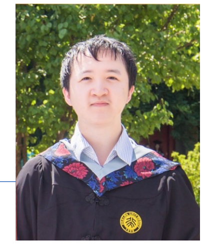
Cycle Representation Learning for Inductive Relation Prediction

Zuoyu Yan, Tengfei Ma, Liangcai Gao, Zhi Tang, Chao Chen



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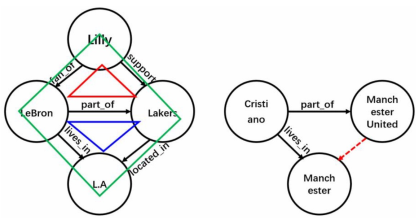
Introduction

- Inductive relation prediction: to predict whether a link (triplet) exists in a totally new knowledge graph (KG) based on rules.
- Motivation: existing inductive relation prediction methods cannot balance computational cost and prediction performance.



- We treat rules as cycles, then the rules in the KG form its cycle space. We use the basis of the cycle space to explore the "right cycles" for
  - Efficient rule learning (decrease the parameter space from exponential to linear).
  - The basis can express all cycles (rules) theoretically.

Cycle Space and Cycle Basis

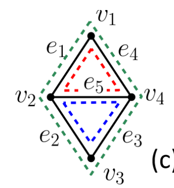
- All cycles in the input KG constitute a vector space under modulo-2 additions and multiplications.
- A cycle basis is a basis spanning the cycle space.
- The number of elements in the basis, is the so-called Betti number, β. The cycle space has size 2^{β}.

Contribution:

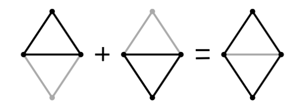
- For the first time, investigate inductive relation prediction through a cycle-centric perspective.
- Efficiently explore rule space through cycle bases
- Propose a novel model CBGNN to learn rules, and achieve SOTA on benchmarks.

Pursuit of Suitable Bases

- Cycle bases that can be easily encoded: shortest path tree (SPT) cycle bases that contain relatively short cycles and can be computed efficiently.
- Cycle bases than can efficiently represent good cycles: multiple SPT cycle bases to ensure locality and sufficient coverage.



(c)



(d)

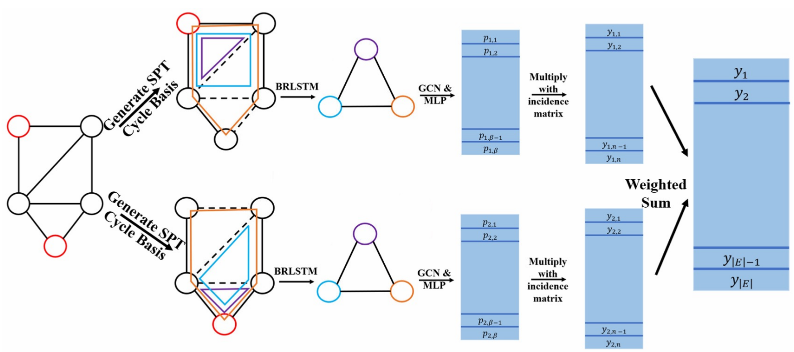
$$\begin{array}{c|ccccc} & e_1 & e_2 & e_3 & e_4 & e_5 \\ \hline v_1 & 1 & 0 & 0 & 1 & 0 \\ v_2 & 1 & 1 & 0 & 0 & 1 \\ v_3 & 0 & 1 & 1 & 0 & 1 \\ v_4 & 0 & 0 & 1 & 1 & 0 \end{array}$$

(e)

$$\begin{array}{c|ccc} & z_r & z_b & z_g \\ \hline e_1 & 1 & 0 & 1 \\ e_2 & 0 & 1 & 1 \\ e_3 & 0 & 1 & 1 \\ e_4 & 1 & 0 & 1 \\ e_5 & 1 & 1 & 0 \end{array}$$

(f)

Cycle Basis Graph Neural Network (CBGNN)



(a) Input KG (b) SPT Cycle Basis (c) Cycle Graph (d) Cycle confidence (e) Triplet confidence

- Construct cycle bases, and build a cycle graph for each cycle basis. In the cycle graph, nodes represent cycles in the basis, edges represent the corresponding cycles have a strong interaction.
- Build a GNN on the cycle graph to learn confidence value for cycles. Then map the cycle confidence to triplet confidence. GNNs among all cycle graphs share weights and their aggregation is used to predict the final confidence value.
- Minimize the cross-entropy loss using negative sampling

Experiments

Table 1. AUC-PR scores of inductive relation prediction, the baseline results are copied from (Teru et al., 2020; Mai et al., 2021).

	WN18RR				FB15K-237				NELL-995			
Method	v1	v2	v3	v4	v1	v2	v3	v4	v1	v2	v3	v4
NeuralLP	86.02	83.78	62.90	82.06	69.64	76.55	73.95	75.74	64.66	83.61	87.58	85.69
DRUM	86.02	84.05	63.20	82.06	69.71	76.44	74.03	76.20	59.86	83.99	87.71	85.94
RuleN	90.26	89.01	76.46	85.75	75.24	88.70	91.24	91.79	84.99	88.40	87.20	80.52
GraIL	94.32	94.18	85.80	92.72	84.69	90.57	91.68	94.46	**86.05**	92.62	93.34	87.50
CoMPILE	98.23	**99.56**	**93.60**	**99.80**	85.50	91.68	93.12	94.90	80.16	**95.88**	96.08	85.48
CBGNN	**98.63**	97.62	89.76	97.80	**96.34**	**96.53**	**96.38**	**95.23**	82.79	94.78	**96.29**	**94.02**

Table 3. Evaluation of computational efficiency (second).

Dataset	WN18RR v1			FB15K-237 v1			NELL-995 v1		
Phase	Preparation	Training	Inference	Preparation	Training	Inference	Preparation	Training	Inference
GraIL	452.36	2230.55	1.07	704.42	9026.21	1.67	402.86	3718.22	1.79
CoMPILE	434.45	2388.28	1.46	706.19	3809.56	2.41	479.21	2868.38	1.23
CBGNN	601.96	952.55	0.52	437.13	901.27	0.75	379.29	175.19	0.14

Table 4. AUC-PR scores of ablation study.

	WN18RR				FB15K-237				NELL-995			
Method	v1	v2	v3	v4	v1	v2	v3	v4	v1	v2	v3	v4
CBGNN-MLP	96.33	97.49	86.86	95.22	90.90	94.07	87.01	87.78	72.29	93.35	94.63	91.29
CBGNN-Random	97.13	76.64	87.30	93.47	96.23	96.07	93.27	94.49	**83.69**	93.73	96.20	92.94
CBGNN-Single	58.96	58.05	55.67	61.61	81.67	84.28	81.75	79.44	72.29	83.79	90.70	80.97
CBGNN-BOW	97.54	96.45	86.83	97.46	96.04	**97.61**	**96.85**	**97.00**	75.31	90.25	91.00	87.53
CBGNN-LSTM	98.26	97.04	89.69	97.75	95.86	91.46	94.56	92.47	71.85	93.33	93.74	85.78
CBGNN	**98.63**	**97.62**	**89.76**	**97.80**	**96.34**	96.53	96.38	95.23	82.79	**94.78**	**96.29**	**94.02**