Towards Human-like Learning from Relational Structured Data

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Research Goal

Relational structured data is a way of representing knowledge using nodes and edges, while also capturing the meaning of that knowledge in a structured form that can be used for machine learning. (Peter W. Battaglia 2018). Compared with vision and natural language data, relational structured data represents and manipulates structured knowledge, which can be beneficial for tasks that involve reasoning or inference. On the other hand, vision and NLP deal more with unstructured data (like images and text), and they often require different types of models and algorithms to extract useful information or features from the data. **Human-like Learning** develops methods that can harness relational structures and learning-to-learn to rapidly acquire and generalize knowledge to new tasks and situations (Lake and Baroni 2023). With Human-like Learning, the learning algorithm is efficient and is able to adapt to new or unseen situations, which is crucial in real-world applications where environments may change unpredictably. Moreover, the models are easier for humans to understand and interpret, which is important for transparency and trust in AI systems.

Roadmap

The key to achieve the above goal is to develop knowledge and data dual-driven learning methods, which should have the following three properties:

- Data-Specific: design the tailored model on different types of data guided by relational knowledge.
- Sample-efficient: extract meaningful meta-knowledge from limited data, allowing it to generalize effectively to new, unseen examples.
- Interpretable: understand and explain how a model makes predictions with structural evidence.

Works to be Covered

Following recent works from our group will be high-lighted

- Data-Specific side: AutoBLM (Zhang, Yao, and Kwok 2022) automatically designs scoring function for KG learning. Human-designed scoring functions struggle to consistently perform well due to the complex patterns exhibited by relations in KGs. AutoBLM proposes to search scoring functions among bilinear models for KG learning with evolutionary algorithm.
- Sample-efficient side: PAR (Wang et al. 2021) addresses few-shot molecular property prediction in drug discovery with meta learning based on a property-aware embedding function, adaptive relation graph learning, and refining embeddings based on the target property.
- Interpretable side: QL-GNN (Qiu et al. 2023) shows that GNN can capture logical rules from graded model logic, providing a new theoretical tool for interpreting the expressiveness of GNN for KG reasoning. It also concludes that state-of-the-art methods are mainly based on labeling trick due to its simplicity in capturing logical rules.
- Scientific application side: EmerGNN (Zhang et al. 2023) predicts interactions between emerging drugs and existing drugs with GNN that considers connections between biomedical entities and relations. It extracts paths between drugs using a flow-based GNN, propagates information from emerging drugs to existing drugs, providing interpretable evidence using attention weights on the edges.

References

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