How to Turn your Knowledge Graph Embeddings into Generative Models

Paper

Code

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TL;DR *"We reinterpret KGE models into generative models of triples, making them to scale to large knowledge graphs, reliable with logical constraints and supporting sampling."*

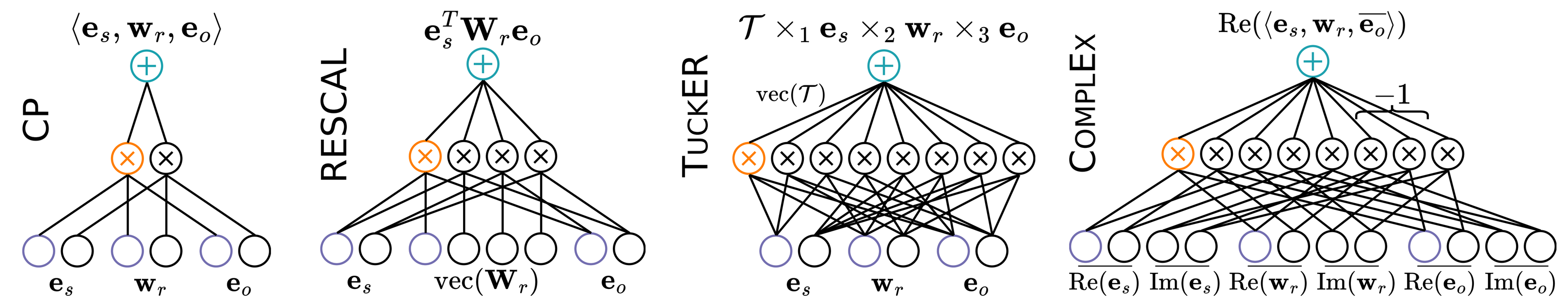
Knowledge graph embedding (KGE) models

Issues?

1 Scores are difficult to interpret, combine, compare [1].
How to measure the confidence of predictions?

2 Link predictions violate logical constraints.
How to guarantee the satisfaction of constraints?

3 KGE models are expensive to learn.
How to scale to KGs with millions of entities?

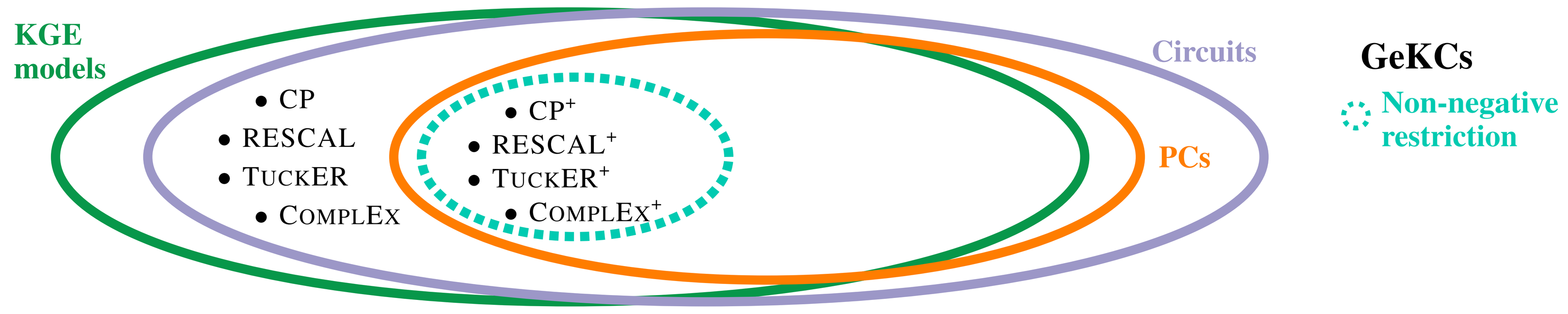


Interpreting the score functions of KGE models as constrained computational graphs: circuits [2]

1 From KGE models to probabilistic circuits (PCs)

We convert score functions (i.e., circuits) into ***probabilistic circuits*** (PCs) [2, 3] without additional memory requirements.

$$p(s,r,o) = \frac{1}{Z}\,\phi_{\mathsf{pc}}(s,r,o) \qquad \text{s.t.} \qquad \phi_{\mathsf{pc}}(s,r,o) \geq 0$$



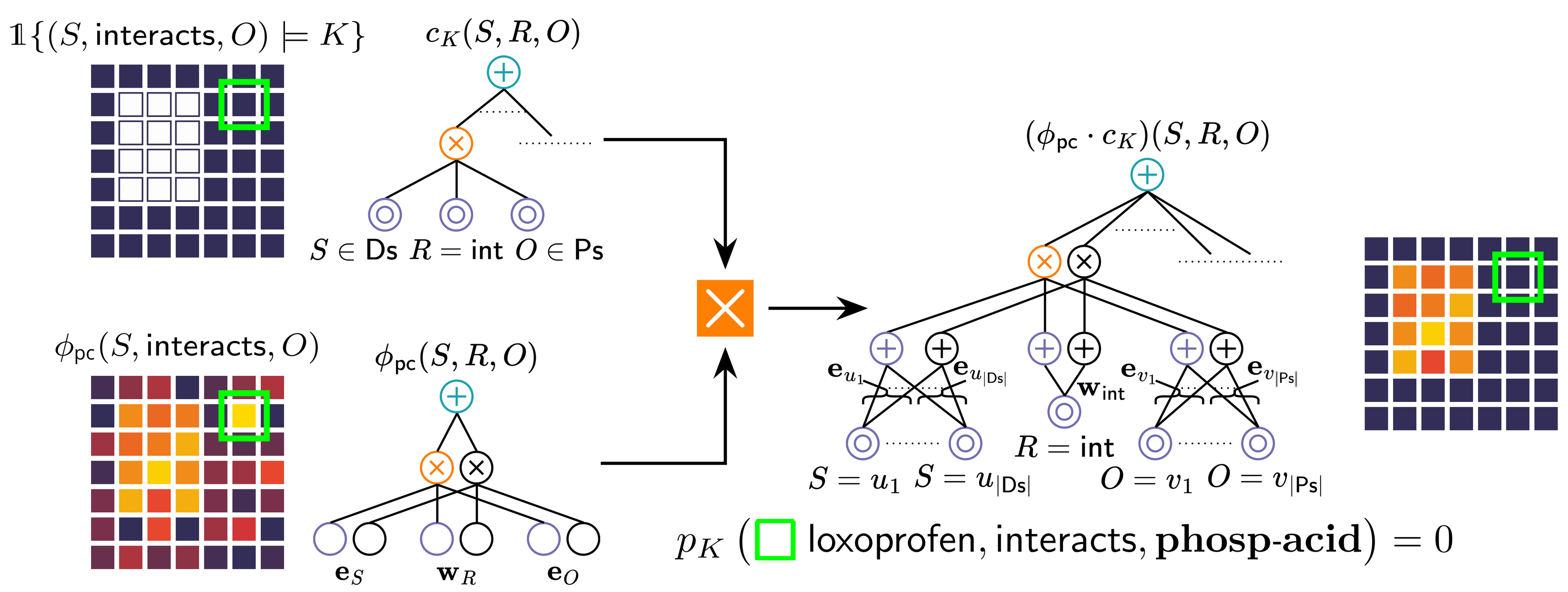
Generative KGE circuits (GeKCs) obtained via:

Non-negative restriction make the embeddings and computational unit activations non-negative;

or **Squaring the score function** square the circuit [4] without restricting the parameters domain, e.g.,

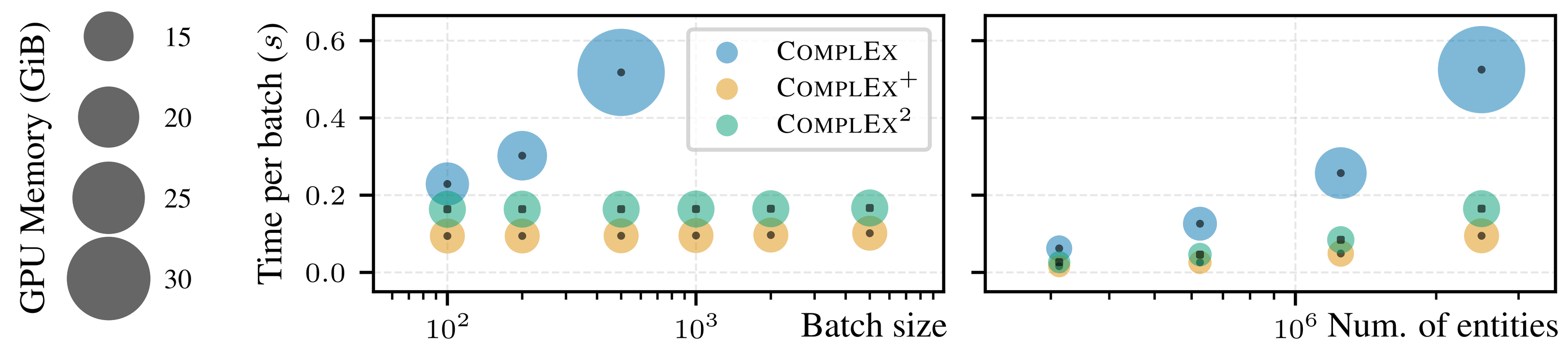
$$\phi_{\mathsf{CP}^2}(s,r,o) = \left(\sum_{i=1}^{d} \mathbf{e}_{si}\mathbf{w}_{ri}\mathbf{e}_{oi}\right)^2 = \sum_{i=1}^{d}\sum_{j=1}^{d} \mathbf{e}_{si}\mathbf{e}_{sj}\mathbf{w}_{ri}\mathbf{w}_{rj}\mathbf{e}_{oi}\mathbf{e}_{oj}$$

2 Integration of constraints with guarantees



[5]

3 Scaling to KGs with millions of entities



Link prediction benchmarks

Model	FB15k-237		WN18RR		ogbl-biokg	
	PLL	MLE	PLL	MLE	PLL	MLE
CP	0.310	—	**0.105**	—	0.831	—
CP+	0.237	0.230	0.027	0.026	0.496	0.501
CP²	**0.315**	0.282	**0.104**	0.091	**0.848**	0.829
ComplEx	**0.342**	—	**0.471**	—	0.829	—
ComplEx+	0.214	0.205	0.030	0.029	0.503	0.516
ComplEx²	0.334	0.300	0.420	0.391	**0.858**	0.840

Bonus *Sampling triples*

$$\mathrm{KTD}(\mathbb{P},\mathbb{Q}) = \|\, \mathbb{E}_{\mathbf{x}\sim\mathbb{P}}[\, \varphi(\psi(\mathbf{x}))\,] - \mathbb{E}_{\mathbf{z}\sim\mathbb{Q}}[\, \varphi(\psi(\mathbf{z}))\,]\,\|^2$$

References

[1] Erik Arakelyan, Pasquale Minervini, and Isabelle Augenstein. *Adapting Neural Link Predictors for Complex Query Answering*. 2023. arXiv: 2301.12313 [cs.LG].

[2] Antonio Vergari, Nicola Di Mauro, and Guy Van den Broeck. "Tractable probabilistic models: Representations, algorithms, learning, and applications". In: *Tutorial at the 35th Conference on Uncertainty in Artificial Intelligence (UAI)* (2019).

[3] YooJung Choi, Antonio Vergari, and Guy Van den Broeck. "Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling". In: (2020).

[4] Antonio Vergari et al. "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference". In: *Advances in Neural Information Processing Systems 34 (NeurIPS)*. Curran Associates, Inc., 2021, pp. 13189–13201.

[5] Kareem Ahmed et al. "Semantic probabilistic layers for neuro-symbolic learning". In: *Advances in Neural Information Processing Systems 35 (NeurIPS)*. Vol. 35. Curran Associates, Inc., 2022, pp. 29944–29959.