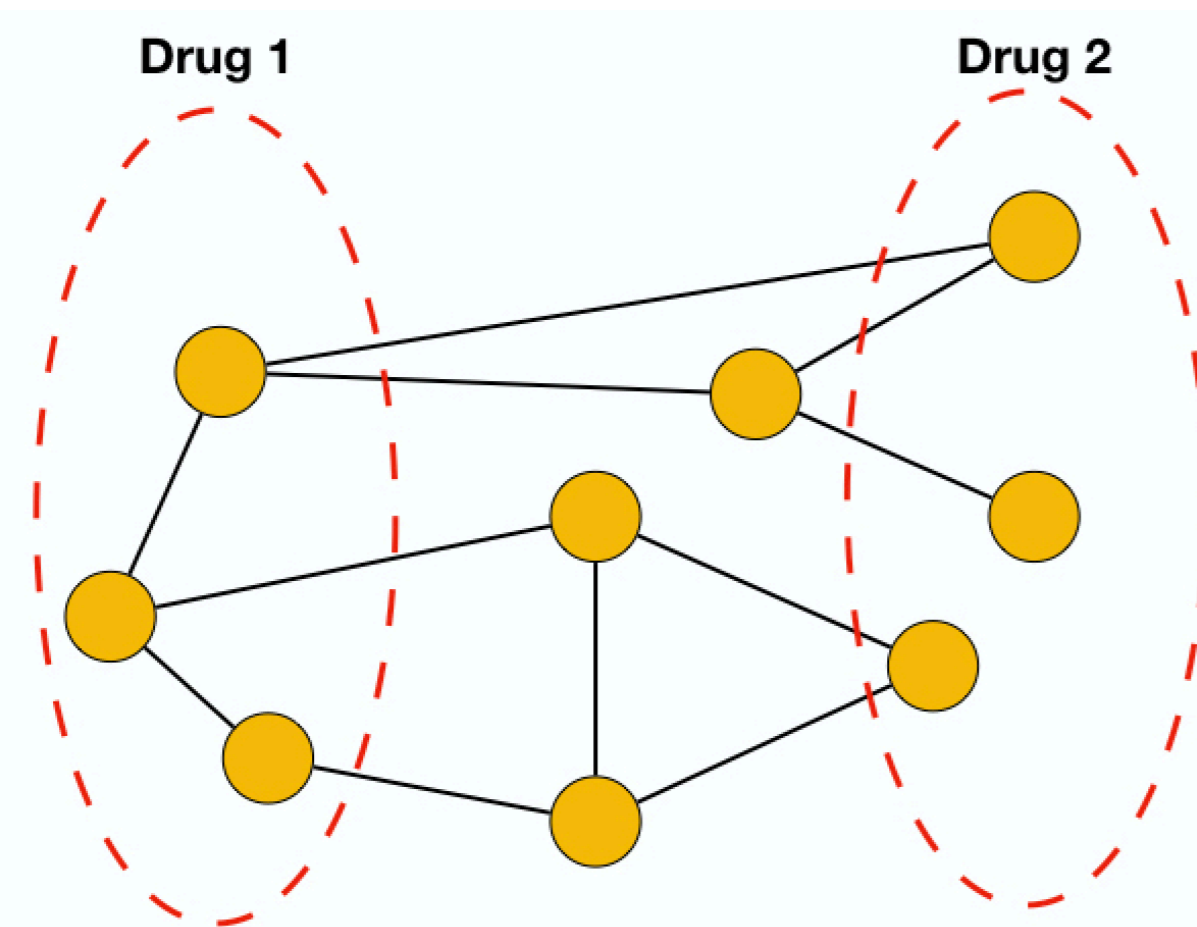
- Low cost
- Time efficiency

Two Views of Drugs

View 1: Molecular Structure View x_c

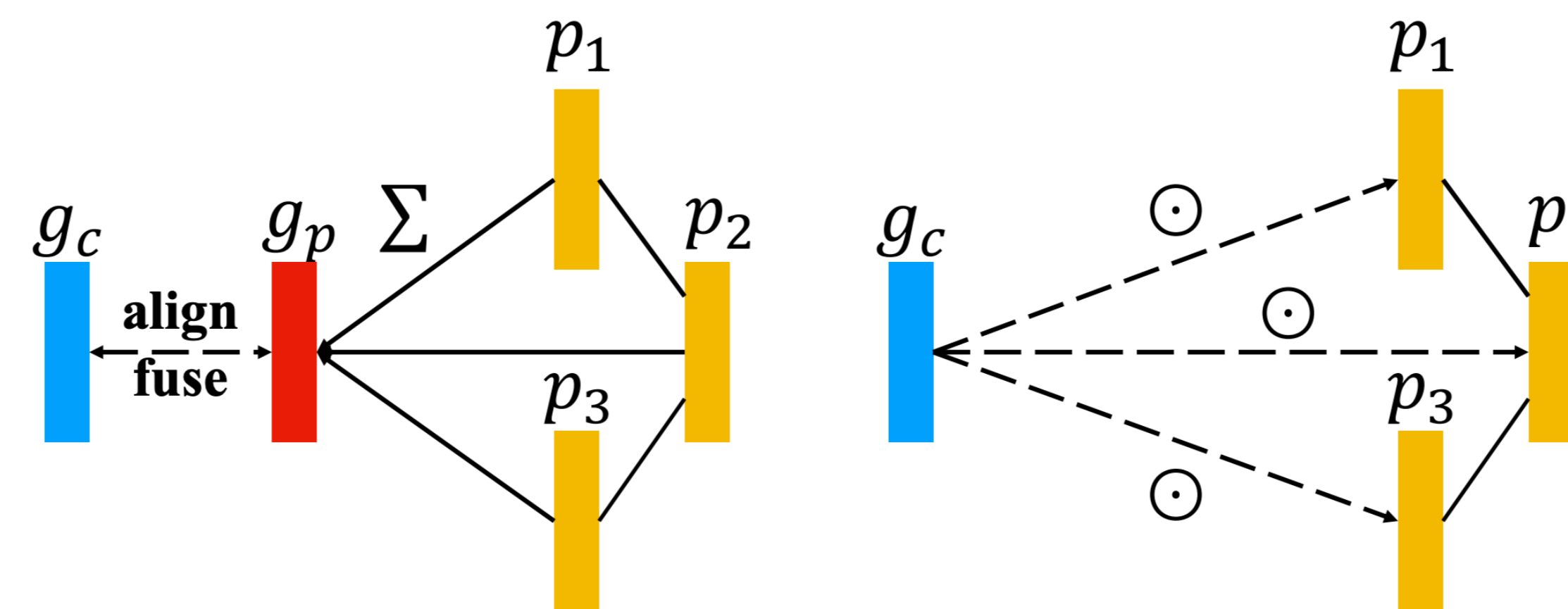


View 2: Protein View x_p

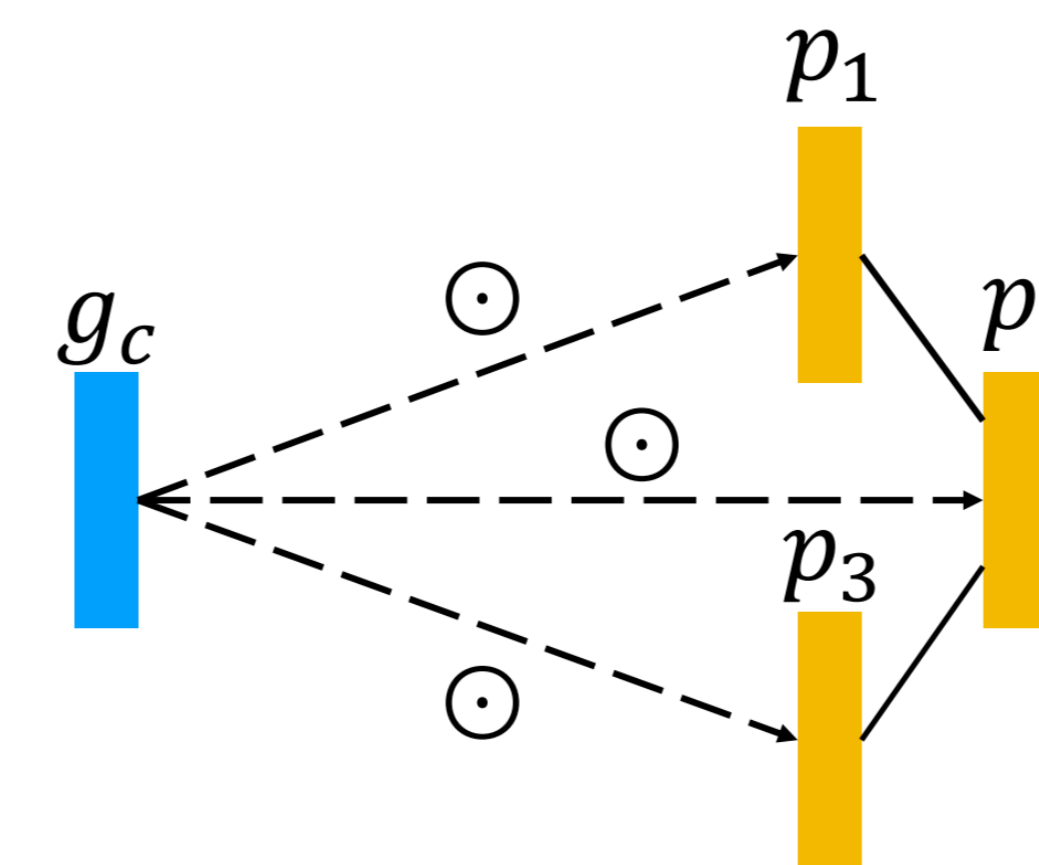


Cross-View Representation Learning

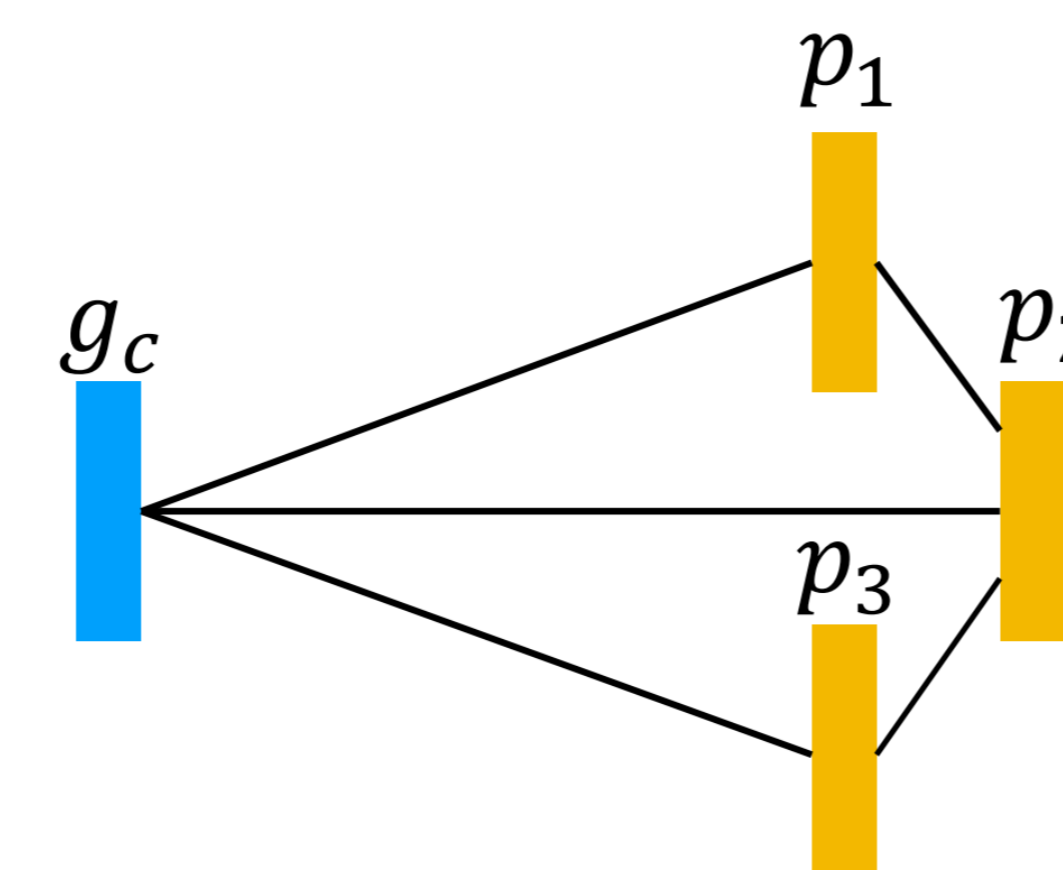
- Unstructured Multi-View Representation (UMVI)
- **Structured Multi-View Representation (SMVI)**
- Context-Protein Attention (CPA)
- Master-Protein Message Passing (MPMP)
- Drug-Protein Message Passing (DPMP)



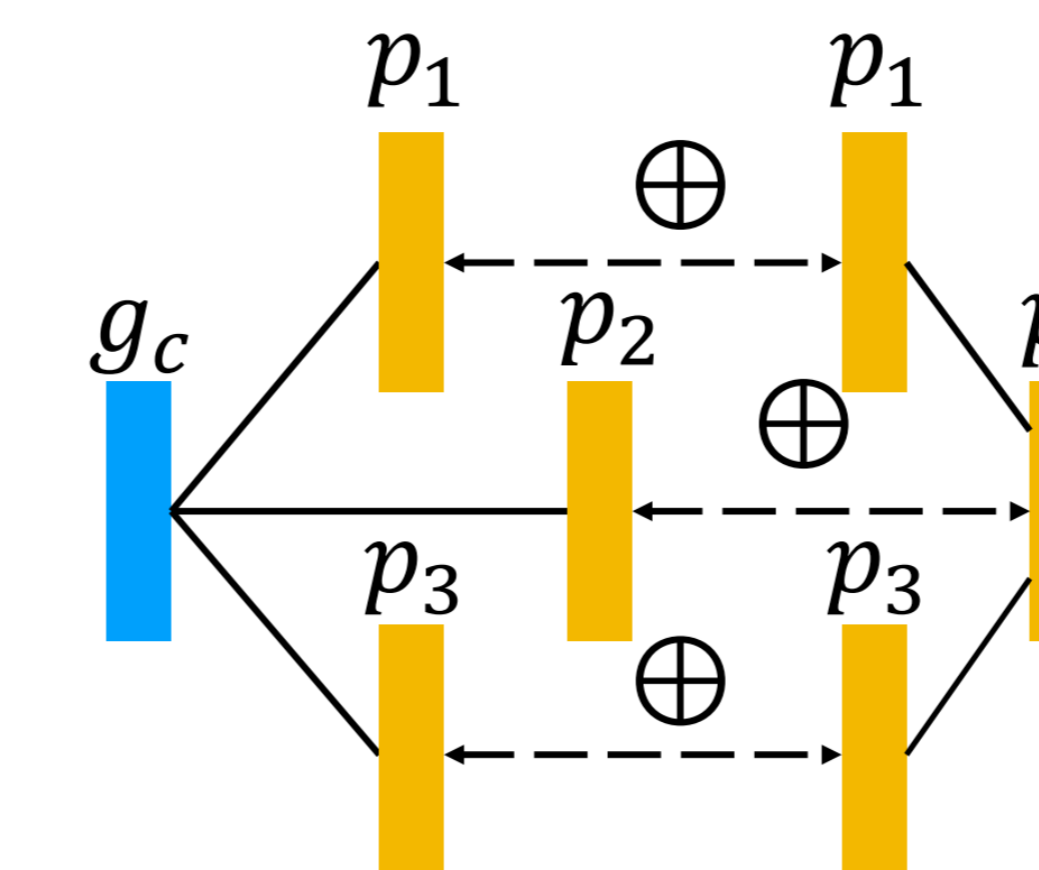
(a) UMVI



(b) CPA



(c) MPMP



(d) DPMP

Experiments

- Representation
 - ECFP for x_c
 - Knowledge graph for x_p
- Data
 - Molecule drug pairs from National Cancer Institute (NCI)
 - Knowledge graph:
 - STITCH-STRING
 - Graph-Based proximity paper

View	Model	NCI-SS		
		RMSE	MAE	
Chemical View	ECFP	27.11 ± 1.58	15.22 ± 0.88	
Protein View	Local PPI	25.95 ± 1.04	15.41 ± 0.43	
Chemical View & Protein View	UMVI	Simple Mean	26.19 ± 1.74	15.30 ± 0.71
		Deep CCA	31.03 ± 1.22	22.32 ± 0.73
		Deep Fusion	26.55 ± 2.22	15.33 ± 0.81
		InfoNCE	26.61 ± 1.61	15.69 ± 0.68
	SMVI	CPA	24.42 ± 1.13	13.70 ± 0.33
		MPMP	25.06 ± 2.33	14.89 ± 0.64
	DPMP	24.79 ± 1.87	15.26 ± 0.81	

View	Model	NCI-GP		
		RMSE	MAE	
Chemical View	ECFP	28.00 ± 3.93	17.24 ± 1.86	
Protein View	Local PPI	27.37 ± 3.64	16.65 ± 1.74	
Chemical View & Protein View	UMVI	Simple Mean	27.12 ± 3.17	16.99 ± 1.33
		Deep CCA	31.47 ± 3.22	22.23 ± 2.59
		Deep Fusion	26.50 ± 3.12	17.00 ± 1.19
		InfoNCE	27.97 ± 3.33	16.88 ± 1.30
	SMVI	CPA	25.94 ± 4.51	15.34 ± 1.56
		MPMP	27.11 ± 2.99	16.66 ± 0.77
	DPMP	26.39 ± 3.93	16.60 ± 1.33	

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