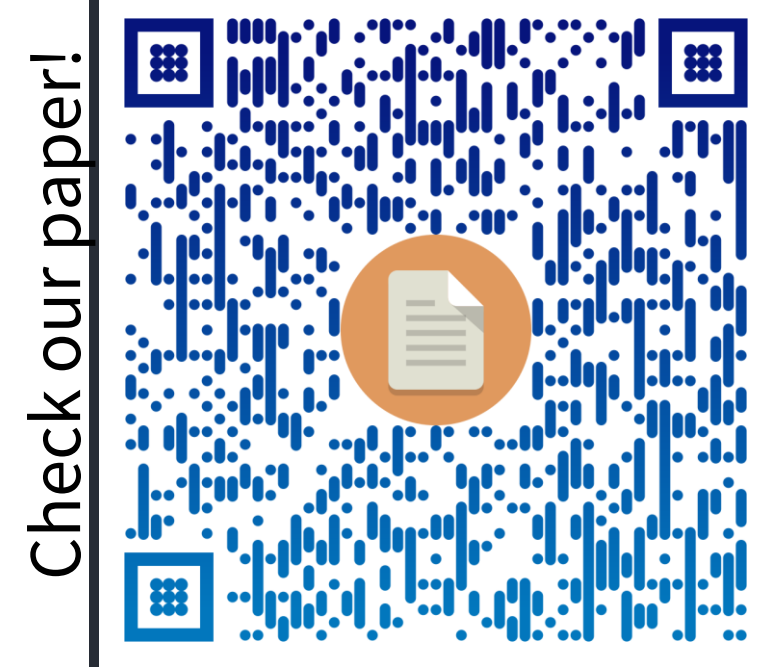


Neuro-Symbolic AI for learning over Knowledge Graphs with contradictions

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1 Motivation

Knowledge Graphs (KGs) often contain contradictions that are not necessarily errors — they can represent polyvocal truths or nuanced realities that, if properly modeled, can enhance the completeness and expressiveness of KG-based machine learning.

< Jerusalem, wiki:country, Palestine > — disputed by Israel, Unites States
< Jerusalem, wiki:country, Israel > — disputed by Palestine, United Nations
Wikidata entry Jerusalem (Q1218)

Current KG Representation Learning is not well-equipped to handle contradictory facts within KGs, especially those that are implicit and context-dependent. There is a lack of mechanisms to explicitly model or leverage contradictions during learning.

Taxonomy of Contradictions

Explicit: Logic-based conflicts that can be detected via rule violations or ontology constraints.

Implicit: Conflicting or context-sensitive facts that do not violate formal logic but may be contradictory under additional assumptions or external knowledge.

2 Hypothesis

An approach that integrates symbolic and sub-symbolic representations can bridge KGs and LLMs to answer:

- **RQ1:** How do contradictions in a KG, implicit and explicit, impact the SOTA KGRL performance for PPIs?
- **RQ2:** Does modeling contradictions onto protein representations improve ML?
- **RQ3:** Can external sources of knowledge such as LLMs be explored to detect implicit contradictions?

3 Challenges

(1) Learning from contradictory statements and particularly with negation must account for:

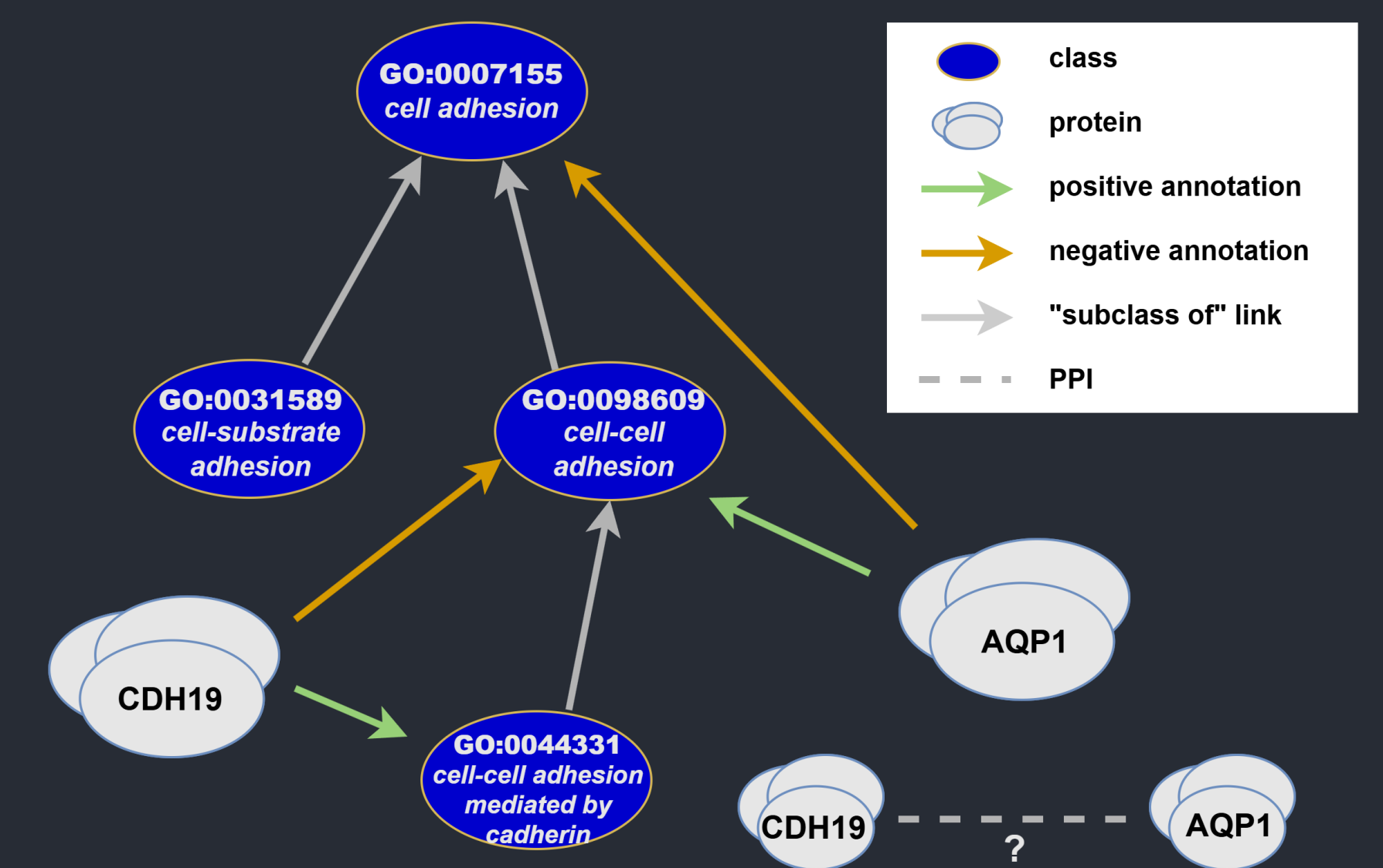
- Inheritance
- Graph closeness \neq Similarity

(2) Not all contradictions are explicit and some are context dependent

rule-based reasoners symbolic + sub-symbolic

Preliminary focus on modeling contradictions stemming from negation:

- Biomedical use-case (Protein-Protein Interaction prediction)
- KG constructed from Protein-Protein Interaction data and positive and negative statements on protein function aspects (Gene Ontology).

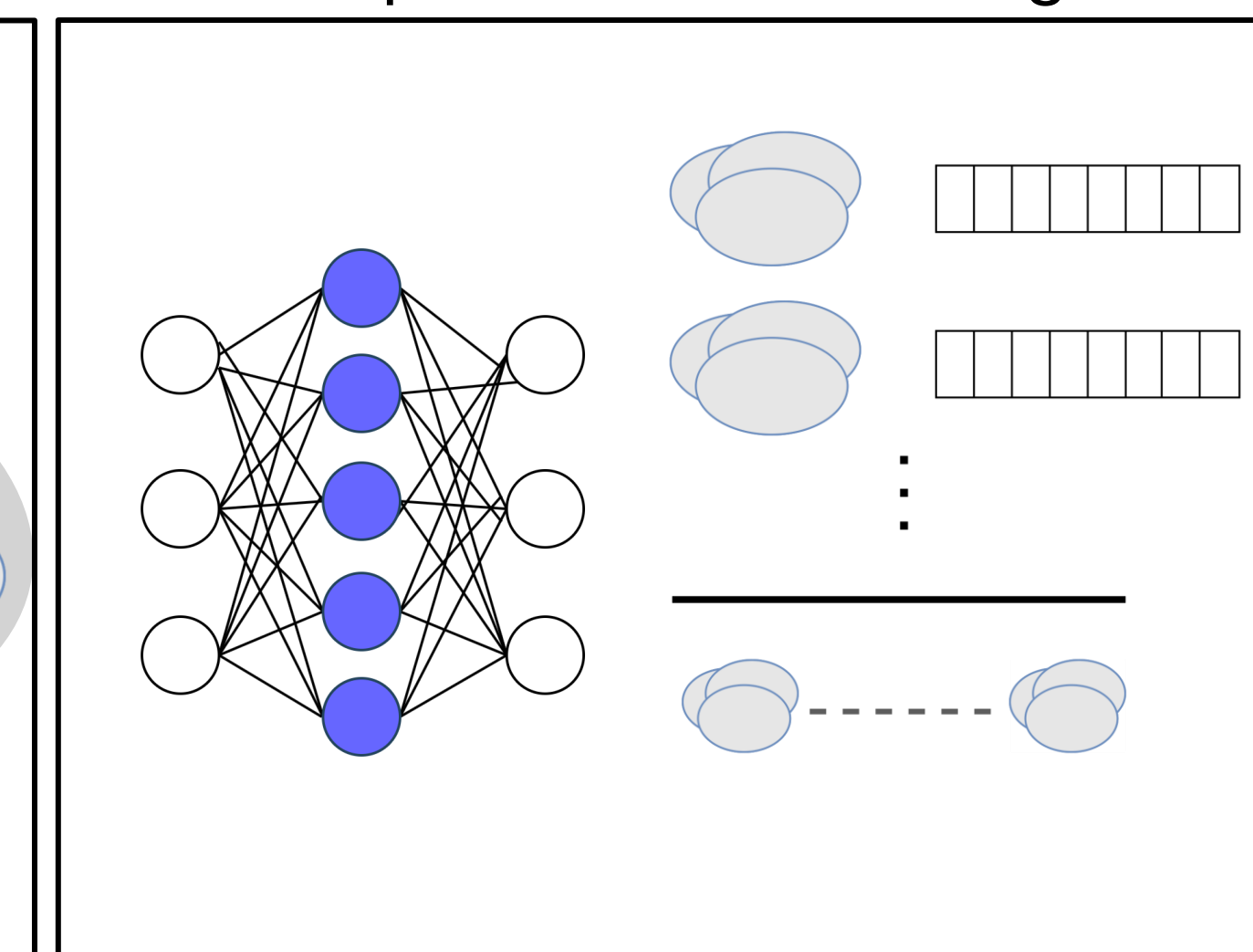
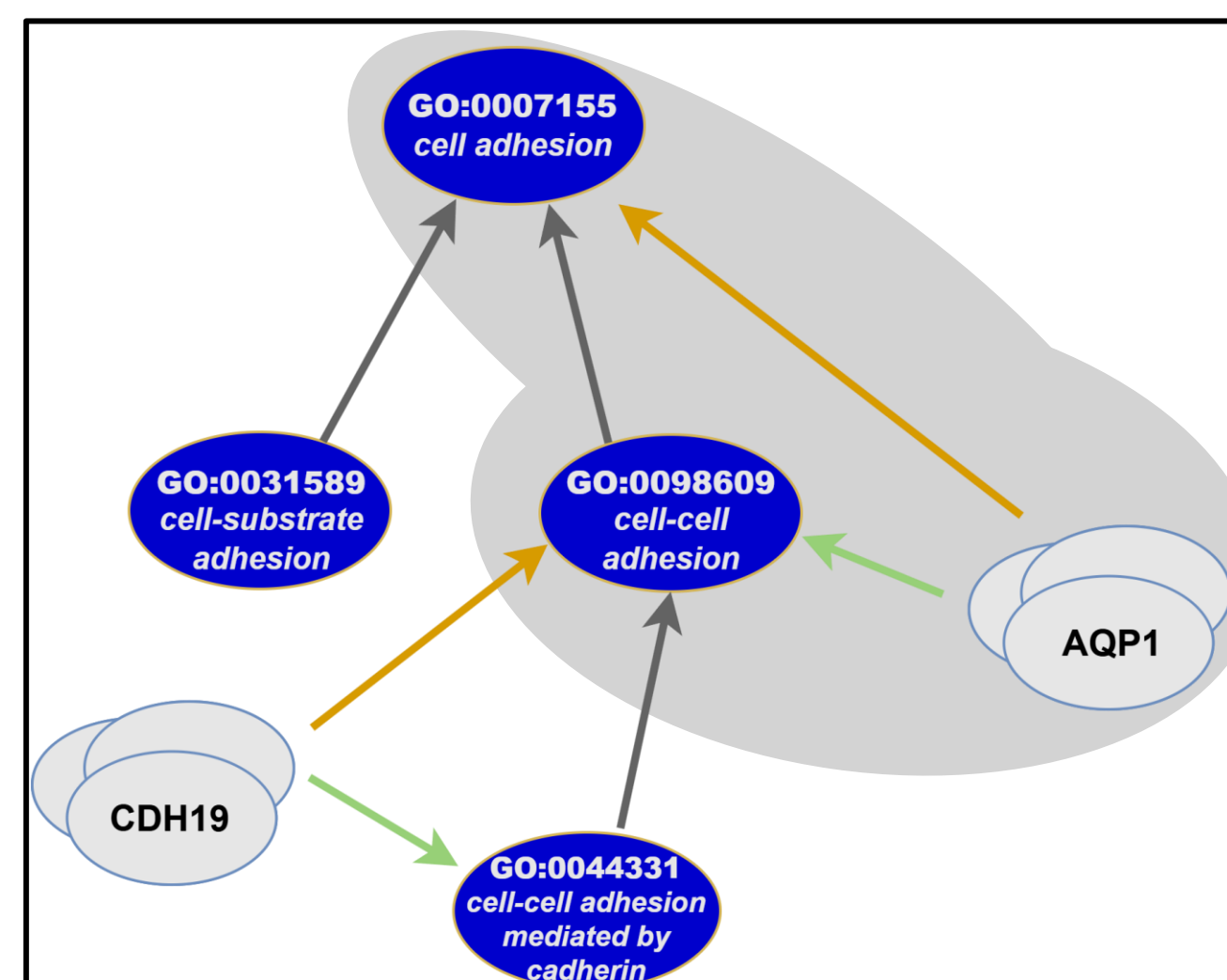
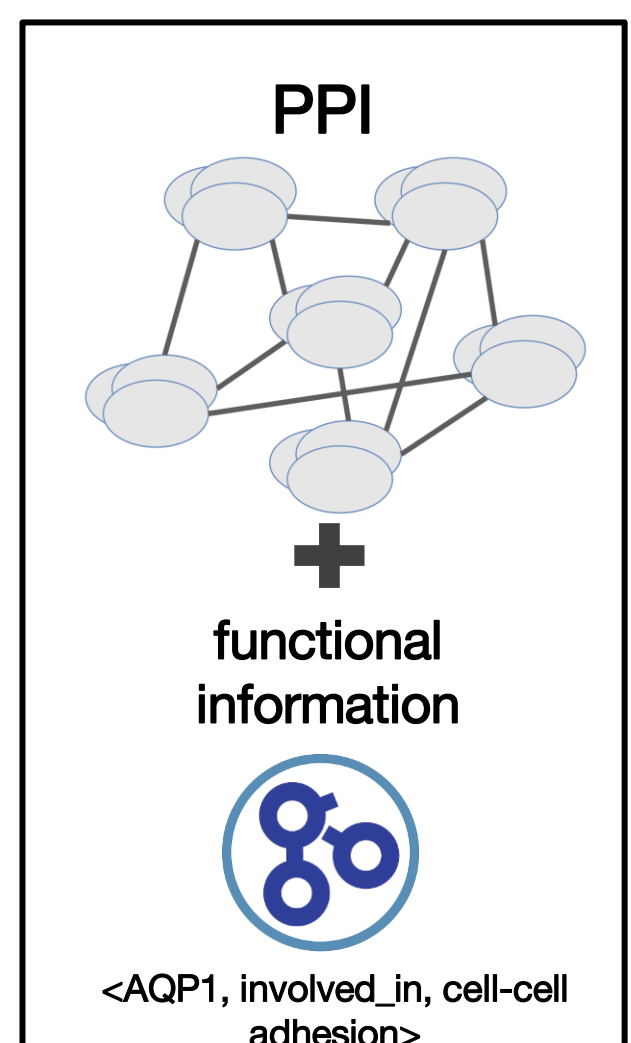


3 Methodology

KG construction

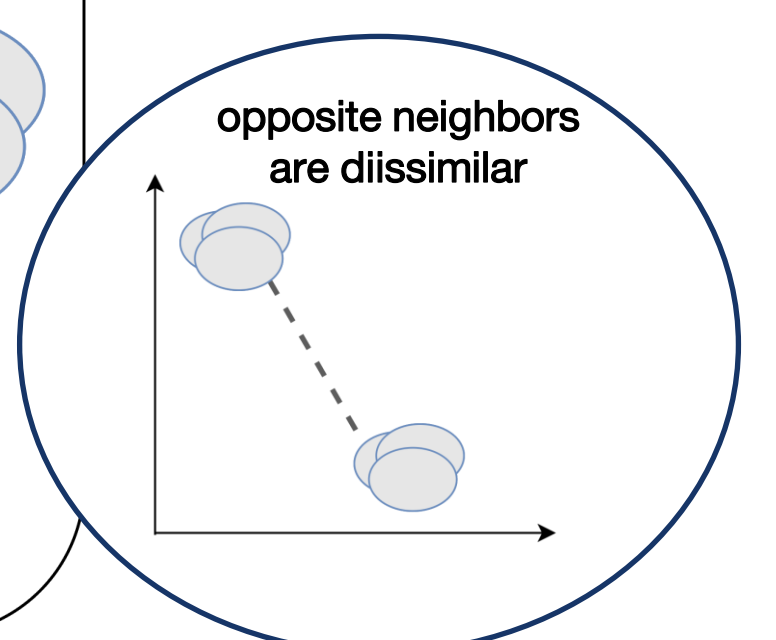
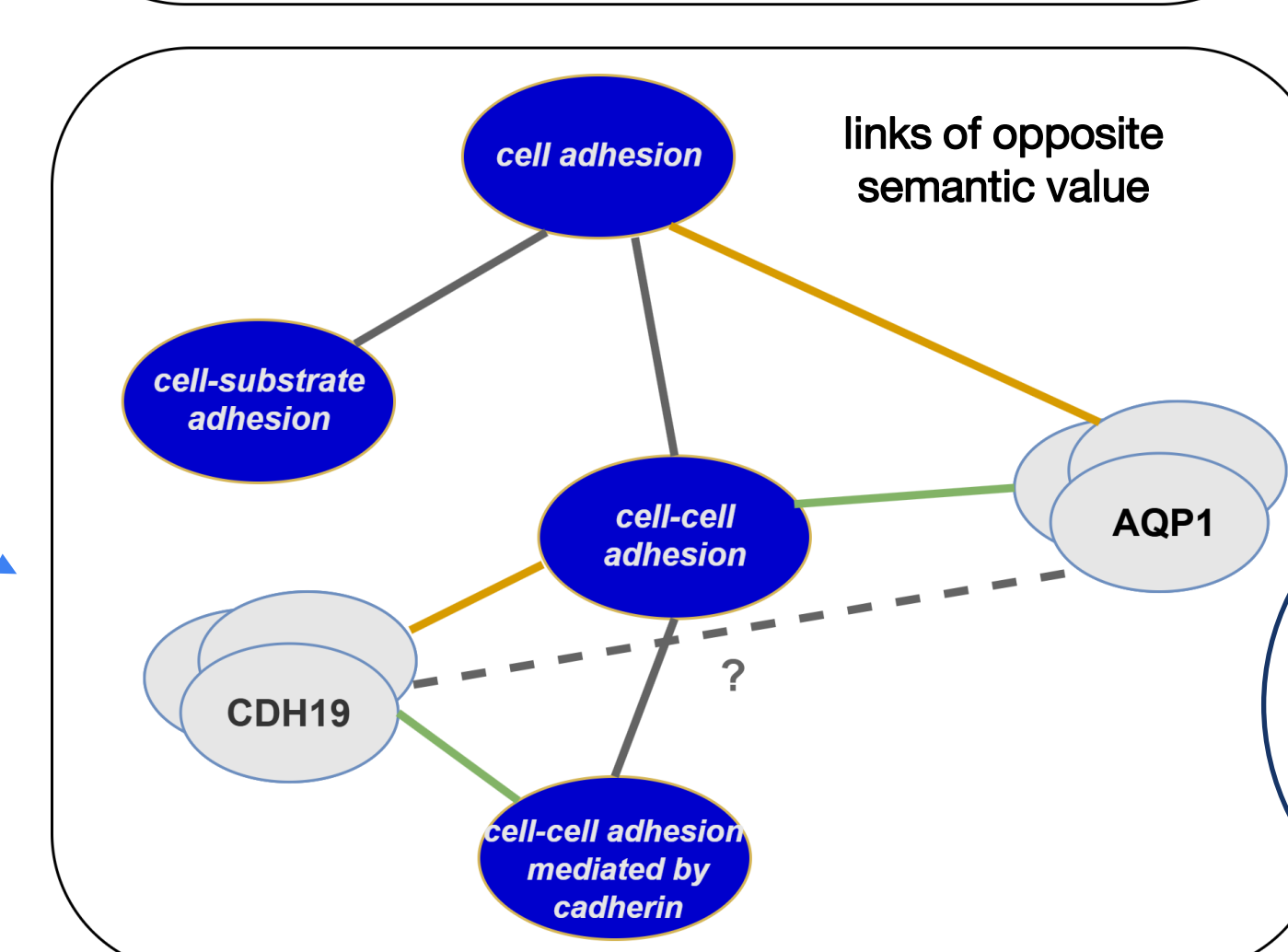
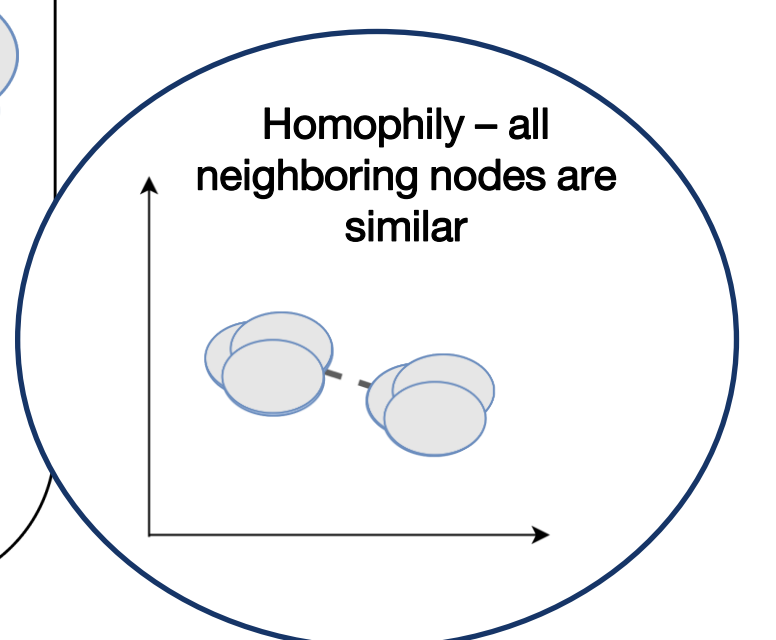
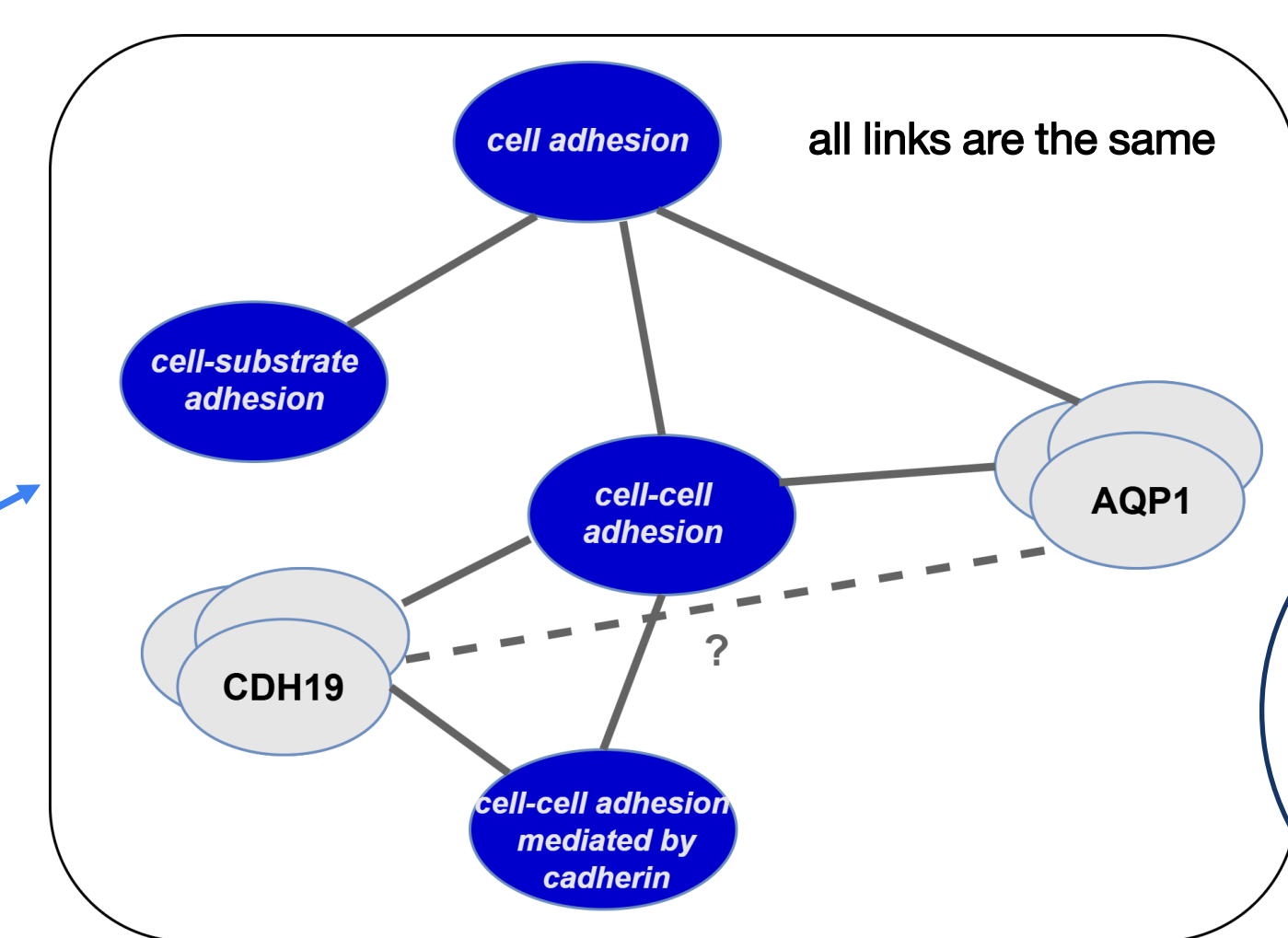
Conflict detection and enrichment

Representation learning



Non-conflict aware

Conflict aware



4 Preliminary experiments

GNN	KG	Acc.	F1	Prec.	Rec.	ROC-AUC	GNN	KG	Acc.	F1	Prec.	Rec.	ROC-AUC
GCN	Full	0.6502	0.6071	0.9440	0.3193	0.9023	GAT	Full	0.5721	0.4795	0.9375	0.1546	0.6913
	w/o contra.	0.6484	0.6041	0.9444	0.3153	0.8998		w/o contra.	0.5690	0.4760	0.9310	0.1491	0.6778
	Negatives	0.6567	0.6175	0.9346	0.3369	0.8954		Negatives	0.6002	0.5287	0.9269	0.2175	0.6777
	Positives	0.6438	0.5970	0.9477	0.3045	0.9007		Positives	0.5672	0.4693	0.9487	0.1419	0.6888
BiGCN	Full	0.6107	0.5451	0.9574	0.2316	0.9002	BiGAT	Full	0.5673	0.4688	0.9452	0.1438	0.6642
	w/o contra.	0.6275	0.5719	0.9546	0.2675	0.8976		w/o contra.	0.5498	0.4420	0.8853	0.1140	0.6255
	Negatives	0.6342	0.5840	0.9391	0.2869	0.8909		Negatives	0.5872	0.5113	0.9105	0.1945	0.6990
	Positives	0.6540	0.6121	0.9475	0.3259	0.9010		Positives	0.5705	0.4743	0.9470	0.1504	0.6636
HGCN	Full	0.6656	0.6294	0.9402	0.3536	0.8916	HGAT	Full	0.5662	0.4702	0.9386	0.1414	0.7030
	w/o contra.	0.6808	0.6501	0.9441	0.3844	0.8888		w/o contra.	0.5661	0.4702	0.9391	0.1415	0.6985
	Negatives	0.6704	0.6358	0.9398	0.3640	0.8904		Negatives	0.5766	0.4891	0.9393	0.1639	0.7021
	Positives	0.6732	0.6396	0.9429	0.3687	0.8912		Positives	0.5506	0.4386	0.9599	0.1057	0.6775

Including contradictions improves performance even if models are not equipped to handle it.

Modeling negative and positive statements separately improves performance.

Potential to increase performance with algorithms that account for contradictions.