Systematic Relational Reasoning With Epistemic Graph Neural Networks

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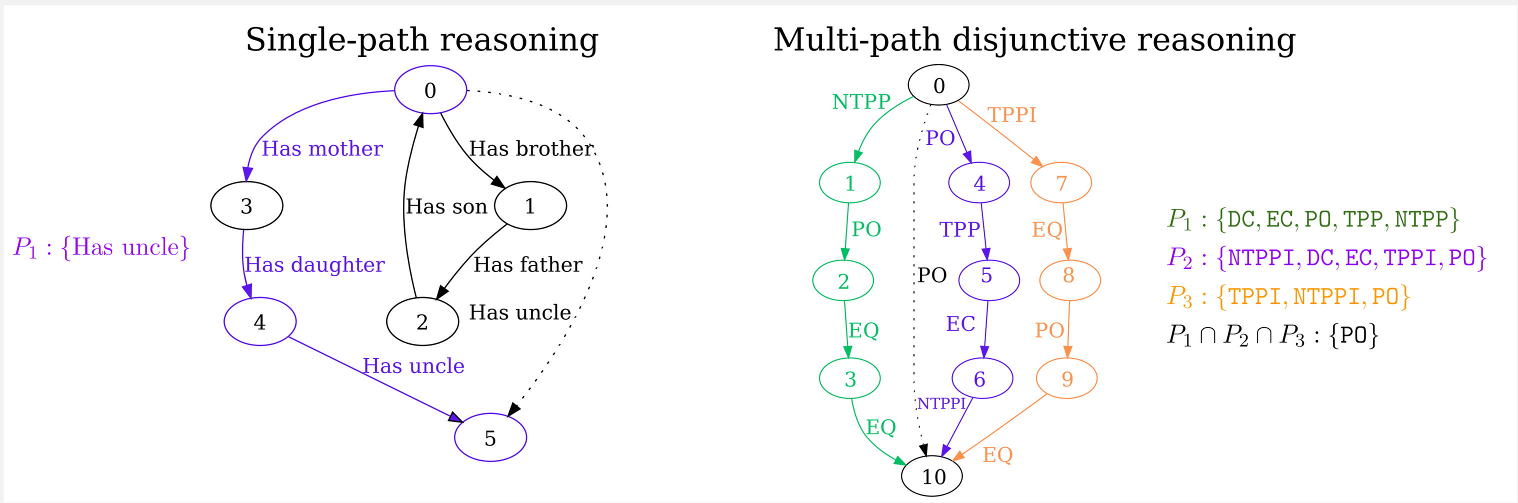
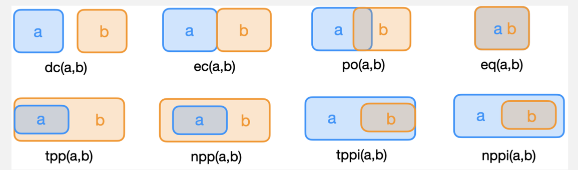
1. TL;DR

1. **Goal:** relational Systematic Generalization (SG) [1] and (generalized) disjunctive reasoning.
2. **New Benchmark:** A novel, multi-path, disjunctive, Spatio-Temporal Reasoning benchmark (STaR) for SG on RCC-8 [2] and Interval Algebra (IA) [3] calculi.
3. **New GNN:** A novel GNN, the Epistemic Graph Neural network (EpiGNN), aligned with directional algebraic closure algorithm that solves disjunctive reasoning.
4. **disjunctive SOTA:** EpiGNN rivals neurosymbolic SOTA on single-path SG, outperforms them on STaR, all while being at least two orders of magnitude more parameter-efficient.
5. **Ability retention:** Designed for SG-type link prediction, EpiGNNs rival specialized SOTA for inductive Knowledge Graph Completion (KGC) drop in performance slightly suggesting inductive bias trade-offs between SG and KGC.

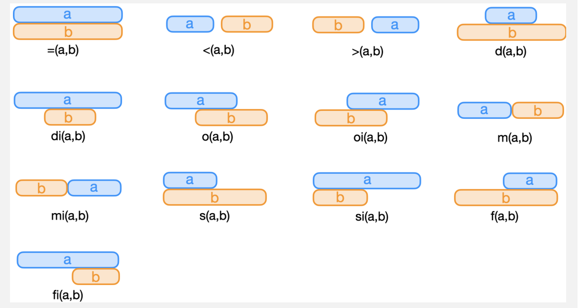
2. Systematic Relational Reasoning and STaR



STaR example



RCC-8 relations [2]



IA relations [3]

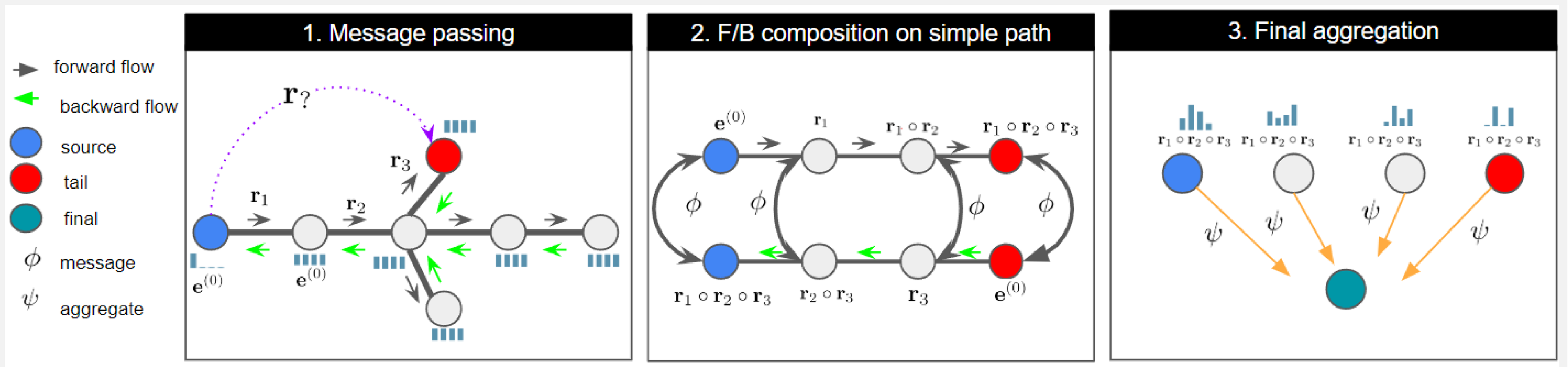
Table 1: Main differences between STaR with previous art.

Previous art e.g. CLUTRR, GraphLOG	STaR
Horn (AND) rules for composition $r(X_1, X_n) \leftarrow r_1(X_1, X_2) \wedge r_2(X_2, X_3)$	Disjunctive (OR) rules for composition $s_1(X_1, X_n) \vee \ldots \vee s_k(X_1, X_n) \leftarrow r_1(X_1, X_2) \wedge r_2(X_2, X_3)$
Single-path based	Multi-path based information aggregation
Random (non-diverse) graph topologies	Rich graph topologies via recursive edge expansion

Spatio-Temporal Reasoning (STaR) benchmark for Systematic Generalization (SG):

- SG is framed as a graph link classification problem $(s, ?, t)$.
- **(Def) SG** is the ability of a model to solve test instances by composing knowledge that was learned from multiple training instances [1], where the test instances are typically larger than the training instances.
- **Problem complexity parameters** : s-t path length k (number of edges) and number of s-t paths b
- **Train/test split:** Train on $k = 2, 3, 4$, $b = 1, 2, 3$, test on $2 \leq k \leq 10$ and $1 \leq b \leq 4$

3. Epistemic Graph Neural Network (EpiGNN)



1. **Message passing:** Independently learn the entity embeddings for the forward and the backward model.
2. **Composition:** Compose the dual entity embeddings on a path between the head and target from the forward and backward model. Each predicts the target relation.
3. **Aggregation:** Combine the evidences over all predictions.

4. Algorithmic alignment with the Algebraic Closure Algorithm

Table 2: Making the GNN epistemic by aligning it with the directional algebraic closure algorithm.

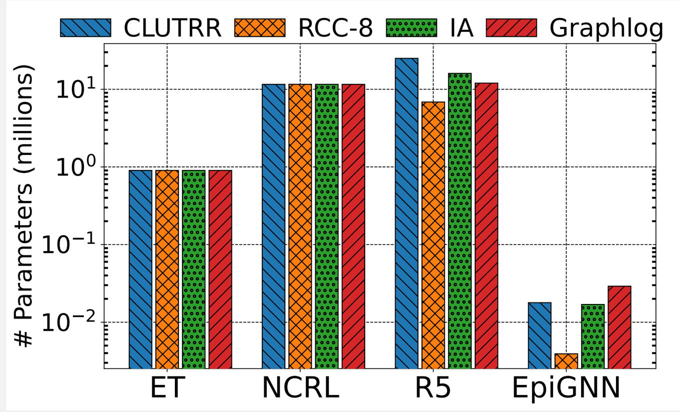
Epistemic GNN	Algebraic Closure Algorithm
Initialize probabilistic embeddings encoding unions $\mathbf{e}^{(0)} = \begin{cases} (1, 0, \ldots, 0) & \text{if } e = h \\ (\frac{1}{n}, \ldots, \frac{1}{n}) & \text{otherwise} \end{cases}$	Initialize node embeddings for all possible relations $X_{ef}^{(0)} = \begin{cases} \{r\} & \text{if } r(e,f) \in \mathcal{F} \text{ or } \{\hat{r}\} \text{ if } r(f,e) \in \mathcal{F} \\ \mathcal{R} & \text{otherwise} \end{cases}$
MESSAGE ϕ simulates discrete relational composition $\phi((f_1, \ldots, f_n), (r_1, \ldots, r_n)) = \sum_{i,j=1}^{n} f_i r_j \mathbf{a}_{ij}$	Compute all possible discrete relational compositions $X_{eg}^{(i-1)} \diamond X_{gf}^{(i-1)} = \bigcup \left\{ r \circ s \middle\vert r \in X_{eg}^{(i-1)}, s \in X_{gf}^{(i-1)} \right\}$
AGGREGATE function ψ simulates intersection $\mathbf{e}^{(l)} = \psi(\{\mathbf{e}^{(l-1)}\} \cup \{\phi(\mathbf{r}, \mathbf{f}^{(l-1)}) \,\vert\, r(e,f) \in \mathcal{F}\})$	Update node embeddings via intersection $X_{ef}^{(i)} = X_{ef}^{(i-1)} \cap \bigcap \{X_{eg}^{(i-1)} \diamond X_{gf}^{(i-1)} \,\vert\, g \in \mathcal{E}\}$

5. Ablations and Parametric efficiency

Table 3: Ablations highlight the usefulness of key alignment components.

	CLUTRR Avg	CLUTRR Hard	RCC-8 Avg	RCC-8 Hard
EpiGNN	0.99	0.99	0.96	0.80
- **With facets=1**	0.94	0.85	0.92	0.68
- **Unconstrained embeddings**	0.36	0.30	0.38	0.21
- **MLP+distmul composition**	0.29	0.31	0.13	0.13
- **Forward model only**	0.94	0.82	0.84	0.51

Figure 1: EpiGNN is at least $O(10^2)$ more parameter efficient compared to SoTA.



6. Systematic Generalization Results

Table 4: EpiGNN matches neuro-symbolic methods on single-path reasoning. Results (accuracy) on CLUTRR. Results marked with * were taken from [9], those with † from [6] and those with 2 from [7]. The best performance for each k is highlighted in **bold**.

	5 Hops	6 Hops	7 Hops	8 Hops	9 Hops	10 Hops
EpiGNN-mul (ours)	0.99±.01	**0.99**±.01	**0.99**±.02	0.99±.03	0.96±.03	**0.98**±.02
EpiGNN-min (ours)	0.99±.01	0.98±.02	0.98±.03	0.97±.06	0.95±.04	0.93±.07
NCRL[2]	**1.0**±.01	**0.99**±.01	0.98±.02	0.98±.03	0.98±.03	0.97±.02
R5[†]	0.99±.02	0.99±.04	0.99±.03	**1.0**±.02	**0.99**±.02	0.98±.03
CTP^*_L	0.99±.02	0.98±.04	0.97±.04	0.98±.03	0.97±.04	0.95±.04
CTP^*_A	0.99±.04	0.99±.03	0.97±.03	0.95±.06	0.93±.07	0.91±.05
CTP^*_M	0.98±.04	0.97±.06	0.95±.06	0.94±.08	0.93±.08	0.90±.09
GNTP*	0.68±.28	0.63±.34	0.62±.31	0.59±.32	0.57±.34	0.52±.32
ET	0.99±.01	0.98±.02	**0.99**±.02	0.96±.04	0.92±.07	0.92±.07
GAT*	0.99±.00	0.85±.04	0.80±.03	0.71±.03	0.70±.03	0.68±.02
GCN*	0.94±.03	0.79±.02	0.61±.03	0.53±.04	0.53±.04	0.41±.04
NBFNet	0.83±.11	0.68±.09	0.58±.10	0.53±.07	0.50±.11	0.53±.08
R-GCN	0.97±.03	0.82±.11	0.60±.13	0.52±.11	0.50±.09	0.45±.09
RNN*	0.93±.06	0.87±.07	0.79±.11	0.73±.12	0.65±.16	0.64±.16
LSTM*	0.98±.03	0.95±.04	0.89±.10	0.84±.07	0.77±.11	0.78±.11
GRU*	0.95±.04	0.94±.03	0.87±.08	0.81±.13	0.74±.15	0.75±.15

Figure 2: EpiGNN outperforms SoTA rule and statistical learners on disjunctive reasoning. RCC-8 and Interval Algebra benchmark results (accuracy). R5 and CTP results for 5+ hops were set to zero since the model took longer than 30 minutes for inference. The best model for all cases is EpiGNN-min.

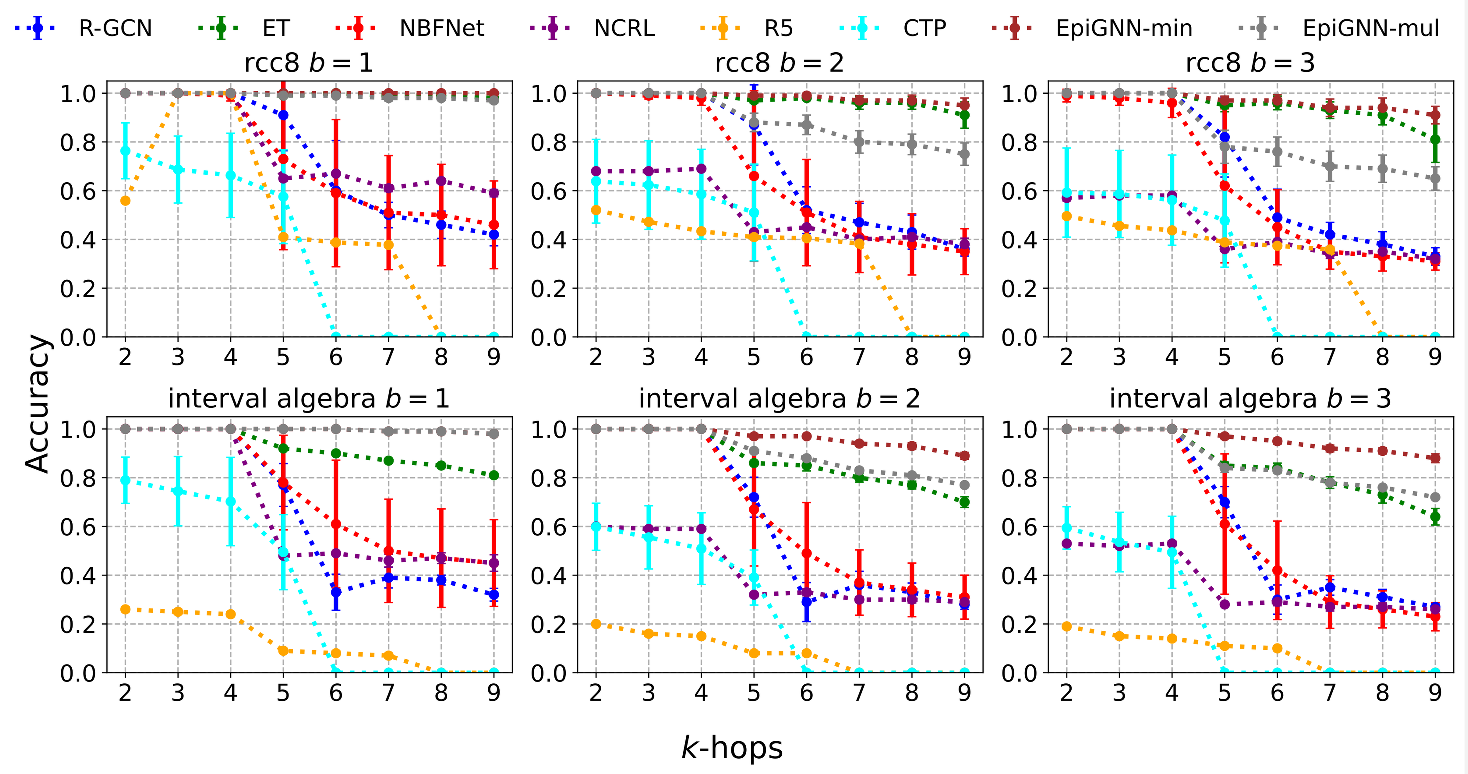
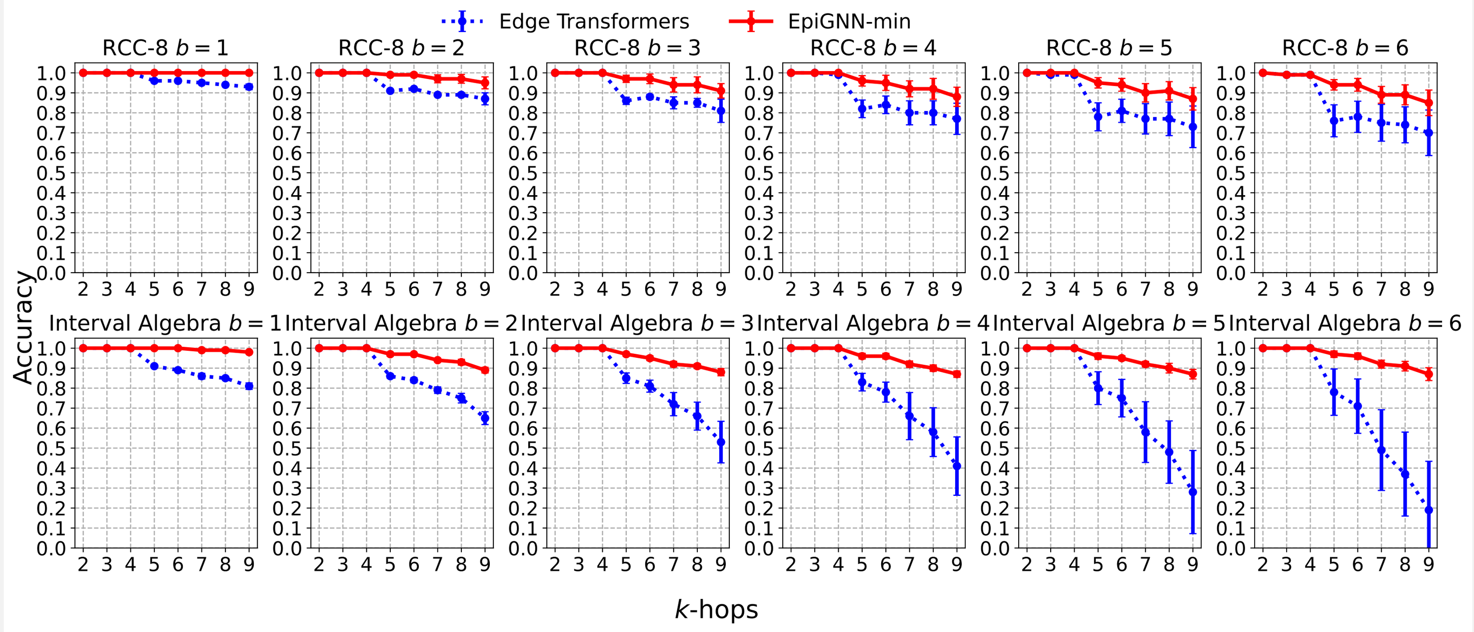


Figure 3: EpiGNN retains its performance wrt. the best STaR baseline for the most challenging splits.



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