How to Turn your Knowledge Graph Embeddings into Generative Models via Probabilistic Circuits

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TL;DR: *"We cast KGE models into generative models supporting exact and efficient marginalisation, sampling and the integration of propositional constraints with guarantees."*

From Knowledge Graph Embeddings ...

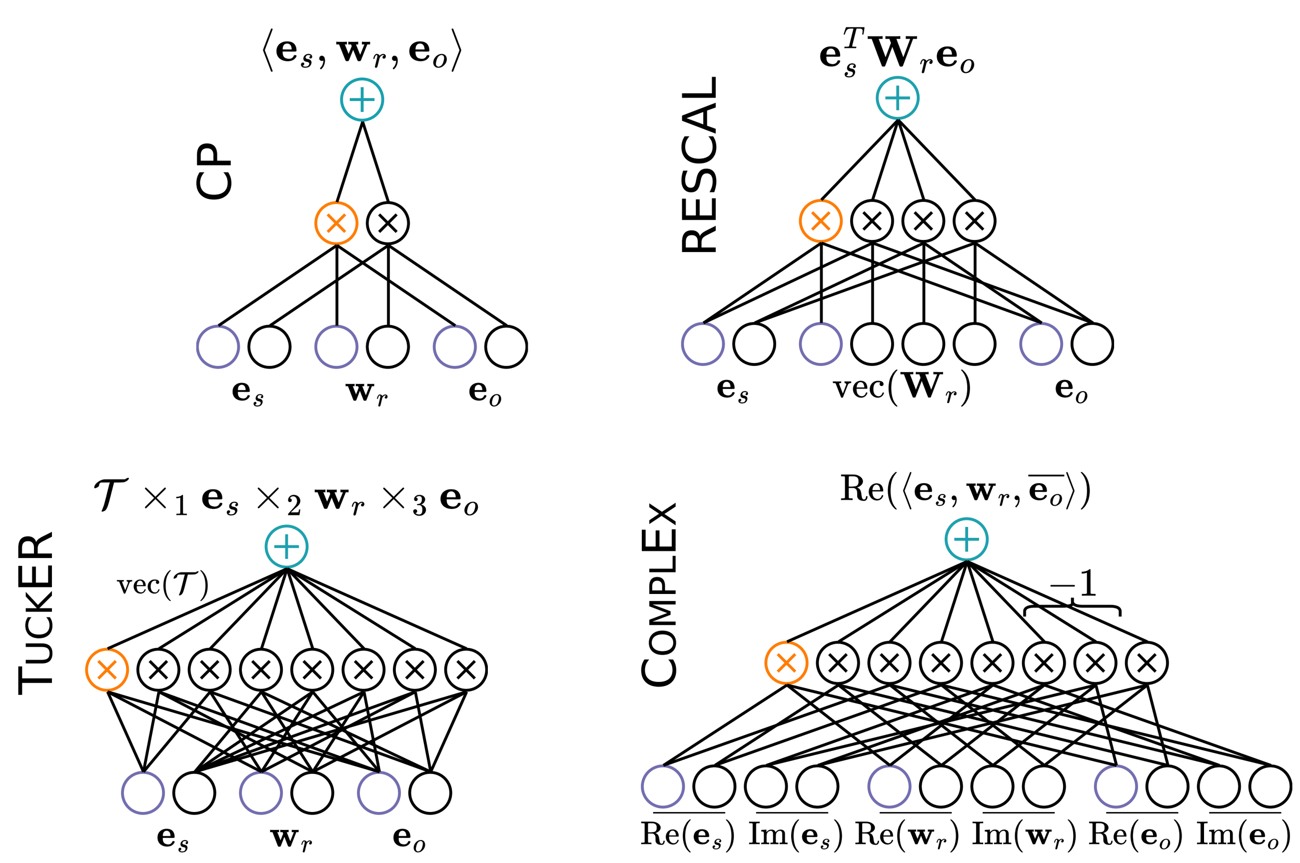
A Knowledge Graph Embeddings (KGE) model can be interpreted as an *energy-based model* defining an unnormalized distribution over triples (S, R, O)

$$p(S=s, R=r, O=o) = \frac{1}{Z}\exp\phi(s,r,o)$$

where $\phi : \mathcal{E}\times\mathcal{R}\times\mathcal{E}\to\mathbb{R}$ is a triple score function.

KGE models have several **shortcomings**:

1. Computing triple probabilities is impractical
   Z requires 10^{11} evaluations of ϕ on FB15K-237 [5]
   thus comparing triple scores is not easy
2. Learning by maximum-likelihood is infeasible
   requires contrastive objectives or
   expensive cross-entropies, e.g., $\log p(o \mid s, r)$ [4]
3. Logical constraints are violated at test time [3]
   e.g., $Q:(\text{loxoprofen}, \text{interacts}, ?)$
   $A:\text{phosphoric-acid}$ *(not a protein!)*
4. No efficient way of sampling new triples
   useful for data augmentation or negative sampling



*Interpreting the score functions of KGE models as constrained computational graph: **circuits**.*

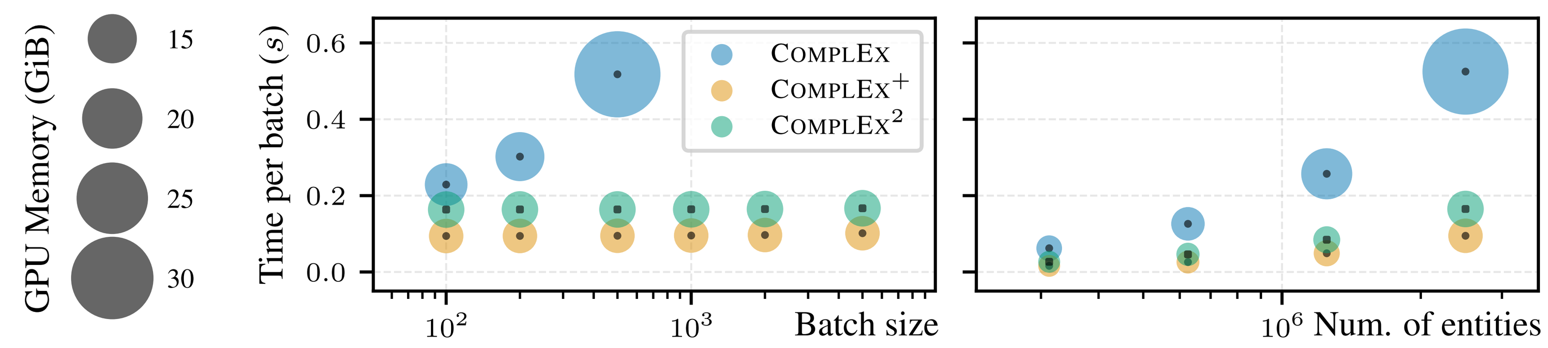
... to Probabilistic Circuits

We cast score functions to *probabilistic circuits* (PCs) [1] ϕ_{pc} without additional memory requirements

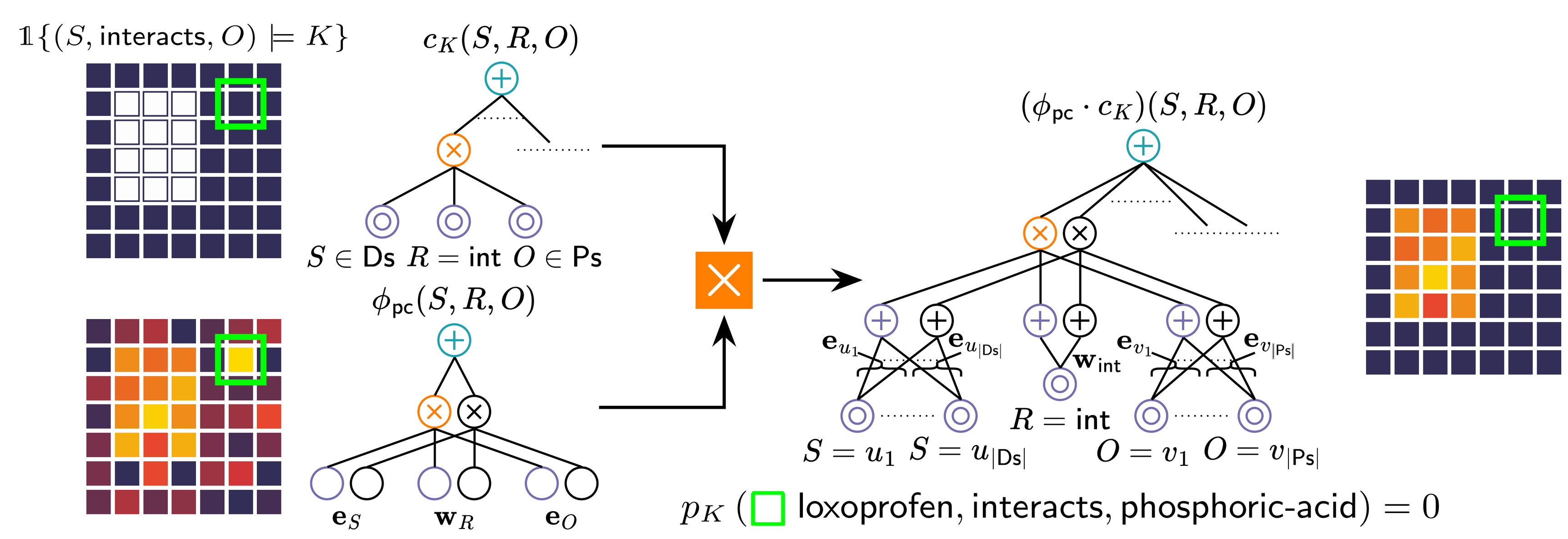
$$p(s,r,o) = \frac{1}{Z}\phi_{\text{pc}}(s,r,o) \quad s.t. \quad \phi_{\text{pc}}(s,r,o)\geq 0$$

- **Non-negative restriction**: make the embeddings and unit activations non-negative [2]
- **Squaring the score function**: square the circuit, without restricting the parameters domain [6], e.g.,

$$\phi_{\text{CP}^2}(s,r,o) = \langle \mathbf{e}_s, \mathbf{w}_r, \mathbf{e}_o\rangle^2 = \sum_{i=1}^{d}\sum_{j=1}^{d} e_{si}e_{sj}w_{ri}w_{rj}e_{oi}e_{oj}$$



Scaling training on KGs with millions of entities.



Integration of domain constraints with guarantees.

The perks

Computing Z and any marginal/conditional probability can be done in time $\mathcal{O}((|\mathcal{E}|+|\mathcal{R}|)\cdot\text{cost}(\phi_{\text{pc}}))$, whilst being more memory efficient at exploiting GPUs

e.g., $Z = \sum_{(s,r,o)}\phi_{\text{CP}}(s,r,o) = \langle \sum_s \mathbf{e}_s, \sum_r \mathbf{w}_r, \sum_o \mathbf{e}_o\rangle$

1. Efficient computation of triple probabilities
   comparable scores across different models and queries
2. More efficient learning by maximum-likelihood and by using classification objectives
3. Propositional logical constraints satisfied *by design*
   e.g., $K := S\in\text{Drugs}\wedge R=\text{interacts}\wedge O\in\text{Proteins}$
   $p_K(\text{loxoprofen}, \text{interacts}, \text{phosphoric-acid}) = 0$
4. Efficient sampling of *high quality* new triples
   via ancestral or inverse transform sampling

Our *Generative KGE Circuits* (GeKCs) are competitive with traditional KGE models, *while coming with the above perks!*

Model	FB15k-237				WN18RR				ogbl-biokg			
	PLL		MLE		PLL		MLE		PLL		MLE	
CP	0.310	(8)	—		**0.105**	(11)	—		0.831	(136)	—	
CP$^+$	0.237	(1)	0.230	(1)	0.027	(1)	0.026	(1)	0.496	(172)	0.501	(142)
CP^2	**0.315**	(8)	0.282	(7)	**0.104**	(23)	0.091	(23)	**0.848**	(66)	0.829	(61)
ComplEx	**0.342**	(36)	—		**0.471**	(16)	—		0.829	(180)	—	
ComplEx$^+$	0.214	(10)	0.205	(5)	0.030	(6)	0.029	(3)	0.503	(245)	0.516	(212)
ComplEx^2	0.334	(10)	0.300	(16)	0.420	(37)	0.391	(19)	**0.858**	(71)	0.840	(59)

References

[1] YooJung Choi, Antonio Vergari, and Guy Van den Broeck. *Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling*. Tech. rep. University of California, Los Angeles (UCLA), 2020.

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[3] Nicolas Hubert et al. "New Strategies for Learning Knowledge Graph Embeddings: The Recommendation Case". In: *EKAW*. Vol. 13514. Lecture Notes in Computer Science. Springer, 2022, pp. 66–80.

[4] Daniel Ruffinelli, Samuel Broscheit, and Rainer Gemulla. "You CAN Teach an Old Dog New Tricks! On Training Knowledge Graph Embeddings". In: *ICLR*. OpenReview.net, 2020.

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[6] Antonio Vergari et al. "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference". In: *Advances in Neural Information Processing Systems*. Vol. 34. 2021, pp. 13189–13201.