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DeepPath: A Reinforcement Learning Method for Knowledge Graph Reasoning

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Relational Message Passing for Knowledge Graph Completion

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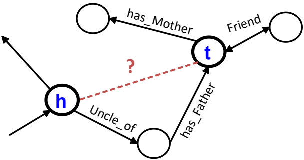
Main interest

- **Knowledge Graph Completion(KGC)**

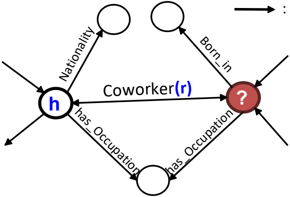
□ Find ? for (h,r,?) or (?,r,t) or (h,?,t)

: entity

: relation



▲ relation prediction



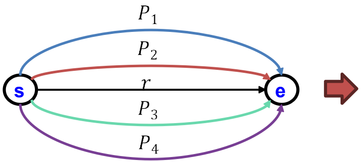
▲ link prediction

Problem with previous models(DeepPath)

- **Problem of PRA**

  □ PRA(2011a), a very impactful random walk based research on KGC

  □ However, operates in a fully <u>discrete</u> space limiting the ability to score and compare results



$$score(e; s) = \sum_{P \in \mathbf{P}_\ell} h_{s,P}(e)\theta_P$$

Architecture(DeepPath)

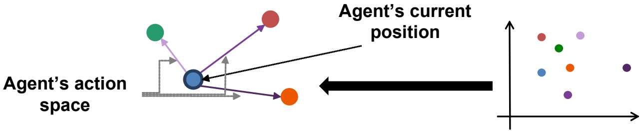
>> Preview of DeepPath

- **Reinforcement learning(RL) based model**

  □ Trains a policy-based RL agent **to find promising reasoning paths**

- **Incorporates translation based KG embedding method**

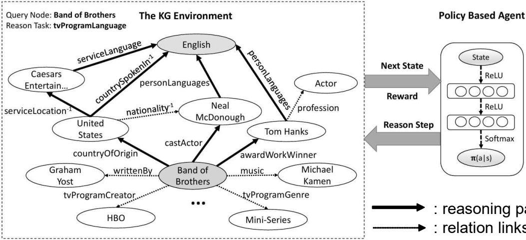
  □ Agent uses embeddings **to navigate the path in a continuous space**



Architecture(DeepPath)

$$< \mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R} >$$

Markov decision process(MDP) = environment



→ : reasoning path found by agent

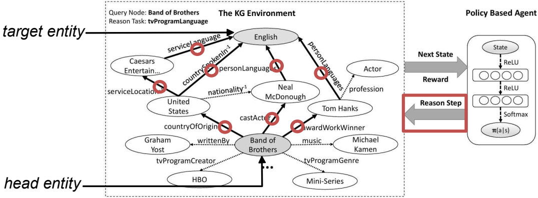
⇢ : relation links(excluding bold ones)

Architecture(DeepPath)

▪ Components of RL environment<S,A,P,R>

Given tirple (h,r,t), we want the agent to find the most informative paths linking the target nodes

□ **Action** : Agent uses policy network to pick the most promising relation to extend the path



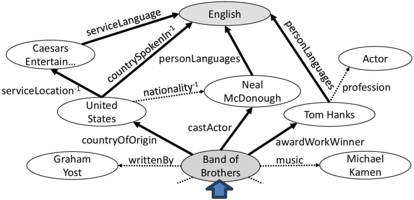
Architecture(DeepPath)

- **Components of RL environment<S,A,P,R>**

  □ **States** : Help define the current circumstance the agent is facing
  $\mathbf{e}$: entity embedding generated from **TransE**

$$\mathbf{s}_t = \mathbf{e}_t \oplus \underbrace{(\mathbf{e}_{target} - \mathbf{e}_t)}$$

equivalent to the sum of relation embeddings of a path which can connect $\mathbf{e}_{target}$ to $\mathbf{e}_t$



$\mathbf{e}_0 = \mathbf{e}_{source}$

since TransE is able to model composition!!

Architecture(DeepPath)

- **Components of RL environment<S,A,P,R>**

□ **Rewards** : 3 segments contribute to enhence the quality of paths found by the agent

1. Global **accuracy**

$$r_{\text{GLOBAL}} = \begin{cases} +1, & \text{if the path reaches } e_{target} \\ -1, & \text{otherwise} \end{cases}$$

2. Path **efficiency**

$$r_{\text{EFFICIENCY}} = \frac{1}{length(p)}$$

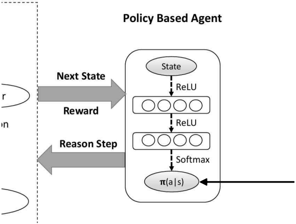
3. Path **diversity**

$$r_{\text{DIVERSITY}} = -\frac{1}{|F|} \sum_{i=1}^{|F|} cos(\mathbf{p}, \mathbf{p}_i)$$

Architecture(DeepPath)

- **Components of RL environment<S,A,P,R>**

□ **Policy network** : neural network that maps state vector to probability distribution of all possible actions



dimension is fixed to the number of total relations in the KG

Architecture(DeepPath)

- **Supervised policy learning inspired by *AlphaGo(2016)***

□ Large action space of KG results in poor convergence with naive trial and error approaches

□ To tackle this problem, **feed paths that connect positive sample first** to better guide the agent (after that, we retrain the model on trial and error)

<expected total rewards for one episode> → *<supervised version of reward gradient>*

$$J(\theta) = \mathbb{E}_{a\sim\pi(a|s;\theta)}\Big(\sum_t R_{s_t,a_t}\Big)$$
$$= \sum_t \sum_{a\in\mathcal{A}} \pi(a|s_t;\theta) R_{s_t,a_t}$$

$$\nabla_\theta J(\theta) = \sum_t \sum_{a\in\mathcal{A}} \pi(a|s_t;\theta)\nabla_\theta \log\pi(a|s_t;\theta)$$
$$\boxed{\approx \nabla_\theta \sum_t \log\pi(a=r_t|s_t;\theta)}$$

- r_t belongs to the supervised path p
- it assumes that all the actions are done with 100% certainty

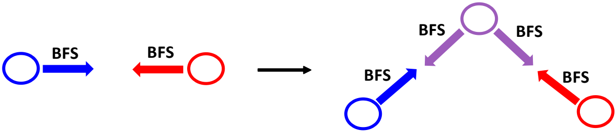
Architecture(DeepPath)

Traditional two-side BFS is not enough

□ Supervised paths are sampled by picking a subset of positive tuples (e_{source}, e_{target}) and conducting BFS from each entity untill they meet

□ **However,** BFS is biased to **short paths** which may hinder generality in retraining process

□ To tackle this, randomly sample a intermediate node and conduct two two-side BFS



Architecture(DeepPath)

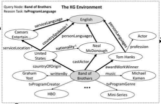
- **Review of DeepPath schema**

<training>

1. Pre-train on supervised paths

2. Retrain on the environment alone

Sample successful paths and re-rank them via linear regression (similar to PRA)



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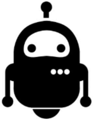


<testing>

Use learned paths as formulas for inference

Use path parameters learned by linear regression as confidence of the path

Experiments(DeepPath)

- **Settings**

☐ **Metric** : MAP(Mean Average Precision)

☐ **Dataset** : FB15k-237, NELL-995(Tasks refer to relations that we will observe in this section)

Dataset	# Ent.	# R.	# Triples	# Tasks
FB15K-237	14,505	237	310,116	20
NELL-995	75,492	200	154.213	12

- **Experiments**

☐ Entity prediction and fact prediction

Experiments(DeepPath)

- **Link prediction and # of collected reasoning paths**

	FB15K-237					NELL-995			
Tasks	PRA	RL	TransE	TransR	Tasks	PRA	RL	TransE	TransR
teamSports	**0.987**	0.955	0.896	0.784	athletePlaysForTeam	0.547	**0.750**	0.627	0.673
birthPlace	0.441	**0.531**	0.403	0.417	athletePlaysInLeague	0.841	**0.960**	0.773	0.912
personNationality	**0.846**	0.823	0.641	0.720	athleteHomeStadium	0.859	**0.890**	0.718	0.722
filmDirector	0.349	**0.441**	0.386	0.399	athletePlaysSport	0.474	0.957	0.876	**0.963**
filmWrittenBy	0.601	0.457	0.563	**0.605**	teamPlaySports	0.791	0.738	0.761	**0.814**
filmLanguage	0.663	**0.670**	0.642	0.641	orgHeadquaterCity	**0.811**	0.790	0.620	0.657
tvLanguage	0.960	**0.969**	0.804	0.906	worksFor	0.681	**0.711**	0.677	0.692
capitalOf	**0.829**	0.783	0.554	0.493	bornLocation	0.668	0.757	0.712	**0.812**
organizationFounded	0.281	0.309	**0.390**	0.339	personLeadsOrg	0.700	**0.795**	0.751	0.772
musicianOrigin	0.426	**0.514**	0.361	0.379	orgHiredPerson	0.599	**0.742**	0.719	0.737
...					...				
Overall	0.541	**0.572**	0.532	0.540		0.675	**0.796**	0.737	0.789

	# of Reasoning Paths	
Tasks	PRA	RL
worksFor	247	25
teamPlaySports	113	27
teamPlaysInLeague	69	21
athletehomestadium	37	11
organizationHiredPerson	244	9
...		
Average #	137.2	20.3

Experiments(DeepPath)

- **Fact prediction**

□ Generate 10 negative triples(fake a certain entity, e.g. (h',r,t)) for each positive

□ Rank all the positive and negative triples(PRA is not able to process fact prediction)

fact check

positive (h,r,t) → $(h,r,t)\ true$

negative

(h,r,t_1') → $(h,r,t_1')\ ture$

...

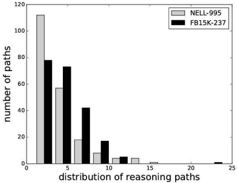
(h,r,t_{10}') → $(h,r,t_{10}')\ false$

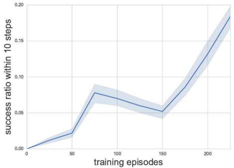
	Fact Prediction Results	
Methods	FB15K-237	NELL-995
RL	**0.311**	**0.493**
TransE	0.277	0.383
TransH	0.309	0.389
TransR	0.302	0.406
TransD	0.303	0.413

Experiments(DeepPath)

- **Other analysis**

Relation	Reasoning Path
filmCountry	filmReleaseRegion featureFilmLocation → locationContains^{-1} actorFilm^{-1} → personNationality
personNationality	placeOfBirth→ locationContains^{-1} peoplePlaceLived → locationContains^{-1} peopleMarriage → locationOfCeremony → locationContains^{-1}
tvProgramLanguage	tvCountryOfOrigin → countryOfficialLanguage tvCountryOfOrigin → filmReleaseRegion^{-1} → filmLanguage tvCastActor → filmLanguage
personBornInLocation	personBornInCity graduatedUniversity → graduatedSchool^{-1} → personBornInCity personBornInCity → atLocation^{-1} → atLocation
athletePlaysForTeam	athleteHomeStadium → teamHomeStadium^{-1} athletePlaysSport → teamPlaysSport^{-1} athleteLedSportsTeam
personLeadsOrganization	worksFor organizationTerminatedPerson^{-1} mutualProxyFor^{-1}





Conclusion(DeepPath)

- **DeepPath for knowledge graph completion**

  □ **First reinforcement learning** based KGC model

  □ Complex reward function to **explore more informative paths**

  □ Adopted embeddings to **define states on a continuous space**

- **Limitations of DeepPath**

  □ **Sparse reward and large action space** is still a problem

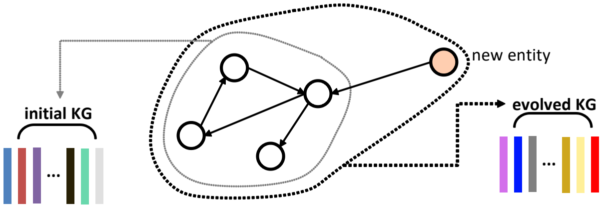
  □ Supervised policy learning is not safe from **bias**(on the other hand, *AlphaGo Zero(2017)*)

  □ **Transductive** nature because of the need to create embeddings for all entities and relations.

Problem with previous models(PathCon)

- **Translation based embedding models's transductive nature**

  □ Embedding based models can't scale to evolving KGs



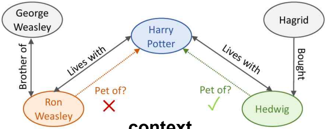
Architecture(PathCon)

- **Considering context and path for link prediction**

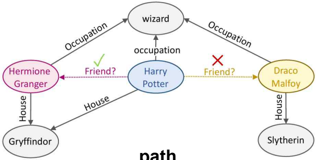
□ Entity type(infered from surrounding relations) = **Context**

□ Relational paths between target nodes = **Path**

Link prediction model
PathCon



context



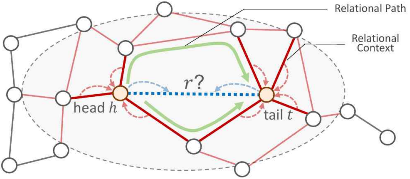
path

Architecture(PathCon)

- **Preview of PathCon**

□ Context obtained by **relational message passing**, detect target entity's **TYPE**

□ Paths detect target nodes **relative positions**



Architecture(PathCon)

- **Problem formulation**

regularization term

link probability distribution → $p(r|h,t) \propto \underline{p(h,t|r)} \cdot p(r)$

$$\underline{p(h,t|r)} = \frac{1}{2}\left(\underline{p(h|r)} \cdot \underline{p(t|h,r)} + \underline{p(t|r)} \cdot \underline{p(h|t,r)}\right)$$

$p(C(h)|r)$ $p(C(t)|r)$

subgraph of entity = **context**

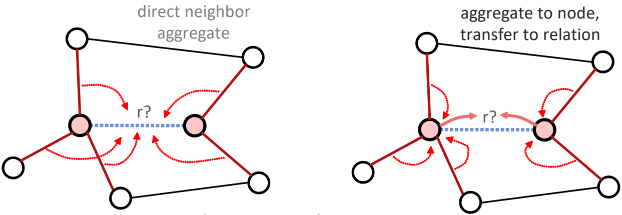
how t(h) can be reached from h(t) = **path**

Architecture(PathCon)

- **Relational message passing(context)**

N : #nodes
M : #edges
Var[d] : variance of node degree

□ Message aggregation between neighbor relations for entity context



$N \cdot \mathrm{Var}[d] + \frac{4M^2}{N}$ ⟵ *cost of message passing* ⟶ $\boxed{6M}$

Architecture(PathCon)

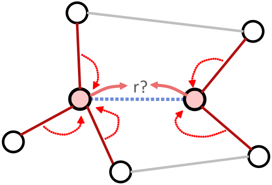
- **Relational message passing(context)**

□ Overview of relational message passing for relational context

$$m_v^i = A_1\left(\{s_e^i\}_{e\in\mathcal{N}(v)}\right), \qquad \text{// node aggregate}$$

$$m_e^i = A_2\left(m_v^i, m_u^i\right),\ v, u \in \mathcal{N}(e), \qquad \text{// aggregate to edge}$$

$$s_e^{i+1} = U\left(s_e^i, m_e^i\right). \qquad \text{// update edge state}$$



$$m_v^i = \sum\nolimits_{e\in\mathcal{N}(v)} s_e^i, \qquad //A_1, A_2$$

$$s_e^{i+1} = \sigma\left(\left[m_v^i, m_u^i, s_e^i\right]\cdot W^i + b^i\right),\ v, u \in \mathcal{N}(e), \qquad //U$$

Architecture(PathCon)

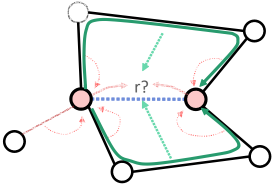
- **Relational paths(path)**

  □ Represents relative position between h and t

  □ Specify embeddings for all possible path combination

$|R|^k, k\ hop\ paths$ ← isn't this too much?

"only 3.2% of all possible paths of length 2 occur in the FB15K dataset"



Architecture(PathCon)

- **Combining relational context and path**

□ Context score vector, path attention and path score vector(K iterations)

$$s_{(h,t)} = \sigma\left(\left[m_h^{K-1}, m_t^{K-1}\right] \cdot W^{K-1} + b^{K-1}\right)$$

$$\alpha_P = \frac{\exp\left(s_P{}^\top s_{(h,t)}\right)}{\sum_{P \in \mathcal{P}_{h \to t}} \exp\left(s_P{}^\top s_{(h,t)}\right)}$$

$$s_{h \to t} = \sum\nolimits_{P \in \mathcal{P}_{h \to t}} \alpha_P s_P$$

□ Optimization process

$$p(r|h,t) = \textsc{SoftMax}\left(s_{(h,t)} + s_{h \to t}\right)$$

$$\min \mathcal{L} = \sum_{(h,r,t) \in \mathcal{D}} J\big(p(r|h,t),\ r\big)$$

The output dimension must match the number of total relations in the KG

Experiments(PathCon)

- **Datasets**

□ FB15k, FB15k-237, WN18, WN18RR, NELL995, DDB14(DDB14 proposed in this paper)

	FB15K	FB15K-237	WN18	WN18RR	NELL995	DDB14
#nodes	14,951	14,541	40,943	40,943	63,917	9,203
#relations	1,345	237	18	11	198	14
#training	483,142	272,115	141,442	86,835	137,465	36,561
#validation	50,000	17,535	5,000	3,034	5,000	4,000
#test	59,071	20,466	5,000	3,134	5,000	4,000
$\mathbb{E}[d]$	64.6	37.4	6.9	4.2	4.3	7.9
$\mathrm{Var}[d]$	32,441.8	12,336.0	236.4	64.3	750.6	978.8

- **Metrics**

□ MRR, Hit@1, 3

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Experiments(PathCon)

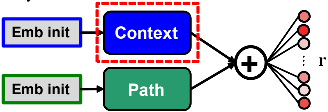
- **Link prediction**

Method	TransE	ComplEx	DisMult	RotatE	SimplE	QuatE	PathCon
#param.	3.7M	7.4M	3.7M	7.4M	7.4M	14.7M	0.06M

	FB15K			FB15K-237			WN18			WN18RR			NELL995			DDB14		
	MRR	Hit@1	Hit@3	MRR	Hit@1	Hit@3	MRR	Hit@1	Hit@3	MRR	Hit@1	Hit@3	MRR	Hit@1	Hit@3	MRR	Hit@1	Hit@3
TransE	0.962	0.940	0.982	0.966	0.946	0.984	0.971	0.955	0.984	0.784	0.669	0.870	0.841	0.781	0.889	0.966	0.948	0.980
ComplEx	0.901	0.844	0.952	0.924	0.879	0.970	0.985	0.979	0.991	0.840	0.777	0.880	0.703	0.625	0.765	0.953	0.931	0.968
DistMult	0.661	0.439	0.868	0.875	0.806	0.936	0.786	0.584	0.987	0.847	0.787	0.891	0.634	0.524	0.720	0.927	0.886	0.961
RotatE	0.979	0.967	0.986	0.970	0.951	0.980	0.984	0.979	0.986	0.799	0.735	0.823	0.729	0.691	0.756	0.953	0.934	0.964
SimplE	0.983	0.972	0.991	0.971	0.955	0.987	0.972	0.964	0.976	0.730	0.659	0.755	0.716	0.671	0.748	0.924	0.892	0.948
QuatE	0.983	0.972	0.991	0.974	0.958	0.988	0.981	0.975	0.983	0.823	0.767	0.852	0.752	0.706	0.783	0.946	0.922	0.962
DRUM	0.945	0.945	0.978	0.959	0.905	0.958	0.969	0.956	0.980	0.854	0.778	0.912	0.715	0.640	0.740	0.958	0.930	0.987
Con	0.962 ± 0.000	0.934 ± 0.000	0.988 ± 0.000	0.978 ± 0.000	0.961 ± 0.001	**0.995** ± 0.000	0.960 ± 0.002	0.927 ± 0.005	0.992 ± 0.001	0.943 ± 0.002	0.894 ± 0.004	0.993 ± 0.003	0.875 ± 0.003	0.815 ± 0.004	0.928 ± 0.003	0.977 ± 0.000	0.961 ± 0.001	0.994 ± 0.001
Path	0.937 ± 0.001	0.918 ± 0.001	0.951 ± 0.001	0.972 ± 0.001	0.957 ± 0.001	0.986 ± 0.001	0.981 ± 0.000	0.971 ± 0.005	0.989 ± 0.001	0.933 ± 0.000	0.897 ± 0.001	0.961 ± 0.001	0.737 ± 0.001	0.685 ± 0.002	0.764 ± 0.002	0.969 ± 0.000	0.948 ± 0.001	0.991 ± 0.000
PathCon	**0.984** ± 0.001	**0.974** ± 0.002	**0.995** ± 0.001	**0.979** ± 0.000	**0.964** ± 0.001	0.994 ± 0.001	**0.993** ± 0.001	**0.988** ± 0.001	**0.998** ± 0.000	**0.974** ± 0.001	**0.954** ± 0.002	**0.994** ± 0.000	**0.896** ± 0.001	**0.844** ± 0.004	**0.941** ± 0.004	**0.980** ± 0.000	**0.966** ± 0.001	**0.995** ± 0.000

Experiments(PathCon)

- **Model variant study(context aggregator)**



□ **Concat aggregator**

$$s_e^{i+1} = \sigma\left(\left[m_v^i, m_u^i, s_e^i\right] \cdot W^i + b^i\right), \ v, u \in \mathcal{N}(e)$$

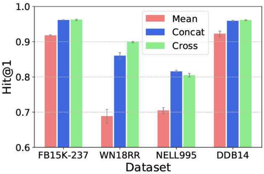
□ **Mean aggregator**

$$s_e^{i+1} = \sigma\left(\frac{1}{3}\left(m_v^i + m_u^i + s_e^i\right) W + b\right), \ v, u \in \mathcal{N}(e)$$

□ **Cross context aggregator**

$$m_v^i {m_u^i}^\top = \begin{bmatrix} {m_v^i}^{(1)} {m_u^i}^{(1)} & \cdots & {m_v^i}^{(1)} {m_u^i}^{(d)} \\ \cdots & & \cdots \\ {m_v^i}^{(d)} {m_u^i}^{(1)} & \cdots & {m_v^i}^{(d)} {m_u^i}^{(d)} \end{bmatrix}$$

$$s_e^{i+1} = \sigma\left(\text{flatten}\left(m_v^i {m_u^i}^\top\right) W_1^i + s_e^i W_2^i + b^i\right), \ v, u \in \mathcal{N}(e)$$



Experiments(PathCon)

- **Model variant study(path representation, path aggregator)**

□ **Independent random initialization**

□ **Learning path representation via RNN**

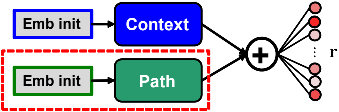
$$s_P = \mathrm{RNN}(r_1, r_2, \ldots)$$

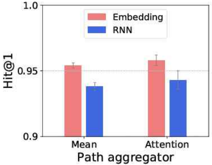
□ **Attention aggregator**

$$s_{h\to t} = \sum_{P\in\mathcal{P}_{h\to t}} \alpha_P s_P$$

□ **Mean aggregator**

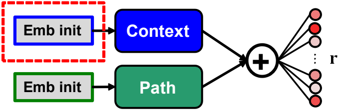
$$s_{h\to t} = \sum_{P\in\mathcal{P}_{h\to t}} s_P$$





Experiments(PathCon)

- **Model variant study(initial edge features)**

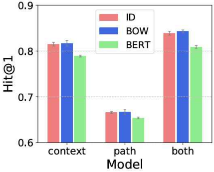


  □ **Identity**(one-hot)

  □ **BOW**(Bag Of Words)

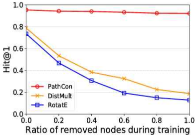
  □ **BERT**(Bidirectional Encoder Representations from Transformers)

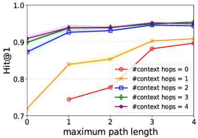
  Input of BOW, BERT are individual relation's english name



Experiments(PathCon)

- **Other analysis**





▼relations of DDB14

0: belong(s) to the category of	7: interacts with
1: is a category subset of	8: belongs to the drug family of
2: may cause	9: belongs to drug super-family
3: is a subtype of	10: is a vector for
4: is a risk factor for	11: may be allelic with
5: is associated with	12: see also
6: may contraindicate	13: is an ingredient of

transformation matrix of path(▼) and context(▶)

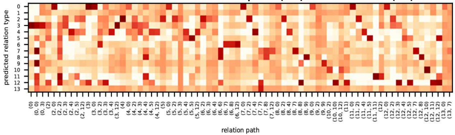


Figure 8: The learned correlation between all relational paths with length ≤ 2 and the predicted relations on DDB14.

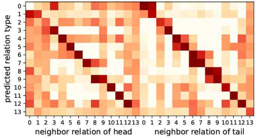
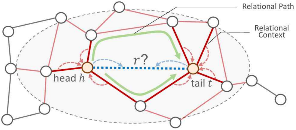


Figure 9: The learned correlation between the contextual relations of head/tail and the predicted relations on DDB14.

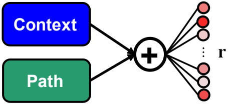
Conclusion(PathCon)



- **Message passing based KGC model**

  □ Novel architecture of **relational message passing**
  □ **Entity-independent** inductive model
  □ Combined **context**(message passing) and **path** for link prediction

- **More stuff to discuss about**



  □ Is it okay to neglect direction attributes of relations?
  □ Why did BERT perform worst in initial edge features?
  □ What happens if new paths are created by new entities?
  □ Need harder negative than random sampling(e.g. (h,r',t)), such as using GAN
  □ Path dependent to context problem

Thank You!

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