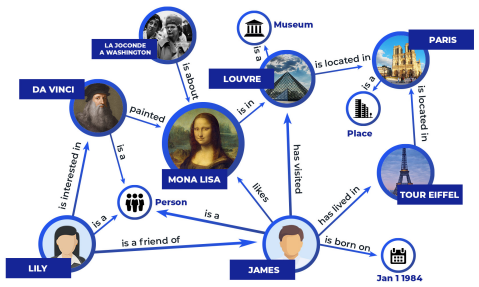
Inductive Relation Prediction Using Analogy Subgraph Embeddings

Jiarui Jin[1], Yangkun Wang[1], Kounianhua Du[1], Weinan Zhang[1], Quan Gan2, Zheng Zhang[2] , Yong Yu[1], David Wipf[2]

[1]Shanghai Jiao Tong University, [2]Amazon

0.0 Background

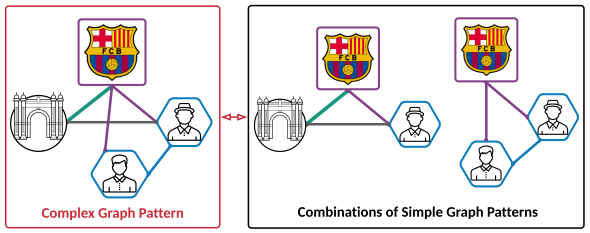
- Knowledge graph is a special heterogeneous graph.
- A set of facts are represented as triples (head entity, relation, tail entity).



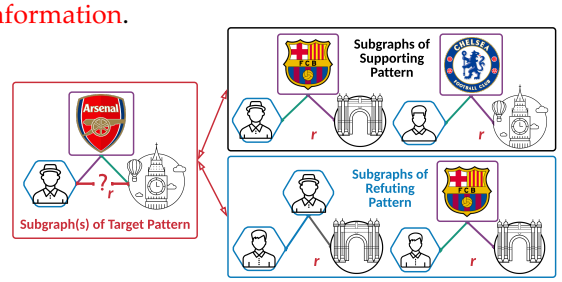
- Inference: Mona Lisa is in Louvre *AND* Louvre is located in Paris → Mona Lisa is in Paris（which constructs a triangle in graph）.

0.1 Logics & Graph patterns

- A relation can often be inferred from other relations with a combination of simple logical rules that do not involve too many nodes.
- This intuitions enable us to only use the simple graph patterns such as pairs, triangles and quadrangles.



- One can predict relation existence by finding whether the subgraphs containing the pair are similar to the (analogy) subgraphs containing an edge with the same relation.
- It allows us to break the limitations of the current graph neural network mainly focusing on the neighborhood information.



1.0 Our Model (GraphANGEL)

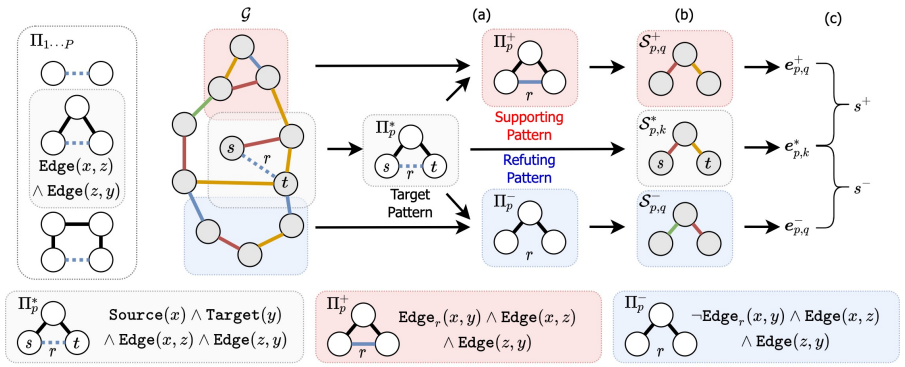


Figure: Overview of GraphANGEL (**AN**alogy sub**G**raph **E**mbedding **L**earning) where different edge colors in the graph represent different relation types, and dashed edge in graph represent the triplet we wish to predict. The left box shows the patterns considered in our implementation, where black edges mean matching edges irrespective of relation types. The bottom boxes show the logical function of the three patterns.

1.1 Search and Retrieval Module

Theorem 1. (Time Complexity of Retrieval and Sampling) *Given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and a graph pattern $\Pi_{3-\texttt{cycle}}$ in 3-cycle and a graph pattern $\Pi_{4-\texttt{cycle}}$ in 4-cycle, the time complexity of retrieving all the (supporting) subgraphs satisfying $\Pi_{3-\texttt{cycle}}$ is $O(|\mathcal{E}|^{\frac{3}{2}})$, of retrieving all the (supporting) subgraphs satisfying $\Pi_{4-\texttt{cycle}}$ is $O(\max(|\mathcal{E}|^{\frac{3}{2}}, N_{4-\texttt{cycle}}))$ where $N_{4-\texttt{cycle}}$ is the number of quadratic cycles in $\mathcal{G}$ and also the trivial lower bound of the time complexity. For uniform sampling algorithms, the time complexity of sampling $n_{4-\texttt{cycle}}$ supporting cases of $\Pi_{4-\texttt{cycle}}$ is $O(|\mathcal{E}|^{\frac{3}{2}} + n_{4-\texttt{cycle}})$. As there are usually more refuting cases than supporting ones, the time complexity of sampling n refuting cases of $\Pi_{3-\texttt{cycle}}$ or $\Pi_{4-\texttt{cycle}}$ is $O(|\mathcal{V}| + |\mathcal{E}| + n)$.*

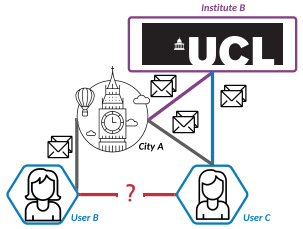
Algorithm 3: Search and Retrieval Algorithm B for $\Pi_{3-\texttt{cycle}}$

$\mathcal{B} \leftarrow \{\}$
foreach $u \in \mathcal{V}$ **do**
  foreach $v \in \mathcal{N}_{\mathcal{G}}(u)$ where $d_v \leq d_u$ **do**
    foreach $w \in \mathcal{N}_{\mathcal{G}}(v)$ where $d_w \leq d_v$ **do**
      if $\langle v, w \rangle \in \mathcal{E}$ **then**
        $\mathcal{B} \leftarrow \mathcal{B} \cup \{(u, v, w)\}$
      end
    end
  end
end

Algorithm 4: Search and Retrieval Algorithm for $\Pi_{4-\texttt{cycle}}$

$\mathcal{B} \leftarrow \{\}$
foreach $u \in \mathcal{V}$ **do**
  $\mathcal{T}_x \leftarrow \{\}$ for each $x \in \mathcal{V}$
  foreach $v \in \mathcal{N}_{\mathcal{G}}(u)$ where $d_v \leq d_u$ **do**
    foreach $w \in \mathcal{N}_{\mathcal{G}}(v)$ where $d_w \leq d_u$ **do**
      foreach $x \in \mathcal{T}_w$ **do**
        $\mathcal{B} \leftarrow \mathcal{B} \cup \{(u, v, w, x)\}$
      end
      $\mathcal{T}_w \leftarrow \mathcal{T}_w \cup \{v\}$
    end
  end
end

1.2 Encoding Algorithms



MESSAGE PASSING:

$$m_v^{t+1} = \sum_{w \in \mathcal{N}(v)} M_t(h_v^t, h_w^t, e_{vw})$$

$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

M_t is message function and U_t is vertex update function, hidden states h_v^t at each node in the graph are updated based on messages m_v^{t+1}.

READOUT:

$$y = R(\{h_v^T | v \in G\})$$

The message function M_t , vertex update function U_t, and readout function R are all learned differentiable function.

1.3 Pros of Our Model

- Our model combines the expressive power of graph neural networks and logical rules.
- Our model breaks the limitation of modelling neighbor connectivity of graph neural networks.
- Each graph pattern explicitly represents a specific logical rule, which contributes to an inductive bias that facilitates generalization to unseen relation types and leads to more explainable predictive models.

2.0 Experiments

Table 2: Patterns Π_p considered in our experiments.

Task	Pair	3-cycle (with type)	4-cycle (with type)
Knowledge Graph Completion	`true`	$\texttt{Edge}(x, z) \wedge \texttt{Edge}(z, y)$	$\texttt{Edge}(x, z) \wedge \texttt{Edge}(z, w) \wedge \texttt{Edge}(w, y)$
Heterogeneous Graph Recommendation	`true`	$\texttt{Edge}_a(x, z) \wedge \texttt{Edge}_b(z, y)$	$\texttt{Edge}_a(x, z) \wedge \texttt{Edge}_b(z, w) \wedge \texttt{Edge}_c(w, y)$

Table 3: Result comparisons with baselines on heterogeneous graph recommendation task.

Models	LastFM			Yelp			Amazon			Douban Book		
	AUC	ACC	F1	AUC	ACC	F1	AUC	ACC	F1	AUC	ACC	F1
HetGNN	0.7936	0.7258	0.7177	0.9083	0.8297	0.8205	0.7744	0.7108	0.7109	0.8737	0.7912	0.7915
HAN	0.8915	0.8337	0.8296	0.9156	0.8488	0.8426	0.8487	0.7682	0.7572	0.9244	0.8501	0.8458
TAHIN	0.8910	0.8463	0.8337	0.9067	0.8490	0.8393	0.8535	0.7718	0.7644	0.9253	0.8497	0.8373
HGT	0.8394	0.7939	0.7882	0.9006	0.8375	0.8334	0.7125	0.6482	0.6296	0.9132	0.8364	0.8222
R-GCN	0.8526	0.8393	0.8341	0.9098	0.8427	0.8323	0.8130	0.7408	0.7366	0.9203	0.8413	0.8271
GraphANGEL$_{3-\texttt{cycle}}$	0.8934	0.8519	0.8465	0.9167	0.8498	0.8514	0.8601	0.7746	0.7746	0.9256	0.8512	0.8479
GraphANGEL$_{4-\texttt{cycle}}$	0.8961	0.8514	0.8467	0.9201	0.8506	0.8521	0.8609	0.7752	0.7716	0.9242	0.8502	0.8378
GraphANGEL	0.8979	0.8524	0.8469	0.9231	0.8512	0.8533	0.8611	0.7790	0.7753	0.9311	0.8601	0.8543
GraphANGEL*	**0.9001**	**0.8611**	**0.8589**	**0.9337**	**0.8701**	**0.8577**	**0.8700**	**0.7810**	**0.7813**	**0.9410**	**0.8640**	**0.8591**

Table 4: Result comparisons with baselines on knowledge graph completion task.

Models	FB15k-237					WN18RR				
	MR	MRR	Hit@1	Hit@3	Hit@10	MR	MRR	Hit@1	Hit@3	Hit@10
pLogicNet	173	0.332	0.237	0.367	0.524	3408	0.441	0.398	0.446	0.537
TransE	181	0.326	0.229	0.363	0.521	3410	0.223	0.235	0.401	0.531
ConvE	244	0.325	0.237	0.356	0.501	4187	0.430	0.400	0.440	0.520
ComplEx	339	0.247	0.158	0.275	0.428	5261	0.440	0.410	0.460	0.510
MLN	1980	0.098	0.067	0.103	0.160	11549	0.259	0.191	0.322	0.361
RotatE	177	0.338	0.241	0.375	0.533	3340	0.476	0.428	0.492	0.571
RNNLogic	232	0.344	0.252	0.380	0.530	4615	0.483	0.446	0.497	0.558
ComplEx-N3	159	0.370	0.272	0.400	0.561	3452	0.491	0.440	0.500	0.581
GraIL	205	0.322	0.223	0.361	0.520	3539	0.401	0.352	0.438	0.501
QuatE	**87**	0.348	0.248	0.382	0.550	**2314**	0.488	0.438	0.508	0.582
GraphANGEL$_{3-\texttt{cycle}}$	159	0.366	0.270	0.398	0.560	2919	0.492	0.463	0.497	0.590
GraphANGEL$_{4-\texttt{cycle}}$	165	0.351	0.239	0.381	0.548	2914	0.493	0.465	0.502	0.587
GraphANGEL	151	**0.374**	**0.275**	**0.408**	**0.564**	2834	**0.504**	**0.470**	**0.515**	**0.598**
	±3	±0.003	±0.002	±0.004	±0.004	±25	±0.003	±0.002	±0.004	±0.004

If you have any question, please feel free to contact Jiarui Jin (jinjiarui97@gmail.com)