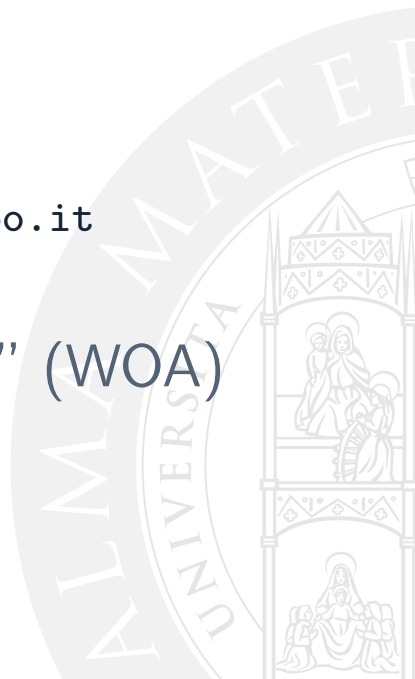
Graph Neural Networks as the Copula Mundi between Logic and Machine Learning: a Roadmap

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Context

- Symbolic and sub-symbolic AI are complementary [2].
- Logic-based techniques are widely used for symbolic approaches.
- Explainable Artificial Intelligence (XAI) is required in modern applications.
- XAI would benefit from the integration between sub-symbolic techniques and symbolic frameworks.



Complex Integration

Combining machine learning (ML) and computational logic (CL) is hard:

- CL relies on symbolic representations.
- ML relies on fixed-size numeric representations.

Complex Integration

Combining machine learning (ML) and computational logic (CL) is hard:

- CL relies on symbolic representations.
- ML relies on fixed-size numeric representations.
- Formulæ vs. Tensors.
- Capability to convert symbols into tensors, and vice versa.



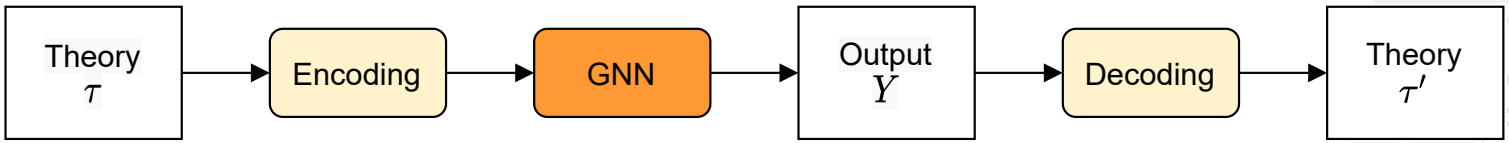
Contribution of the paper

Our contributions

1. Categorise CL problems which may take great advantage from GNN.
2. Discuss how CL problems can be mapped into graph-based tasks.
3. Present end-to-end scenario where GNN are applied to a simple logic knowledge base to detect missing facts.
4. Provide a research roadmap for future works in the integration among CL and GNN.

Framework

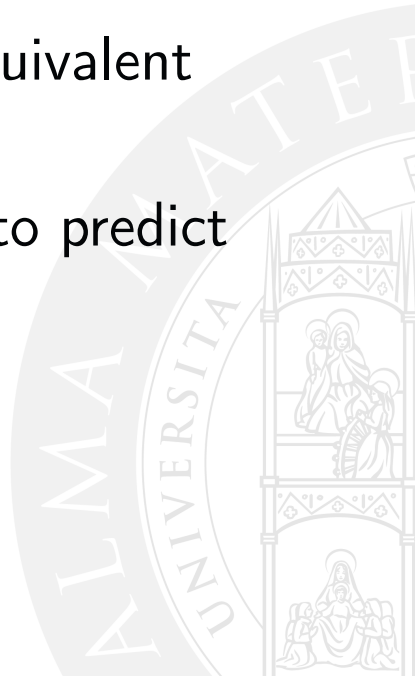
- Knowledge is expressed in terms of logic theories, made up of several logic clauses.
- Knowledge bases can be encoded into graphs aggregating graphs of contained clauses.
- GNN [3] can accept a knowledge base as input to perform sub-symbolic computations on it.
- If needed, obtained graph is decoded to a novel knowledge base.



Logical tasks

There exist relevant tasks hard to formalise or solve into the logic realm:

- **Knowledge filling**, i.e. completing a *fragmented* logic theory.
- **Knowledge inclusion**, i.e. check if theories are complementary and match them.
- **Program equivalence**, i.e. computing a simpler and equivalent theory τ' starting from a theory τ.
- **Resolution speed-up**, i.e. sub-symbolic helper trained to predict frequent queries outcome, speeding up resolution.



Knowledge filling

- Logic reasoners struggle processing knowledge they do not have.
- In sub-symbolic realm, semantic similarities among entities and relations help reconstruct missing facts.
- Map entities of theory to vertices of graph.
- Rules and relations mapped to vectorised arcs between the graph vertices.
- **Knowledge filling** $\rightarrow$ **Link prediction**.



Knowledge inclusion

- Logic reasoners struggle comparing equivalent theories defined differently.
- Requires semantic knowledge of the theory to be taken into account.
- Map entities of theory to vertices of graph.
- Rules and relations mapped to vectorised arcs between the graph vertices.
- **Knowledge Inclusion** $\rightarrow$ **Graph matching**.



Program equivalence

- Logic reasoners struggle to identify compressible theories.
- May require to identify new rules or only drop unnecessary relations.
- Semantic knowledge depends on complexity of compression requirements.
- Mapping between logic and graph is highly dependent on the compression requirements.
- Decoding required to obtain corresponding compressed knowledge base.
- **Program equivalence** $\rightarrow$ **Graph compression**.



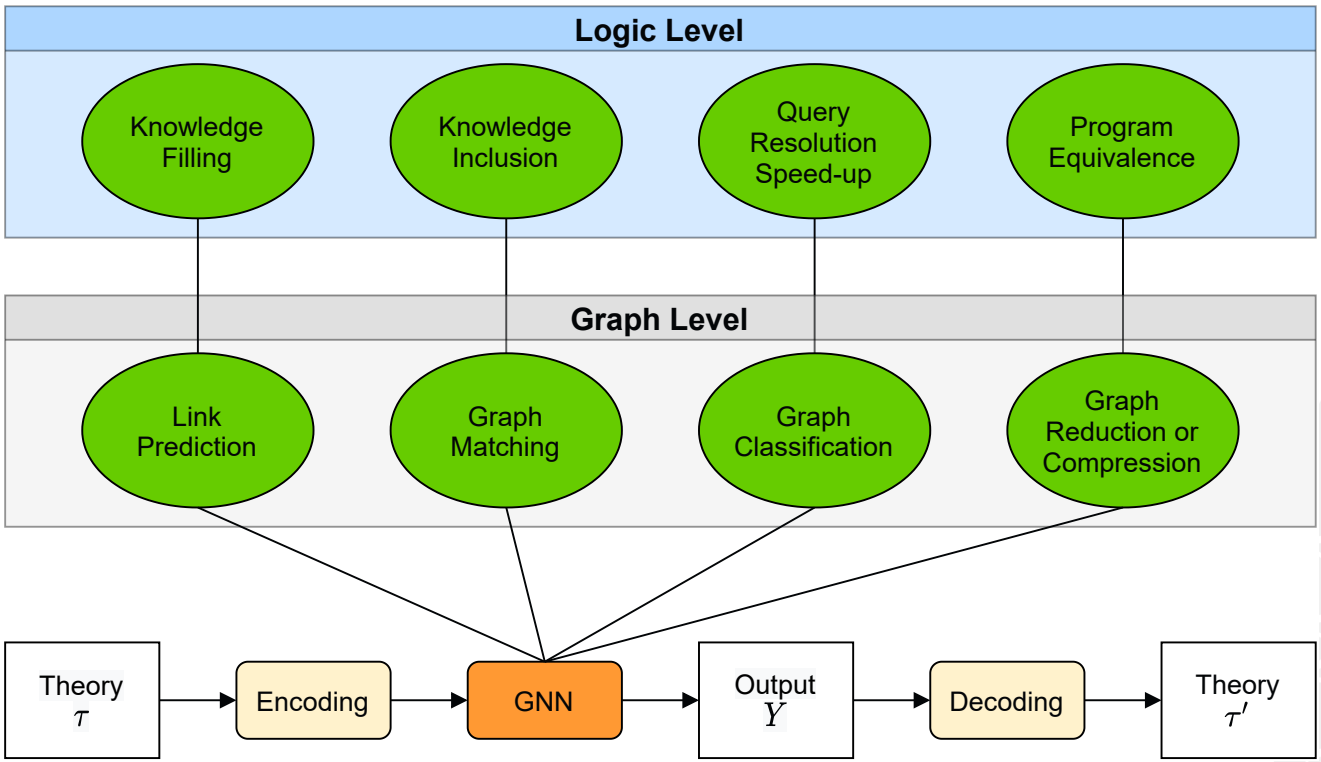
Query resolution speed-up

- Logic reasoners may benefit from sub-symbolic execution to speed-up resolution.
- Semantic knowledge may be required depending on complexity of speed-up.
- Map queries to graphs, rather than whole theory to single graph.
- Query solution is considered the graph label.
- Decoding is not strongly required.
- **Query resolution speed-up** $\rightarrow$ **Graph classification**.



Roadmap

- Logic tasks mapped to graph tasks via encoding.
- Graphs tasks solved sub-symbolically using GNNs.
- If necessary, manipulated knowledge base obtained via decoding.



Case study

- Knowledge filling task for this case study.
- Knowledge base representing kinship relations—i.e. family tree.
- *Mutilate* the knowledge base
- Use remaining knowledge base to reconstruct missing information via proposed framework.



Graph mapping

- Map entities of theory to vertices of graph.
- Rules and relations mapped to vectorised arcs between the graph vertices.

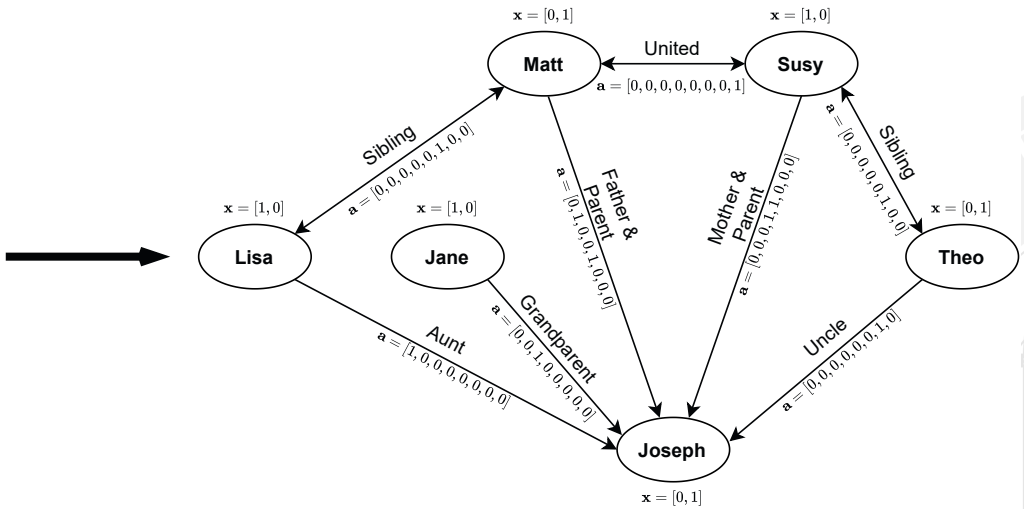
```
sibling(X, Y) :- parent(Z, X), parent(Z, Y), X \= Y.
united(X, Y) :- parent(X, Z), parent(Y, Z), X \= Y.
grandparent(C,D) :- parent(C,E), parent(E,D).
aunt(X, Y) :- female(X), sibling(X, Z), parent(Z, Y).
uncle(X, Y) :- male(X), sibling(X, Z), parent(Z, Y).

male(matt).
male(theo).
male(joseph).

female(susy).
female(lisa).
female(jane).

parent(matt, joseph).
parent(susy, joseph).
parent(jane, matt).

sibling(susy, theo).
sibling(theo, susy).
sibling(matt, lisa).
sibling(lisa, matt).
```



Graph manipulation

- Given graph G representing mutilated theory, task is train GNN mining missing arcs.
- GNN should also classify the arc—i.e. which relation(s) the arc is representing.
- Given nature of graphs, two approaches:

Plain approach

- Consider G as a unique entity [1].
- Predict one solution for each couple of vertices.

Subsampling approach

- Consider G as a pool of subgraphs [4].
- Each subgraph is used to predict if one arc exists.

Results

- Arc classes can overlap—e.g. parent & mother.
- Proposed approach is effective.
- Subsampling approach performs better due to focus on local connections.

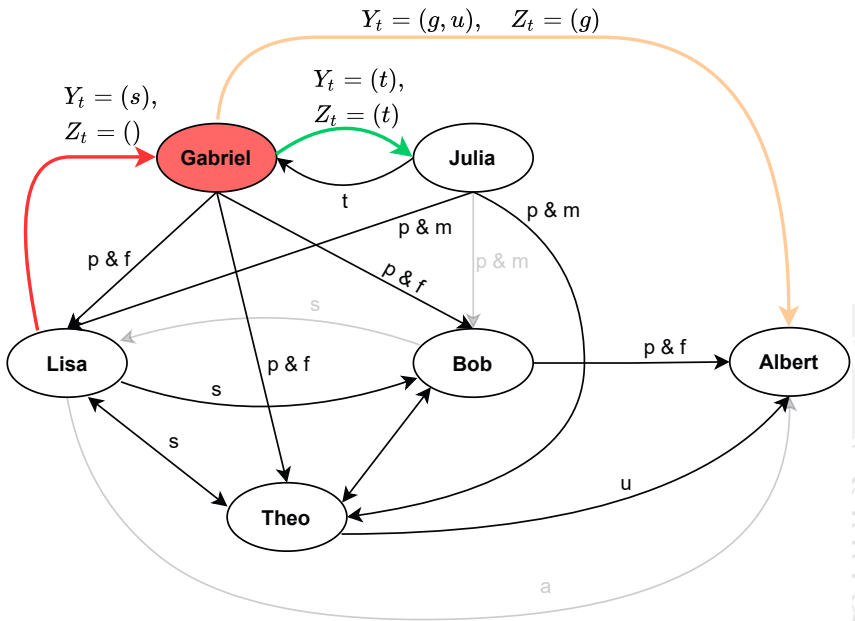
Approach	*Edge Existence*			*Edge Class*		
	AUC	**AP**	**Accuracy**	**EMR**	**F_1**	**PEA**
Plain	0.786	0.786	0.786	0.143	0.148	0.768
Subsampling	0.908	0.892	0.906	0.691	0.386	0.911

- Avoiding class overlap increases effectiveness.

Approach	*Edge Existence*			*Edge Class*		
	AUC	**AP**	**Accuracy**	**EMR**	**F_1**	**PEA**
Plain	0.857	0.857	0.857	0.286	0.214	0.738
Subsampling	0.949	0.961	0.938	0.670	0.340	0.935

Results

- GNNs highly effectively detect missing links.
- Sometimes multiple relations are predicted—NNs suffer multi-labelling.
- GNNs seem to identify missing relations that should exist, even when not defined.



Conclusions

Summing up

- Propose a flexible framework and a roadmap for integrating CL and ML.
- Identify relevant logical problems and describe how they benefit from sub-symbolical techniques.
- Identify possible mappings between logical problems and graph tasks counterpart.
- Demonstrate potential applications and success of the framework.
- Give a future road for research in the area.

Future works

Future research directions

- Apply our framework for tackling relevant logical tasks in CL.
- Deal with GNNs limitations concerning:
  - Hypergraphs.
  - High dimensional vectors for arcs.
  - Relevance of arc attributes.

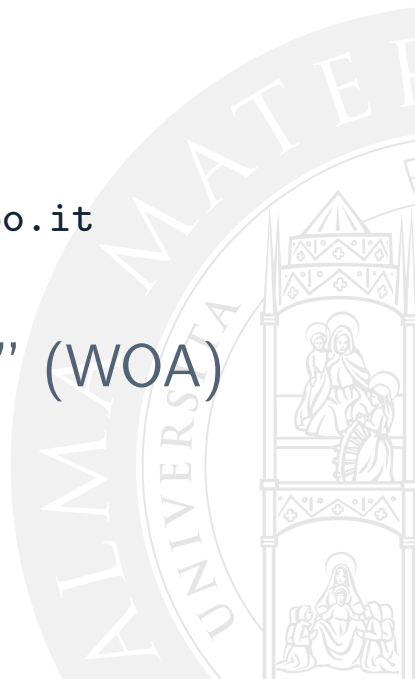


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