AAAI 2022 Tutorial

Automated Learning from Graph-Structured Data

Quanming Yao[1], Huan Zhao[2], Yongqi Zhang[2]

[1]*Department of Electronic Engineering, Tsinghua University*

[2]*4Paradigm Inc.*

https://quanmingyao.github.io/AutoML.github.io/aaai22-tutorial.html



Schedule at a Glance

Time	Event
00-45 minutes	**Part 1**: Automated Graph Neural Network
	Speaker: Huan Zhao
45-90 minutes	**Part 2**: Hyper-parameter Tuning for Graph-Structured Data
	Speaker: Quanming Yao
90-135 minutes	**Part 3**: Automated Knowledge Graph Reasoning: from Triplets to Subgraphs
	Speaker: Yongqi Zhang
135-150 minutes	**Part 4**: Discussion

Code Repo.

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Automated Learning from Graph Structured Data Tutorial

Part 3: Automated Knowledge Graph Reasoning from Triplets to Subgraphs

Yongqi Zhang

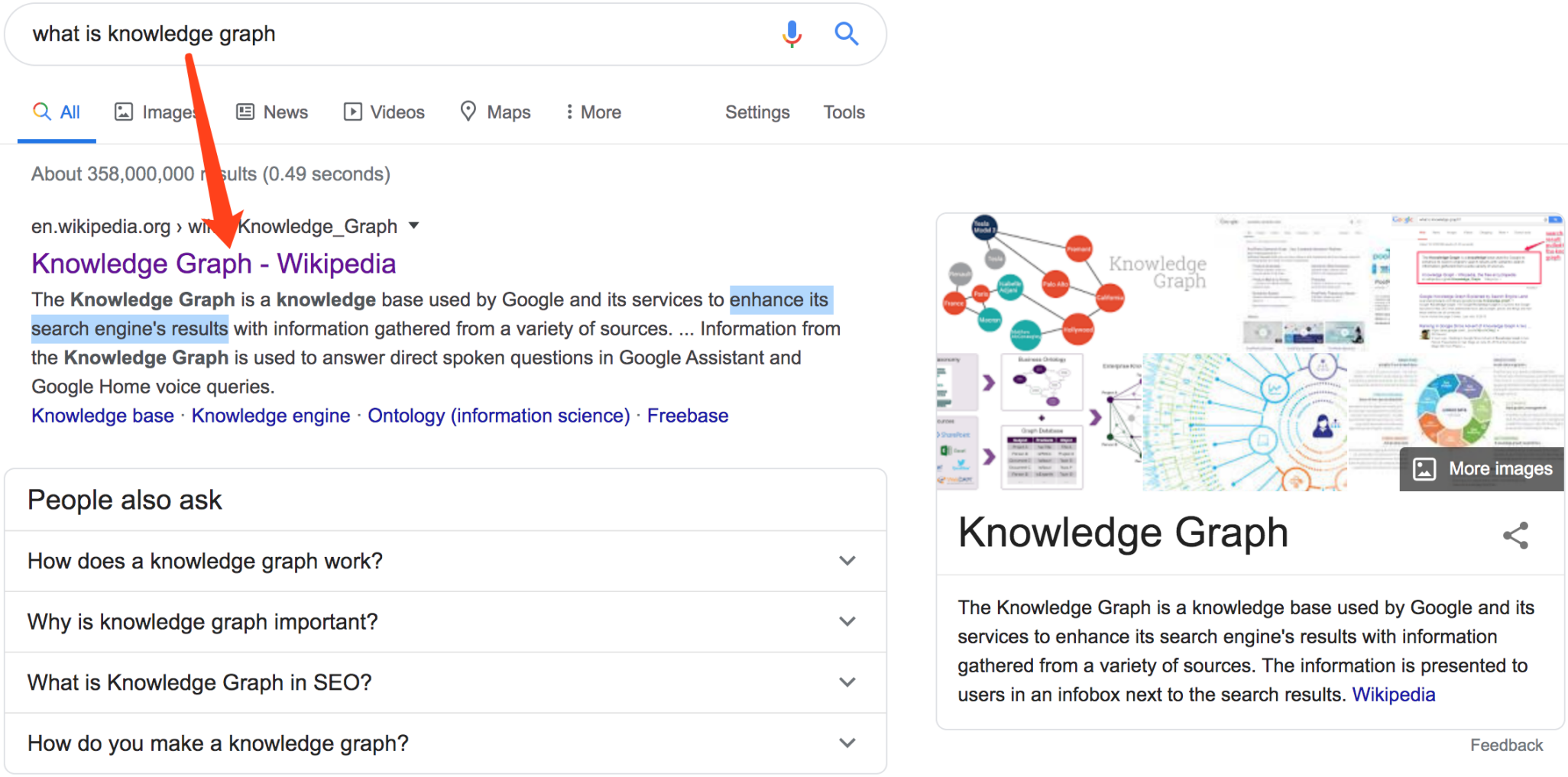
4Paradigm Inc.

zhangyongqi@4paradigm.com

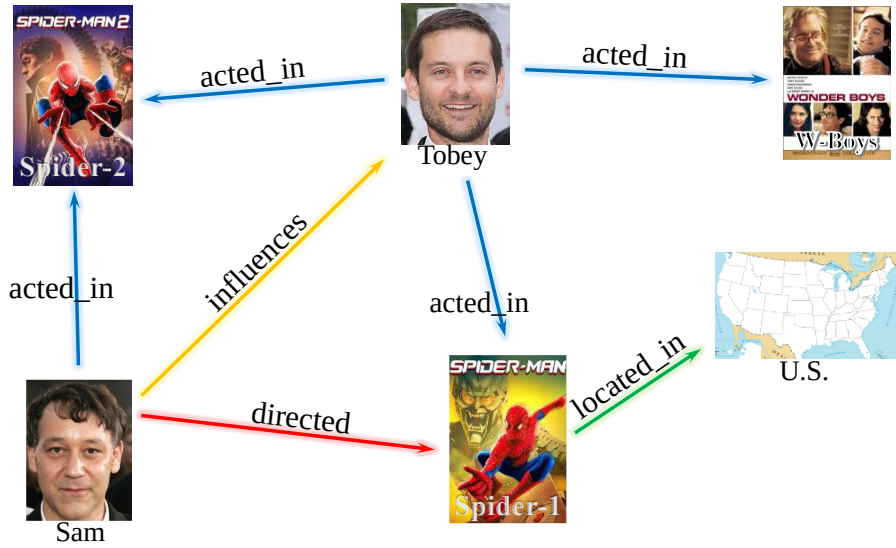
Outline

1. Background
   - Knowledge Graph (KG)
   - KG reasoning (KGR)
2. AutoML for model design
3. Model design
   - Triplet-based
   - Path-based
   - Subgraph-based
4. Summary

Knowledge graph by Google



Knowledge graph (KG)



Graph representation: $\mathcal{G} = (\mathcal{E}, \mathcal{R}, \mathcal{S})$.

Entities $\mathcal{E}$: real world objects or abstract concepts.

Relations $\mathcal{R}$: interactions between/among entities.

Fact/triples $\mathcal{S}$: the basic unit in form of (head entity, relation, tail entity), (h, r, t).

Other related information:

- Types/attributes of entities/relations.
- Text descriptions on entities and relations.
- Ontologies: concept level description.
- Logic rules: regular expressions.

Google Knowledge Graph

范式星图 地址知识图谱工具

WIKIDATA

Freebase™

BIO2RDF

KG – important applications

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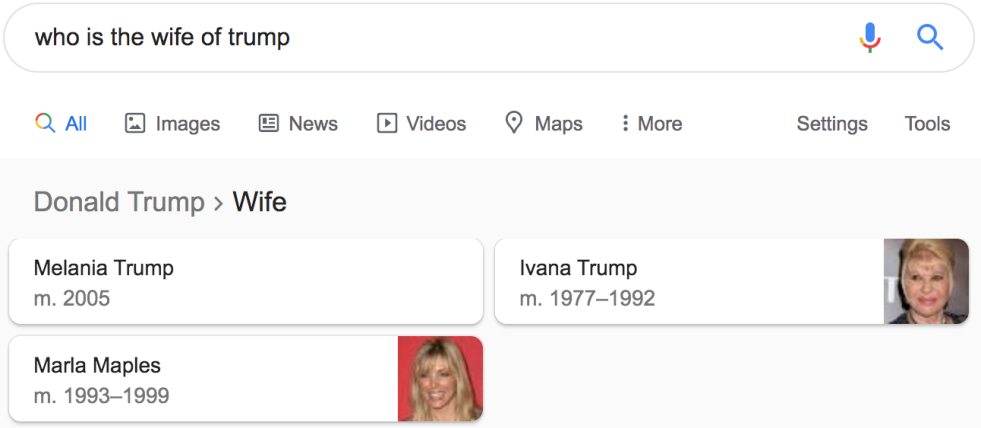
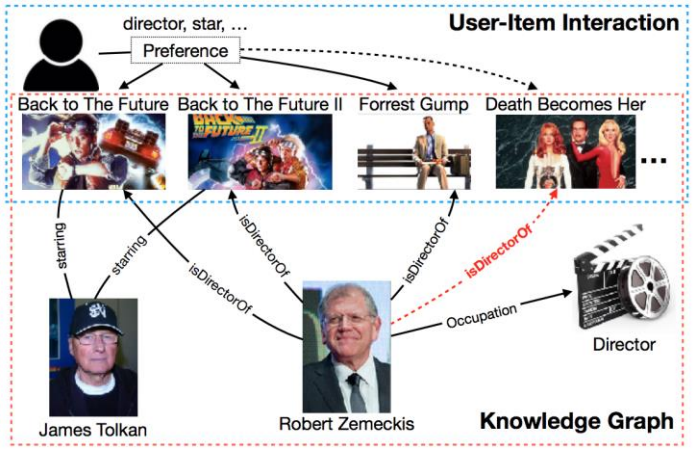
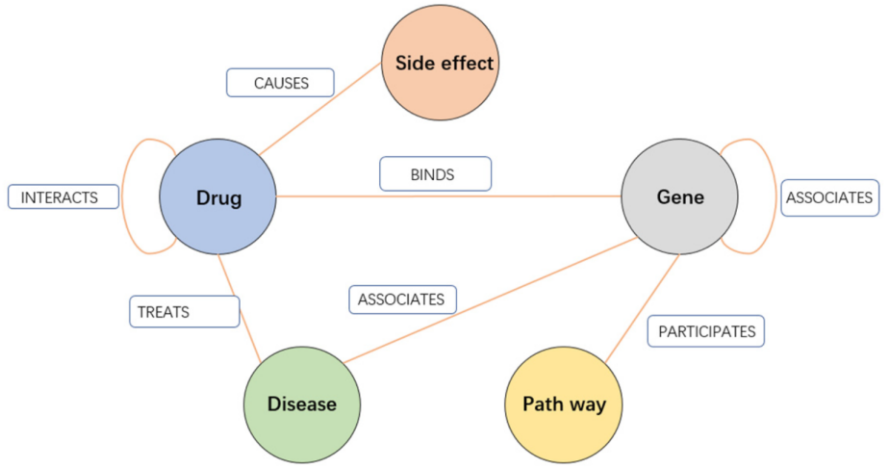
KGQA:



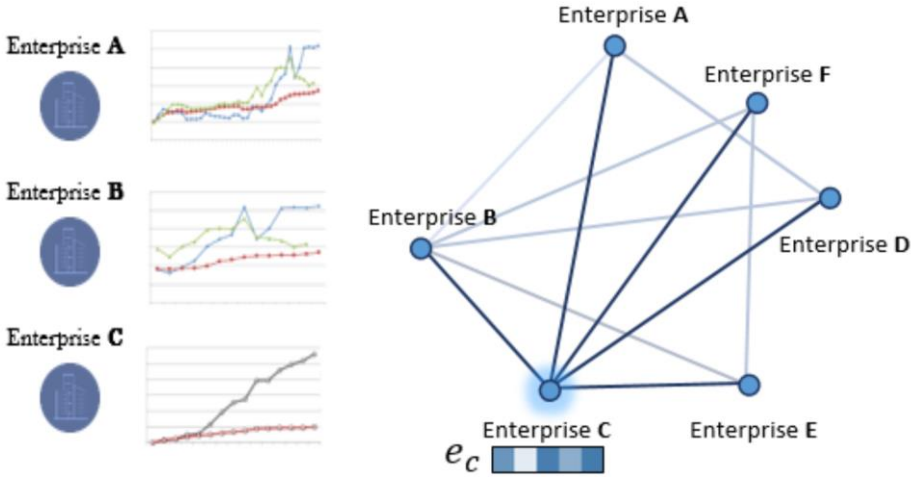
Recommendation:



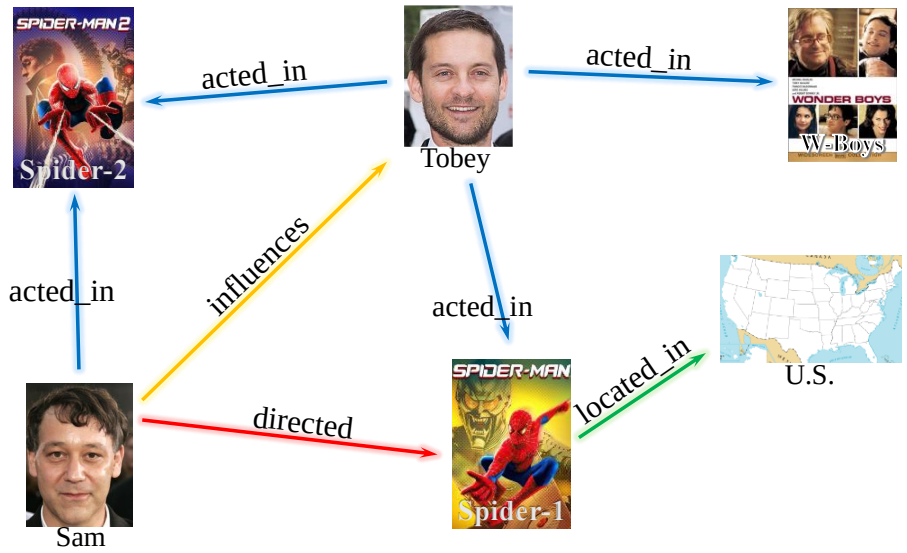
Drug discovery:



Stock prediction:



Representation learning

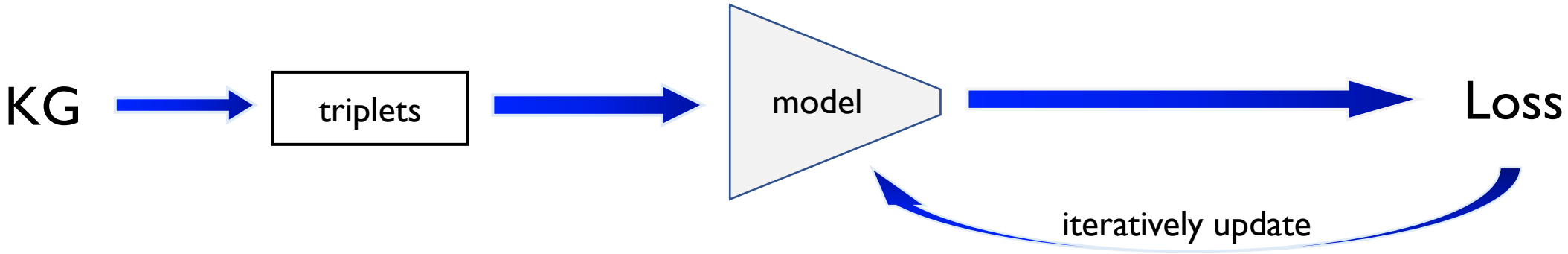


Observed triplets S^+:
maximize score

(Sam, directed, Spider-1)
(Tobey, acted_in, Spider-2)
(Spider-1, located_in, U.S.)
…

Unobserved triplets S^-:
minimize score

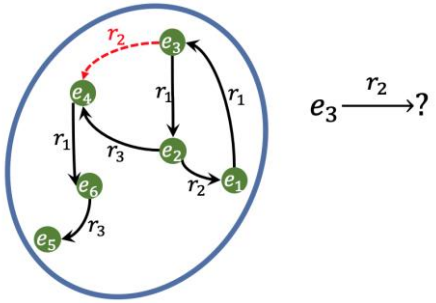
(Tobey, directed, Spider-1)
(Tobey, acted_in, U.S.)
(Spider-1, directed, U.S.)
…



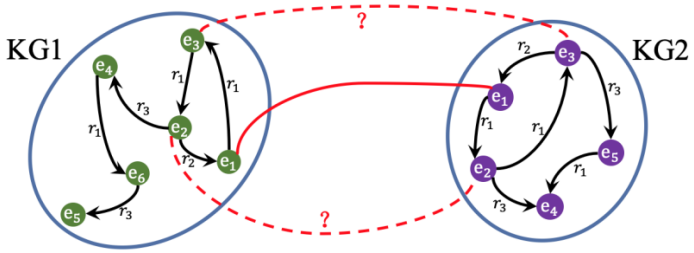
➢Objective: Preserve as much information on original graph as possible.

Basic tasks

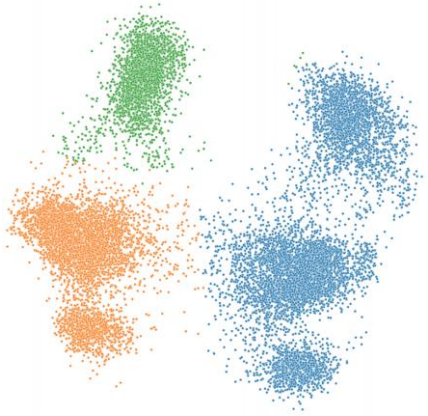
- Knowledge graph completion
  - Link prediction / triple classification: predicting missing links



- Entity alignment
  - Align the same entities in two KGs, e.g. cross-lingual KGs



- Entity classification
  - Predict the type of entities



Evaluation

- Link prediction as an example.

- Evaluation on (h, r, t):
  - head/tail prediction: $(?, r, t)$ or $(h, r, ?)$
  - get the rank of (h, r, t) over $\{(e, r, t): e \in \mathcal{E}\}$ or $\{(h, r, e): e \in \mathcal{E}\}$

- Metrics:

$$MR = \frac{1}{|\mathcal{S}_{\text{tst}}|} \sum_{i \in \mathcal{S}_{tst}} \text{rank}_i \qquad MRR = \frac{1}{|\mathcal{S}_{\text{tst}}|} \sum_{i \in \mathcal{S}_{tst}} \frac{1}{\text{rank}_i} \qquad H@K = \frac{|\{i \in \mathcal{S}_{\text{tst}}: \text{rank}_i \leq K\}|}{|\mathcal{S}_{\text{tst}}|}$$

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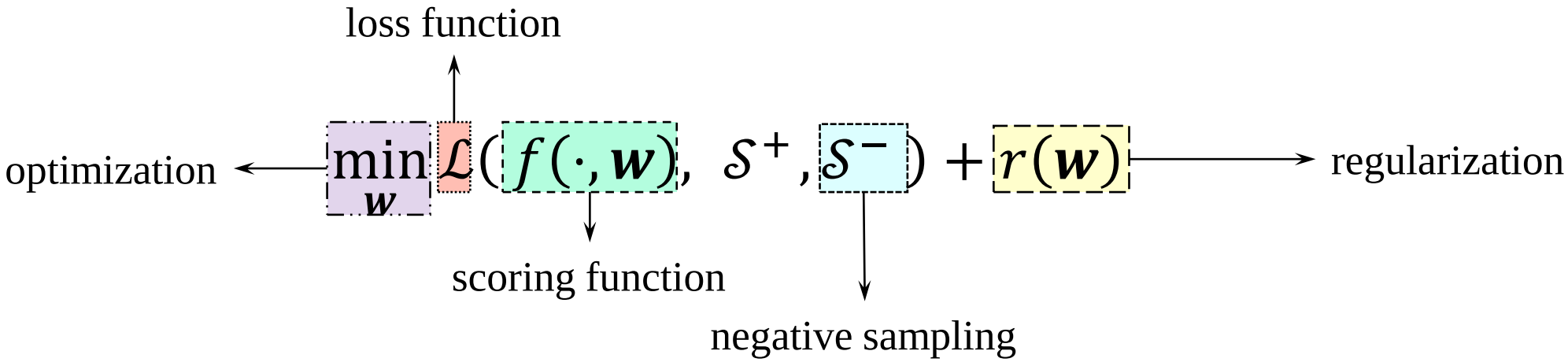
Learning problem in KGR

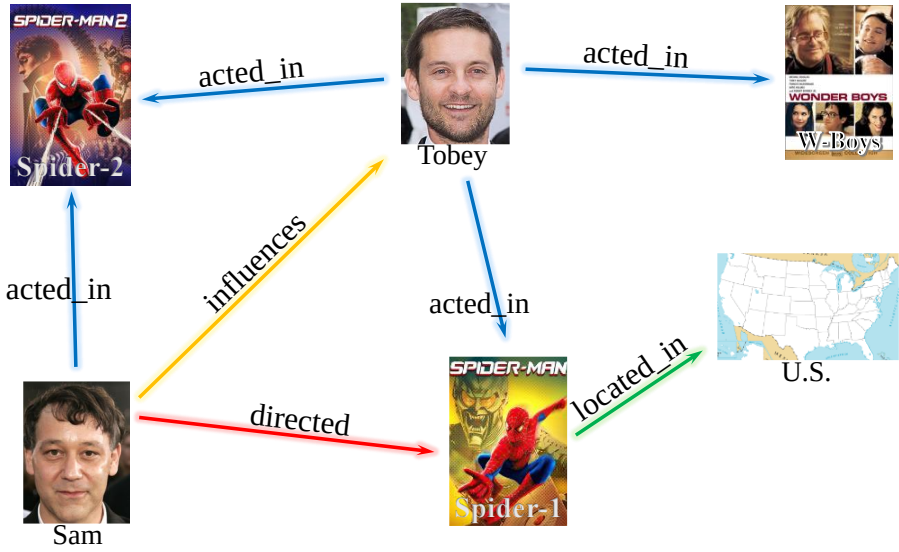
- As a learning problem, the KG reasoning problem contains the following important components:



Models

Query: (Sam, *directed*, ?)

Answer: Spider-1, Spider-2



triplet-based

(Sam, *directed*, Spider-2)

RESCAL [Nickel et. al. 2011]
TransE [Bordes et. al. 2013]
ComplEx [Trouillion et. al. 2017]
ConvE [Dettmers et. al.]
AutoSF [Zhang et. al. 2020]

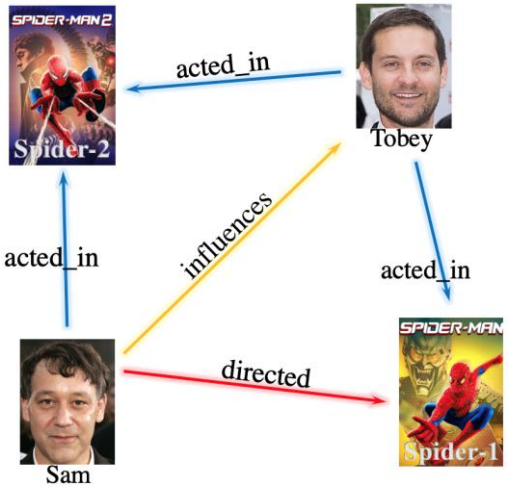
path-based

$$\text{Sam} \xrightarrow{directed} \text{Spider-1} \xrightarrow{acted\_in} \text{Tobey} \xrightarrow{acted\_in} \text{Spider-2}$$

$$\text{Sam} \xrightarrow{influences} \text{Tobey} \xrightarrow{acted\_in} \text{Spider-2}$$

PTransE [Lin et. al. 2015]
RSN [Dettmers et. al.]
Interestellar [Zhang et. al. 2020]

subgraph-based



GraIL [Teru et. al. 2019]
NBFNet [Zhu et. al. 2021]
RED-GNN [Zhang et. al. 2022]

AutoML – Recall

1. Define an AutoML problem

- Derive a **search space** from insights in specific domains
- **Search objective** is usually validation performance
- **Search constraint** is usually resource budgets
- **Training objective** usually comes from classical learning models

$$\min_{\lambda \in \mathcal{S}} M(F(w^*; \lambda), D_{\text{val}})$$ ← Search Objective

Search Space →

$$\text{s. t.} \quad \min_{w} L(F(w; \lambda), D_{\text{tra}})$$ ← Training Objective

$$G(\lambda) \leq C$$ ← Search Constraints

2. Design or select proper search algorithm

- Reduce model training cost (time to get w^*)

AutoML – KGE

Search space:

hyper-parameter, scoring function

Search objective:

ranking-based metrics

Training objective:

loss function

Search constraint:

overall time for searching

Search algorithm:

- grid search, random search, greedy algorithm, evolutionary algorithm
- Bayesian optimization, Reinforcement learning, Gradient descent

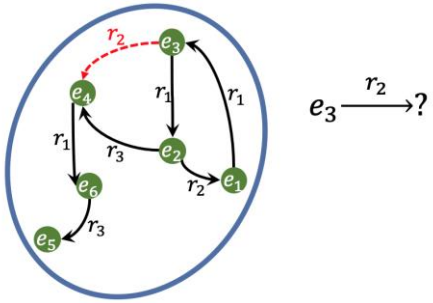
Why AutoML for KGR?

- Various benchmarks

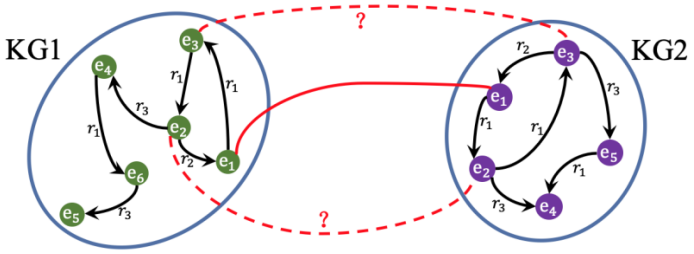
	WN18	FB15k	WN18RR	FB15k-237	YAGO3-10	ogbl-biokg	ogbl-wikikg2
# entities	41k	15k	41k	15k	123k	94k	2,500k
# relations	18	1345	11	237	37	51	535
# triplets	151k	593k	93k	210k	1,080k	5,089k	17,136k

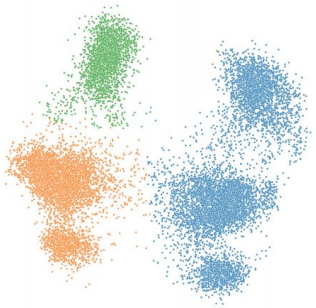
- Different relation patterns:
  - symmetric, anti-symmetric, inverse, asymmetric, composition…

- Different tasks:



$e_3 \xrightarrow{r_2} ?$





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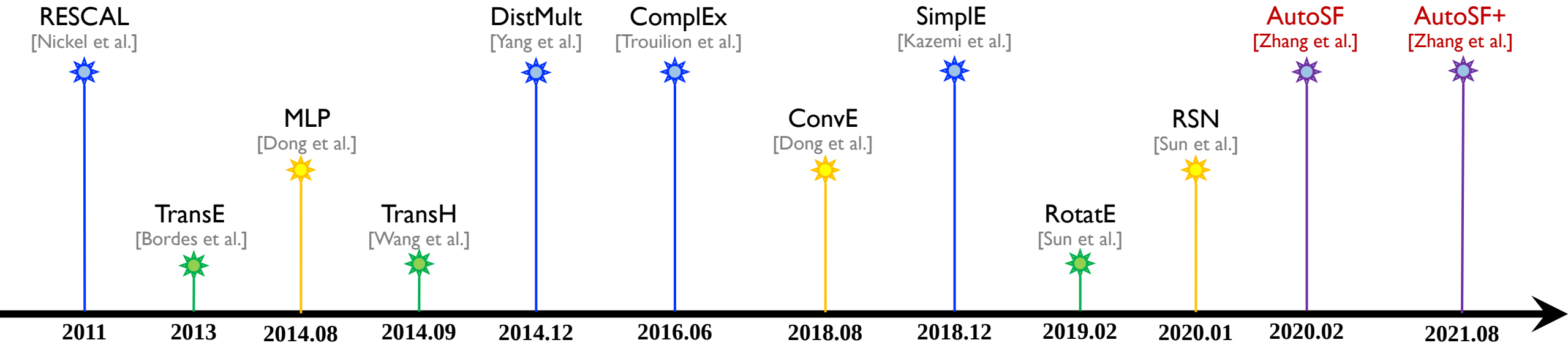
Triplet-based models

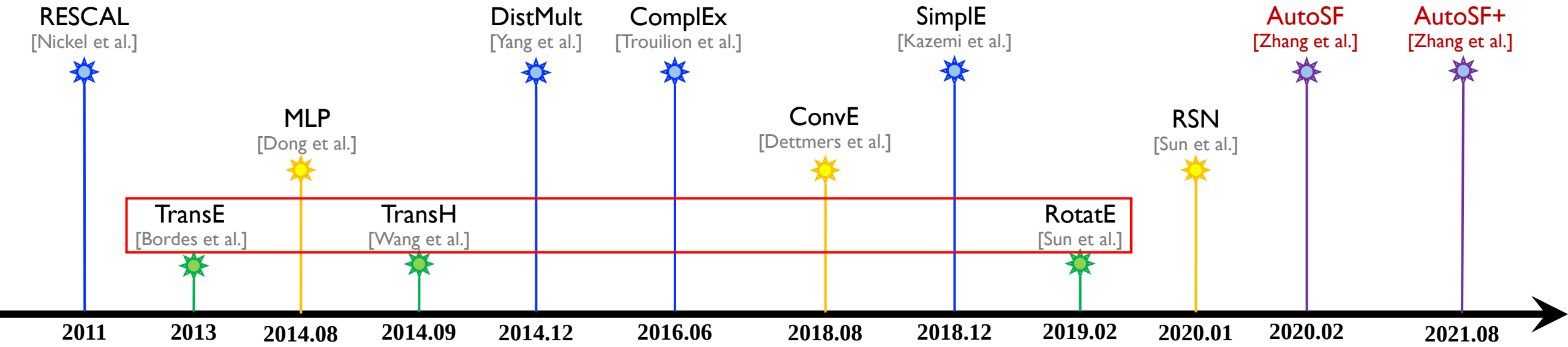


A large amount of scoring functions (SFs) $f(h, r, t)$ are defined to measure the plausibility of triplets $\{(h, r, t)\}$ in KG.

Capture important properties:

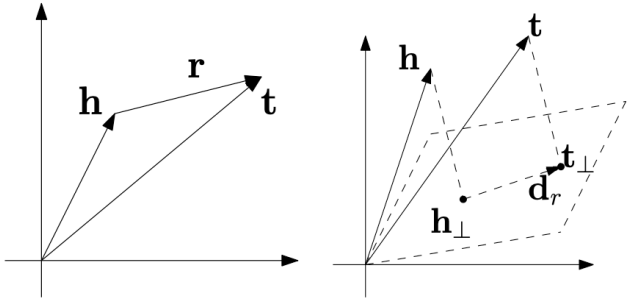
- symmetric, anti-symmetric, inverse, asymmetric…

Translational Distance Model (TDM)



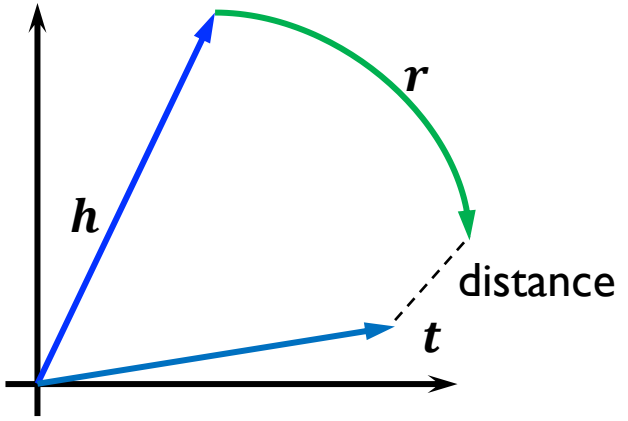
TransE: $f(h,r,t) = -\|(\boldsymbol{h}+\boldsymbol{r})-\boldsymbol{t}\|_p$

TransH: $f(h,r,t) = -\|(\boldsymbol{h}'+\boldsymbol{r})-\boldsymbol{t}'\|_p$



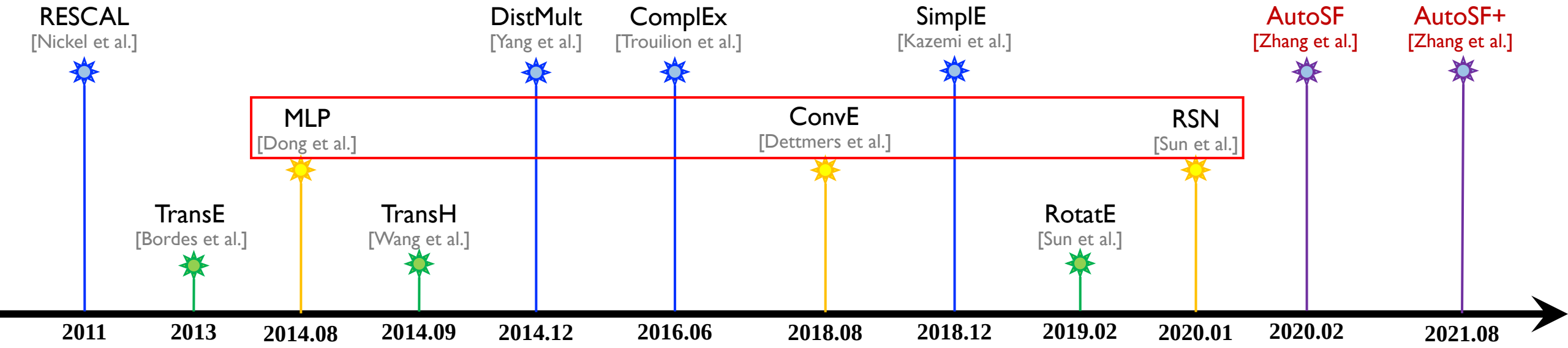
(a) TransE (b) TransH

RotatE: $f(h,r,t) = -\|(\boldsymbol{h}\circ\boldsymbol{r})-\boldsymbol{t}\|_p$

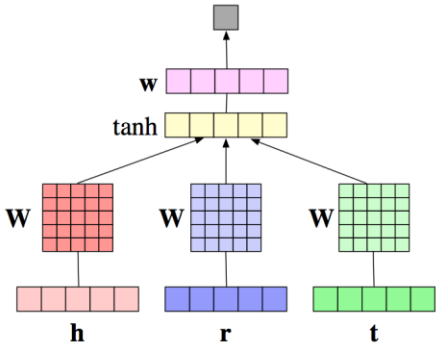


less expressive

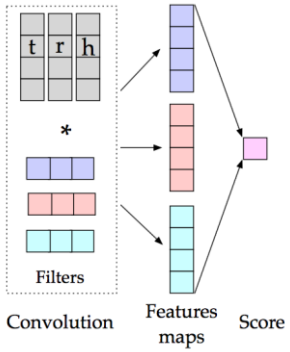
Neural Network Model (NNM)



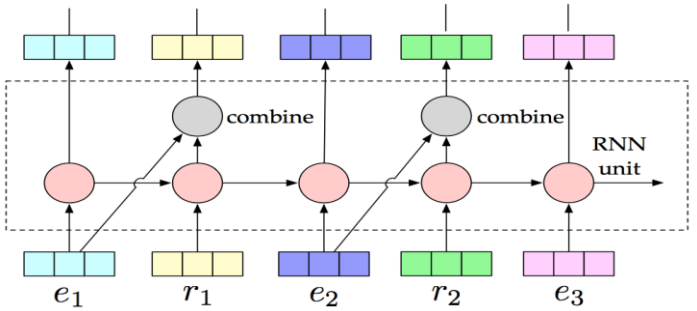
MLP



ConvE

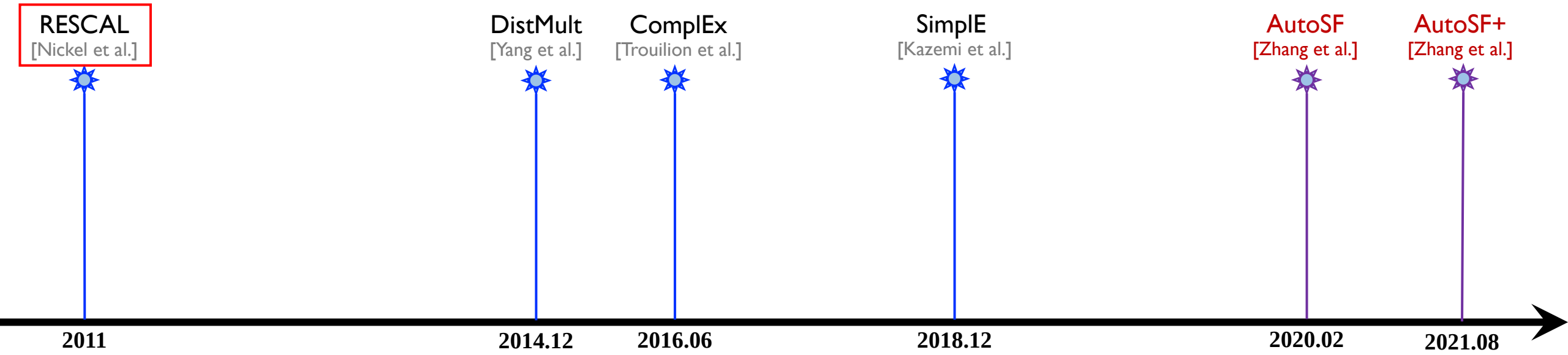


RSN

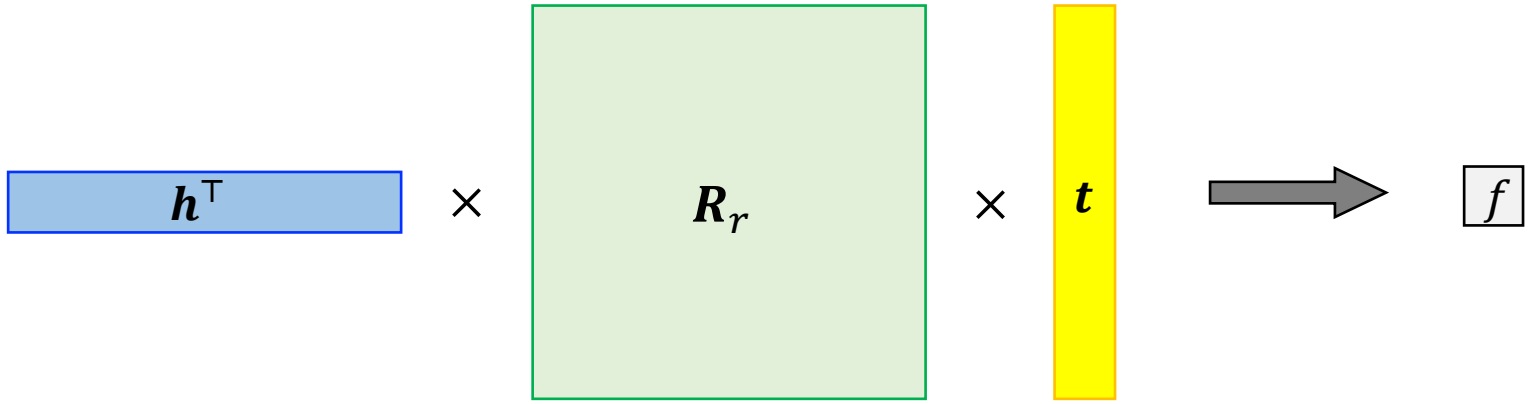


complex
and
difficult to train

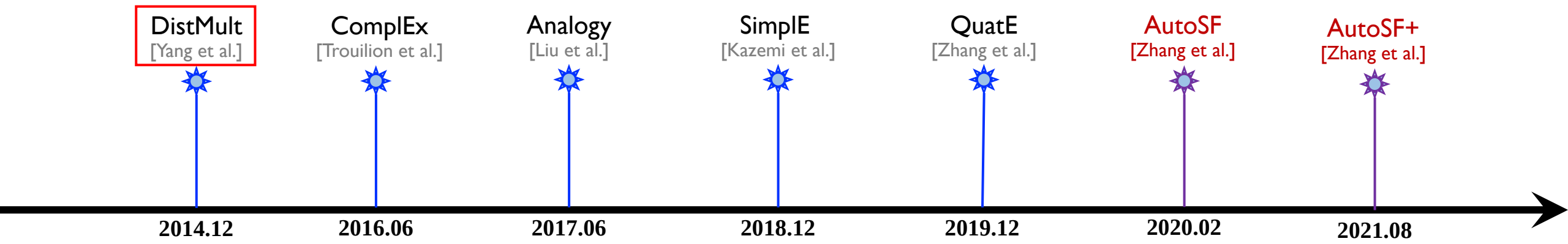
BiLinear Model (BLM)



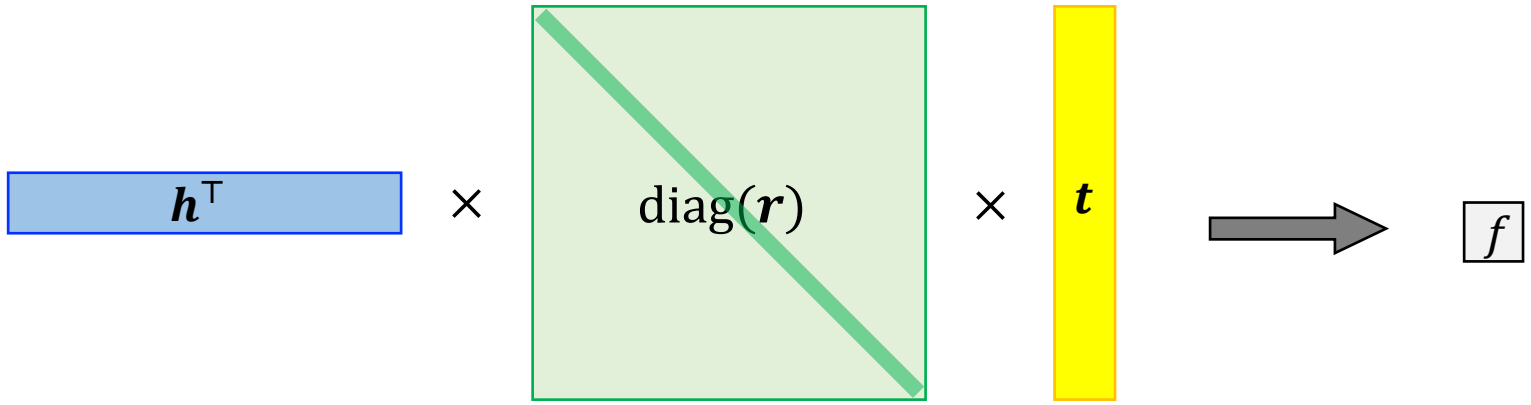
RESCAL: $f(h, r, t) = \boldsymbol{h}^\top \boldsymbol{R}_r \boldsymbol{t}$



DistMult



DistMult: $f(h,r,t) = \boldsymbol{h}^\top \mathrm{diag}(\boldsymbol{r})\boldsymbol{t} = \langle \boldsymbol{h}, \boldsymbol{r}, \boldsymbol{t} \rangle$

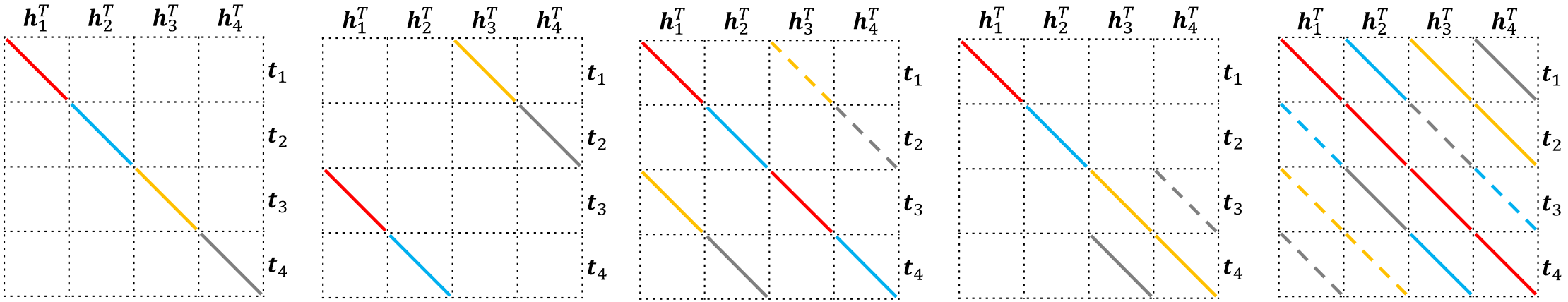


BLMs – unified form

- With unified representation.
- State-of-the-art performance.
- Fully expressive.

- No absolute winner as KGs have different properties.
- How to balance expressiveness and generalization.

AutoSF: searching!



(a) DistMult. (b) SimplE. (c) ComplEx. (d) Analogy. (e) QuatE.

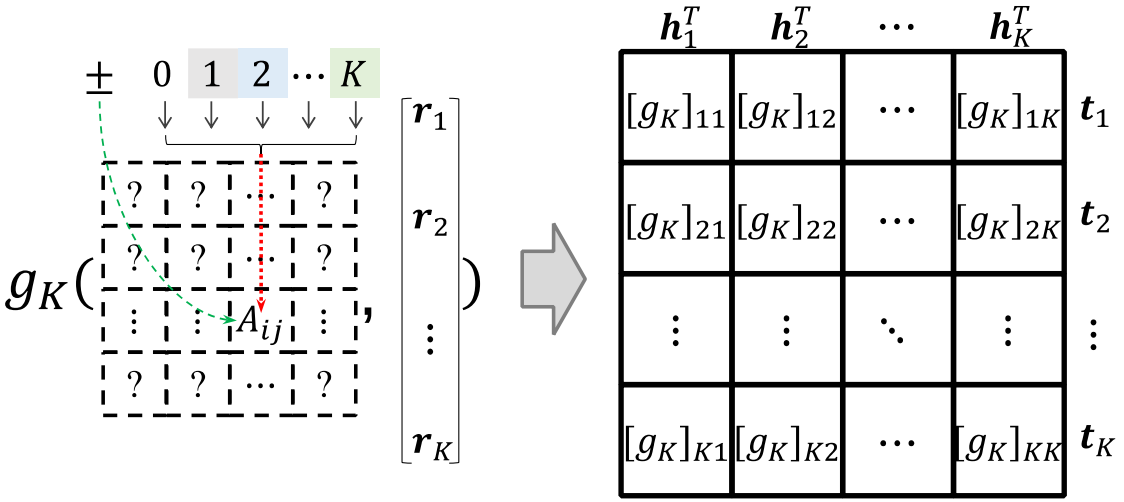
Search problem

$(2K+1)^{K^2}$

Definition 4 (Bilinear Model Search (AutoBLM)). *Let $F(\boldsymbol{P};\boldsymbol{A})$ be a KG embedding model (where $\boldsymbol{P}$ includes the entity embedding matrix $\boldsymbol{E}$ and relation embedding matrix $\boldsymbol{R}$, and $\boldsymbol{A}$ is the structure matrix) and $M(F,\mathcal{S})$ be the performance of F on triples $\mathcal{S}$ (the higher the better). The AutoBLM problem is formulated as:*

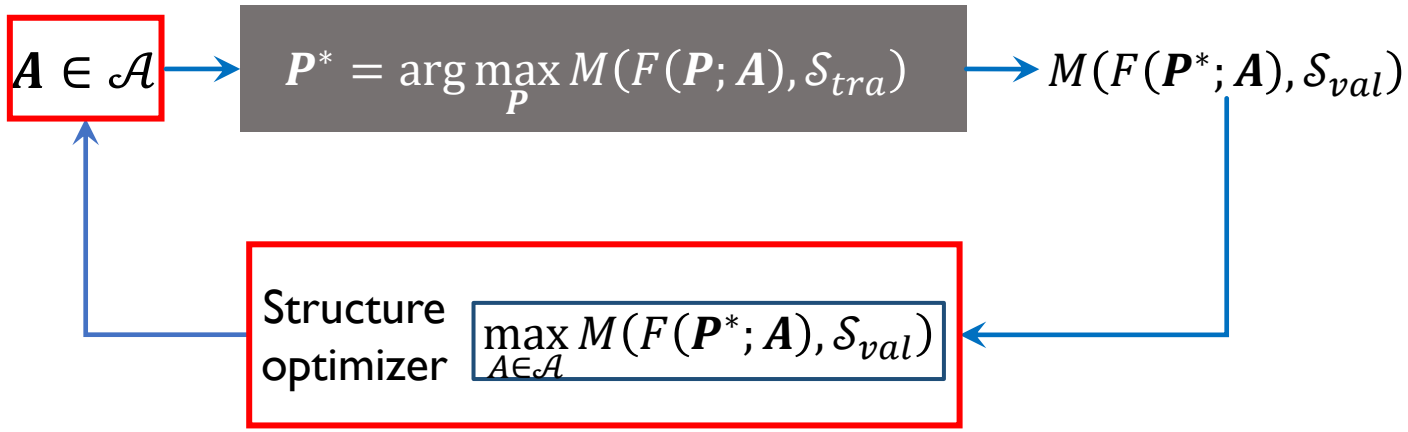
$$\boldsymbol{A}^* \in \operatorname{Arg\,max}_{\boldsymbol{A}\in\mathcal{A}} M\left(F(\boldsymbol{P}^*;\boldsymbol{A}),\mathcal{S}_{val}\right) \quad (9)$$

$$s.t. \quad \boldsymbol{P}^* = \arg\max_{\boldsymbol{P}} M\left(F(\boldsymbol{P};\boldsymbol{A}),\mathcal{S}_{tra}\right), \quad (10)$$



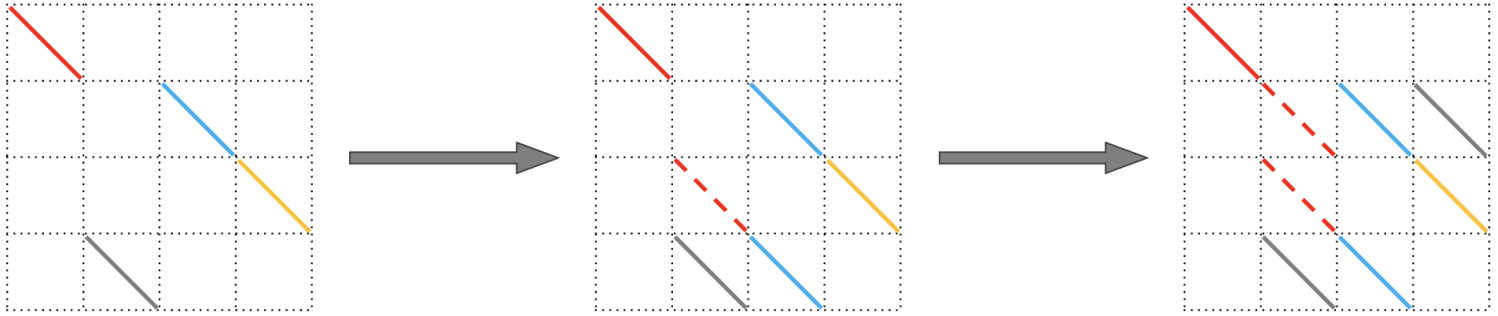
Search space:
What to be searched

Validation performance

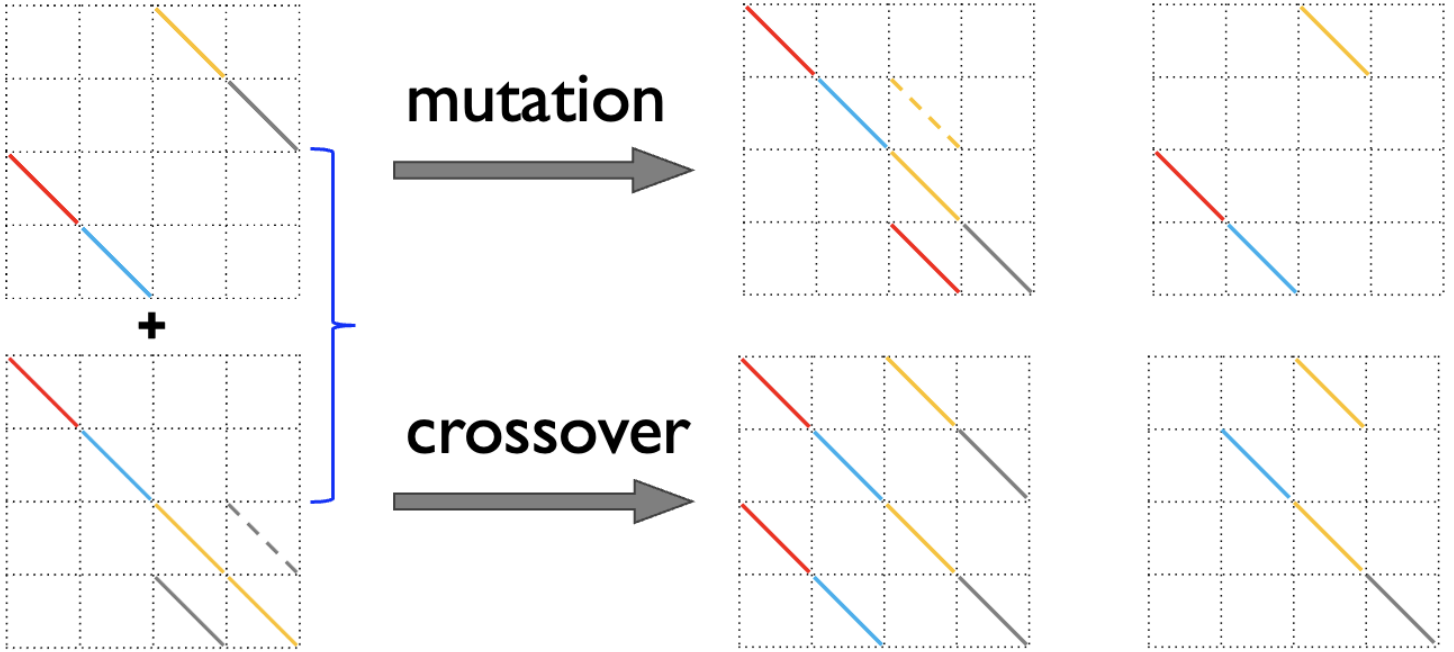


Search algorithms

AutoSF: [Zhang et. al. 2020]
progressive algorithm



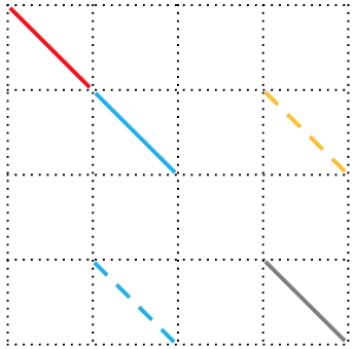
AutoSF+: [Zhang et. al. 2022]
evolutionary algorithm



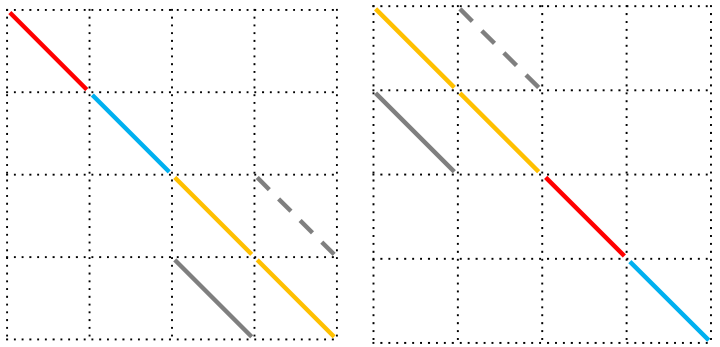
Domain properties

- **Filter:** avoid redundant evaluation

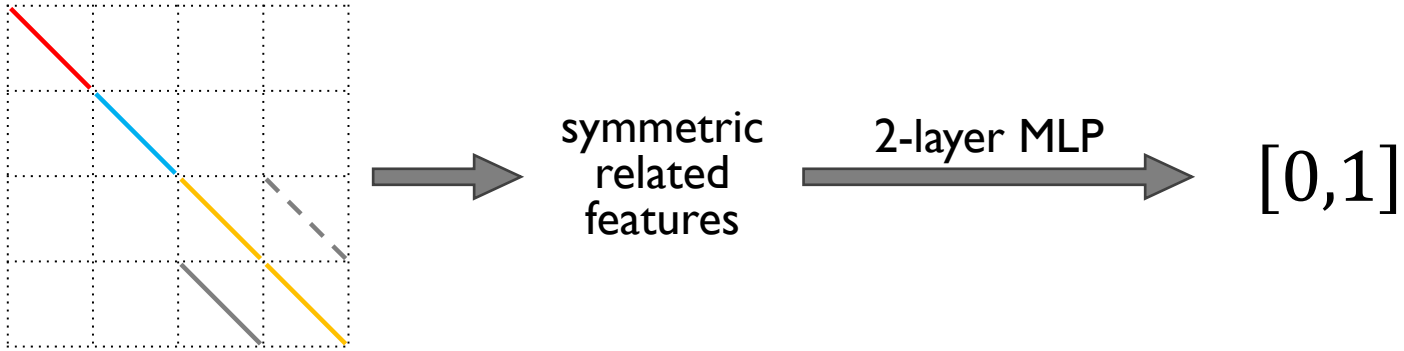
Degenerate



Equivalent

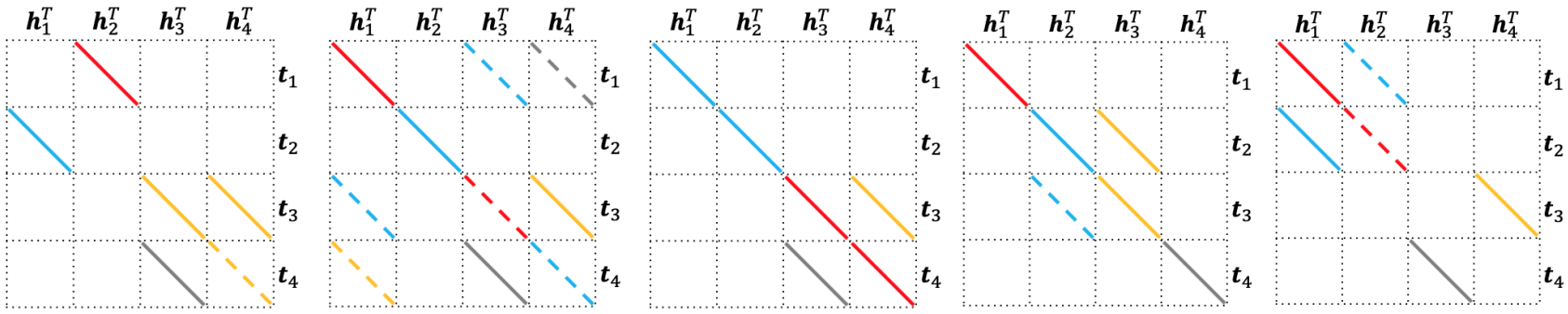


- **Predictor:** estimate the mapping from structure to performance



Expressiveness

	model	WN18			FB15k			WN18RR			FB15k237			YAGO3-10		
		MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10
(TDM)	TransH	0.521	—	94.5	0.452	—	76.6	0.186	—	45.1	0.233	—	40.1	—	—	—
	RotatE	—	—	—	0.797	74.6	88.4	0.476	42.8	57.1	0.338	24.1	53.3	0.488	39.6	66.3
	PairRE	—	—	—	0.811	76.5	89.6	—	—	—	0.351	25.6	54.4	—	—	—
(NNM)	ConvE	0.942	93.5	95.5	0.745	67.0	87.3	0.46	39.	48.	0.316	23.9	49.1	0.52	45.	66.
	RSN	0.94	92.2	95.3	—	—	—	—	—	—	0.28	20.2	45.3	—	—	—
	CompGCN	—	—	—	—	—	—	0.479	44.3	54.6	0.355	26.4	53.5	—	—	—
(BLM)	TuckER	**0.953**	**94.9**	95.8	0.795	74.1	89.2	0.470	44.3	52.6	0.358	26.6	54.4	—	—	—
	DistMult	0.821	71.7	95.2	0.775	71.4	87.2	0.443	40.4	50.7	0.352	25.9	54.6	0.552	47.1	68.9
	SimplE/CP	0.950	94.5	95.9	0.826	79.4	90.1	0.462	42.4	55.1	0.350	26.0	54.4	0.565	49.1	71.0
	HolE/ComplEx	0.951	94.5	95.7	0.831	79.6	90.5	0.471	43.0	55.1	0.345	25.3	54.1	0.563	49.0	70.7
	Analogy	0.950	94.6	95.7	0.816	78.0	89.8	0.467	42.9	55.4	0.348	25.6	54.7	0.557	48.5	70.4
	QuatE	0.950	94.5	95.9	0.782	71.1	90.0	0.488	43.8	**58.2**	0.348	24.8	55.0	0.556	47.4	70.4
	AutoSF	0.952	94.7	**96.1**	0.853	82.1	91.0	0.490	45.1	56.7	0.360	26.7	55.2	0.571	50.1	**71.5**
	AutoSF+	0.952	94.7	**96.1**	**0.861**	**83.2**	**91.3**	**0.492**	**45.2**	56.7	**0.364**	**27.0**	**55.3**	**0.577**	**50.2**	**71.5**



(a) WN18. (b) FB15k. (c) WN18RR. (d) FB15k237. (e) YAGO3-10.

Measurements

- Given a triplet (h, r, t);
- Compute the score of $(h', r, t), \forall h' \in \mathcal{E}$;
- Get the rank of h among all h';

Metrics

- MRR: $\frac{1}{|\mathcal{S}|}\sum_{i=1}^{|\mathcal{S}|}\frac{1}{\text{rank}_i}$
- Hit@k: $\frac{1}{|\mathcal{S}|}\sum_{i=1}^{|\mathcal{S}|}\mathbb{I}(\text{rank}_i < 10)$

Summary

- Bilinear models are the best choice in triplet-based models.
- AutoSF(+): An AutoML approach to design bilinear scoring functions.
- Search space:
  - Unified bilinear models
  - Guaranteed with *expressiveness*
- Search algorithm:
  - *Progressive* and *Evolutionary* algorithm
  - Tackle domain properties by filter and predictor

Outline

1. Background
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Relational path

Triplets (s, r, o)

Relational path

consecutively connected

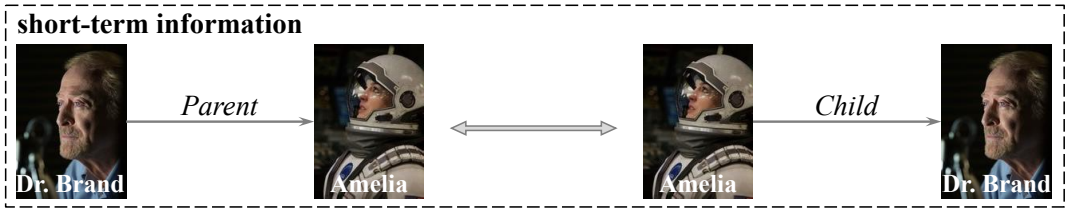
$s_1 \xrightarrow{r_1} s_2 \xrightarrow{r_2} s_3 \cdots s_L \xrightarrow{r_L} s_{L+1}$

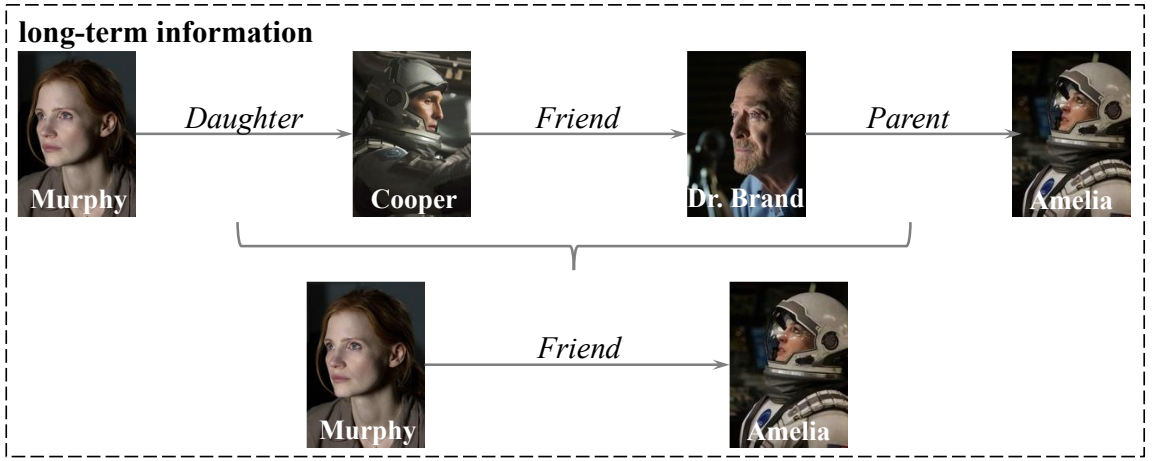
[Guu et al. 2015, Lin et al. 2015, Guo et al. 2019]

short-term information inside triplets.

composition of relations.

long-term information across multiple triplets.





PTransE [Lin et al. 2015]

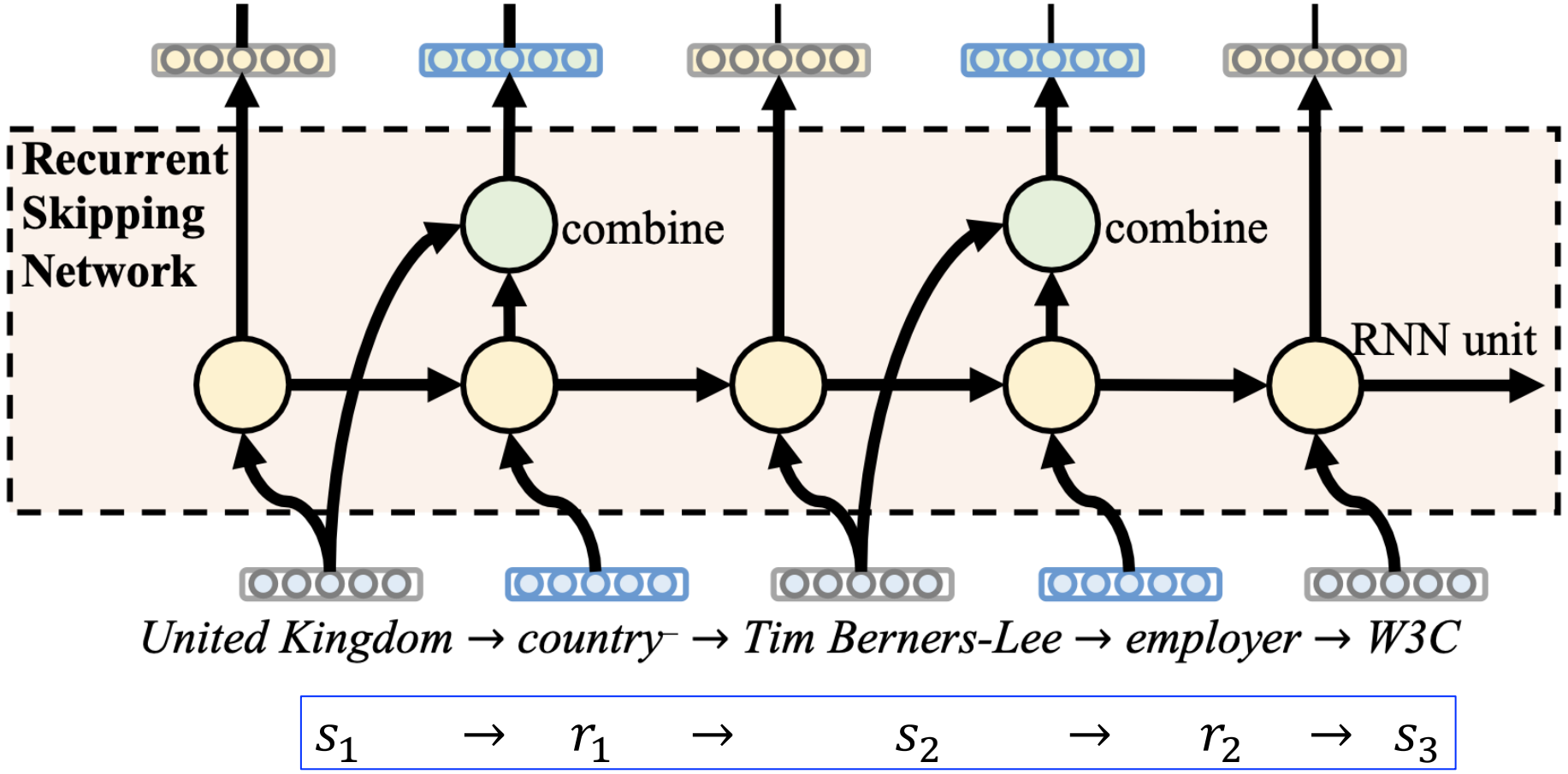
- Models composition of relations

$$s_1 \xrightarrow{r_1} \cdot \xrightarrow{r_2} \cdots \xrightarrow{r_{L-1}} s_L$$

- With condition

$$\boldsymbol{s}_L \approx \boldsymbol{s}_1 + \boldsymbol{r}_1 + \boldsymbol{r}_2 + \cdots \boldsymbol{r}_{L-1}$$

RSN [Guo et al. 2019]

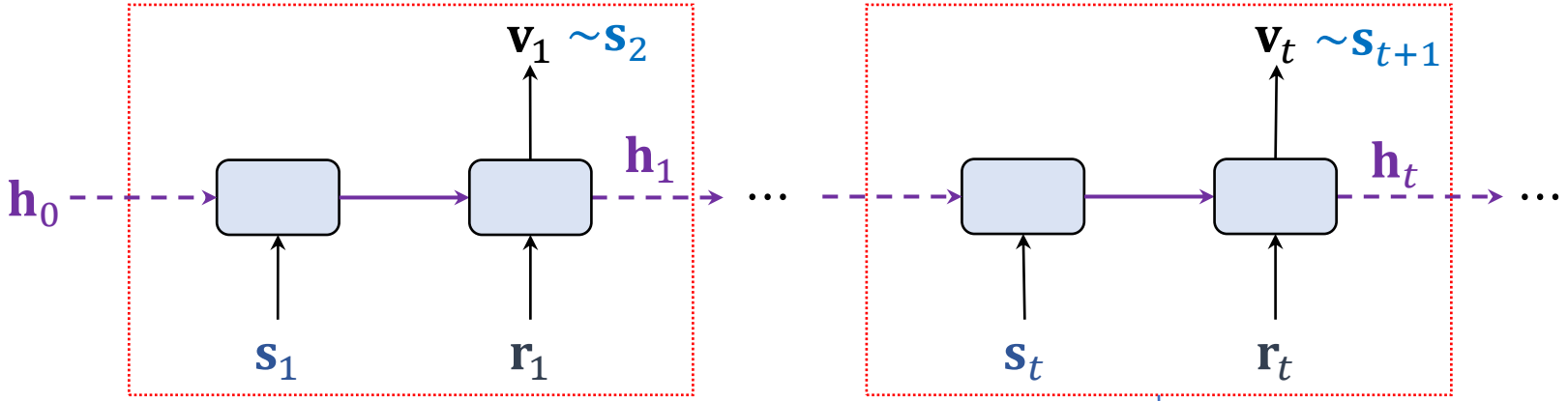


Models long-term information well, but is limited in modeling short-term information.

Interstellar [Zhang et al. 2020]

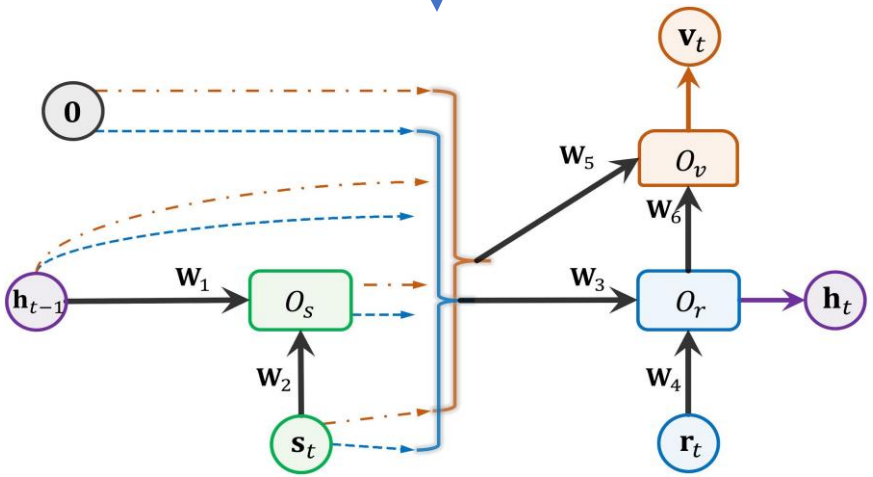
AAAI-22

Recurrently process the path by $[\mathbf{v}_t, \mathbf{h}_t] = f(\mathbf{s}_t, \mathbf{r}_t, \mathbf{h}_{t-1}), \quad \forall t = 1 \ldots L$



Searching !

macro-level	connections	$\mathbf{h}_{t-1}, O_s, \mathbf{0}, \mathbf{s}_t$
$\hat{\boldsymbol{\alpha}} \in \hat{\mathcal{A}}$	combinators	$+, \odot, \otimes$, gated
micro-level	activation	identity, tanh, sigmoid
$\check{\boldsymbol{\alpha}} \in \check{\mathcal{A}}$	weight matrix	$\{\mathbf{W}_i\}_{i=1}^{6}, \mathbf{I}$



Hybrid search algorithm

Search appropriate $\alpha \in \mathcal{A}$ that maximize the validation performance

$$\boldsymbol{\alpha}^* = \arg\max_{\boldsymbol{\alpha}\in\mathcal{A}} \mathcal{M}\left(f(\boldsymbol{F}^*;\boldsymbol{\alpha}), \mathcal{G}_{\text{val}}\right), \quad \text{s.t.} \quad \boldsymbol{F}^* = \arg\min_{\boldsymbol{F}} \mathcal{L}\left(f(\boldsymbol{F};\boldsymbol{\alpha}), \mathcal{G}_{\text{tra}}\right)$$

Stand-alone approach:

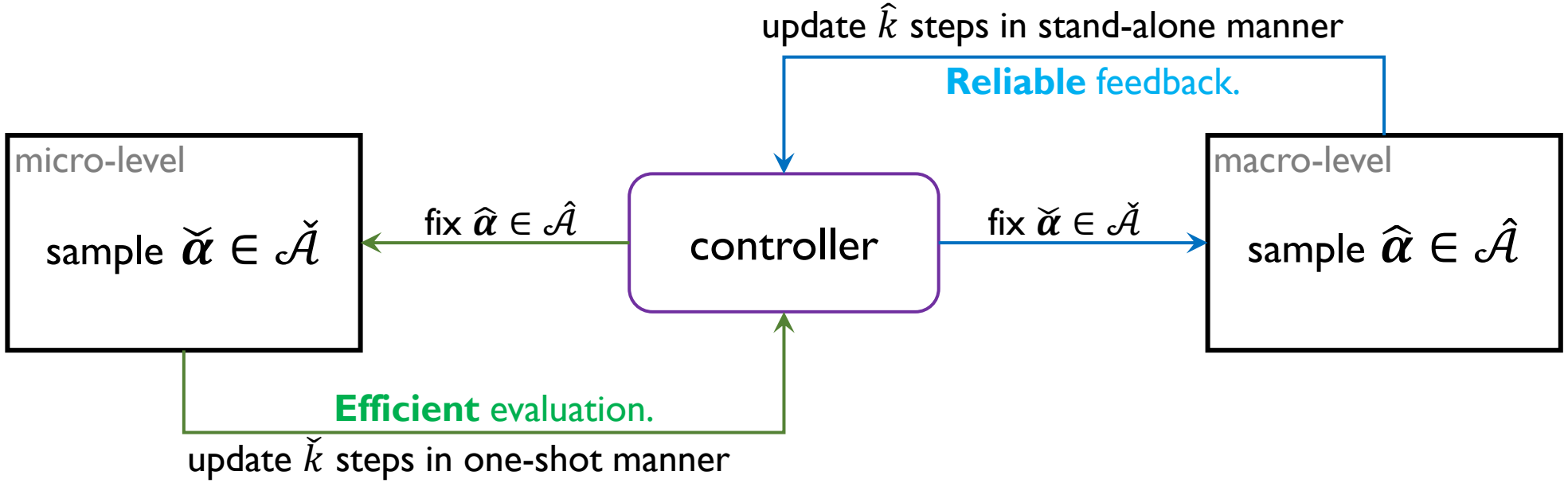
- $\mathcal{M}$ is accurate;
- $\boldsymbol{F}^*$ needs high cost.

[Zoph and Le 2017]

One-shot approach:

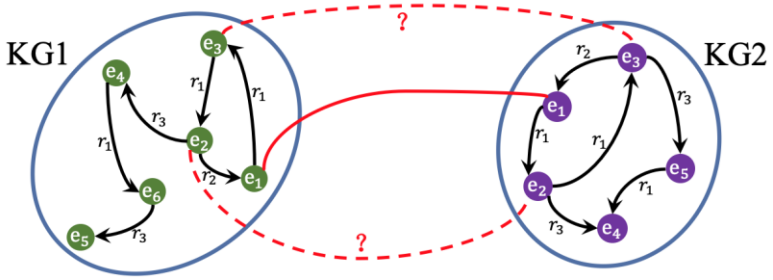
- $\boldsymbol{F}^*$ is shared and efficient;
- $\mathcal{M}$ is not always reliable.

[Pham et al. 2018, Liu et al. 2019]

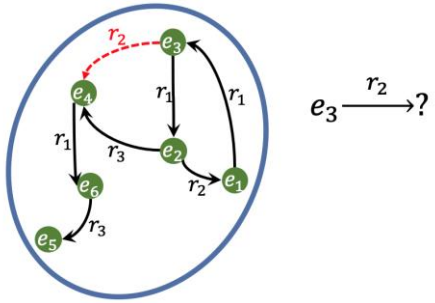


Effectivess

	models	DBP-WD			DBP-YG			EN-FR			EN-DE		
		H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR
triplet	TransE	18.5	42.1	0.27	9.2	24.8	0.15	16.2	39.0	0.24	20.7	44.7	0.29
	TransD*	27.7	57.2	0.37	17.3	41.6	0.26	21.1	47.9	0.30	24.4	50.0	0.33
	BootEA*	32.3	63.1	0.42	31.3	62.5	0.42	31.3	62.9	0.42	44.2	70.1	0.53
GCN	GCN-Align	17.7	37.8	0.25	19.3	41.5	0.27	15.5	34.5	0.22	25.3	46.4	0.22
	VR-GCN	19.4	55.5	0.32	20.9	55.7	0.32	16.0	50.8	0.27	24.4	61.2	0.36
	R-GCN	8.6	31.4	0.16	13.3	42.4	0.23	7.3	31.2	0.15	18.4	44.8	0.27
path	PTransE	16.7	40.2	0.25	7.4	14.7	0.10	7.3	19.7	0.12	27.0	51.8	0.35
	IPTransE*	23.1	51.7	0.33	22.7	50.0	0.32	25.5	55.7	0.36	31.3	59.2	0.41
	Chains	32.2	60.0	0.42	35.3	64.0	0.45	31.4	60.1	0.41	41.3	68.9	0.51
	RSN*	38.8	65.7	0.49	40.0	67.5	0.50	34.7	63.1	0.44	48.7	72.0	0.57
	Interstellar	**40.7**	**71.2**	**0.51**	**40.2**	**72.0**	**0.51**	**35.5**	**67.9**	**0.46**	**50.1**	**75.6**	**0.59**



models	WN18-RR			FB15k-237			YAGO3-10		
	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR
TransE	12.5	44.5	0.18	17.3	37.9	0.24	10.3	27.9	0.16
ComplEx	41.4	49.0	0.44	22.7	49.5	0.31	40.5	62.8	0.48
RotatE*	43.6	54.2	0.47	**23.3**	50.4	**0.32**	40.2	63.1	0.48
R-GCN	-	-	-	15.1	41.7	0.24	-	-	-
PTransE	27.2	46.4	0.34	20.3	45.1	0.29	12.2	32.3	0.19
RSN	38.0	44.8	0.40	19.2	41.8	0.27	16.4	37.3	0.24
Interstellar	**44.0**	**54.8**	**0.48**	**23.3**	**50.8**	**0.32**	**42.4**	**66.4**	**0.51**



Outline

1. Background
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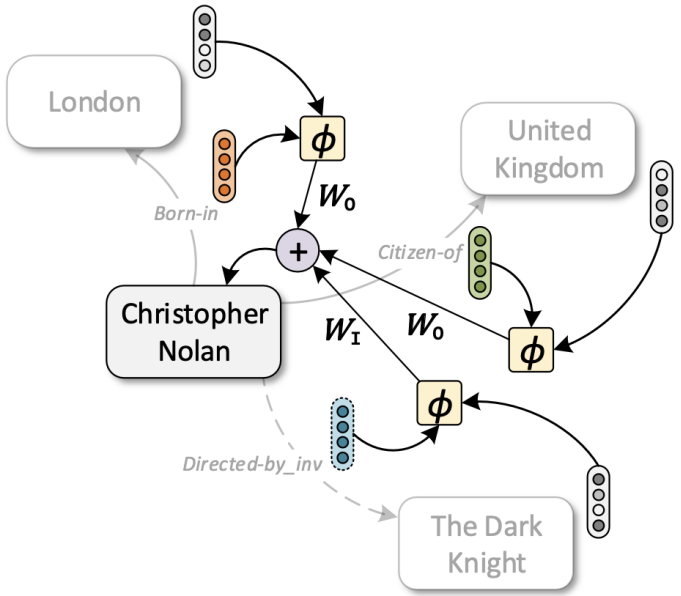
GCN-variants

R-GCN
[Schlichtkrull et. al. 2017]

CompGCN
[Vashishth et. al. 2020]

KE-GCN
[Yu et. al. 2021]



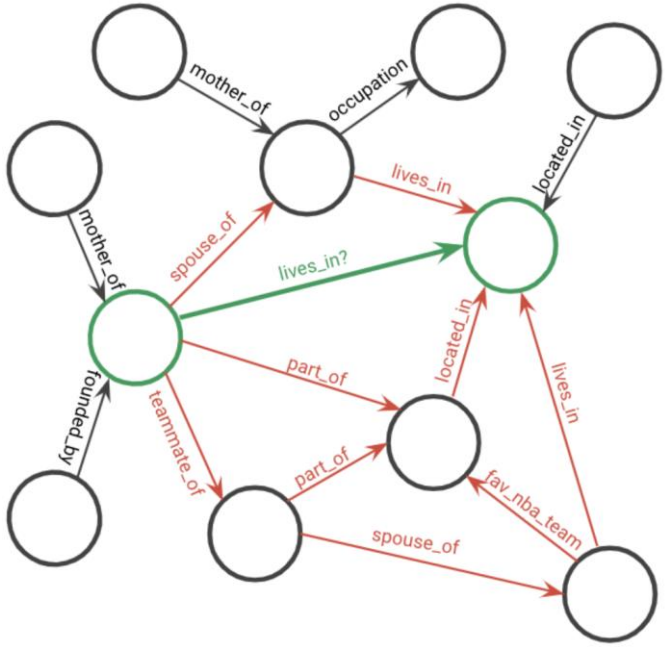
- Not scalable.
- Have little improvement.
- Depends on the scoring function

low-level embeddings → aggregate by relational GNNs → high-level embeddings → TransE / ConvE / DistMult / … → scores

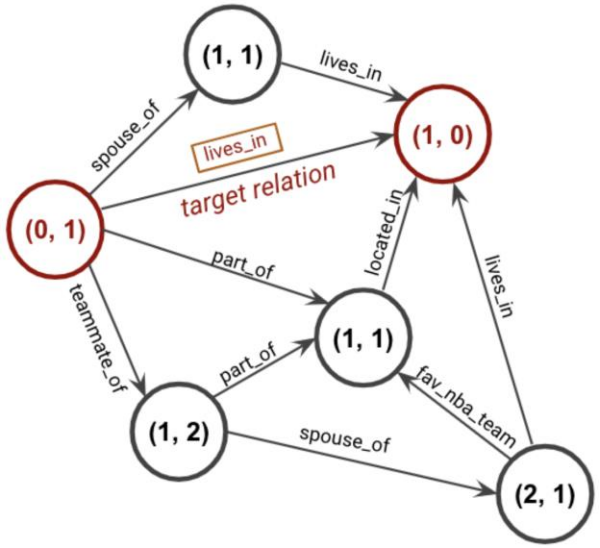
GraIL [Teru et. al. 2020]

AAAI-22

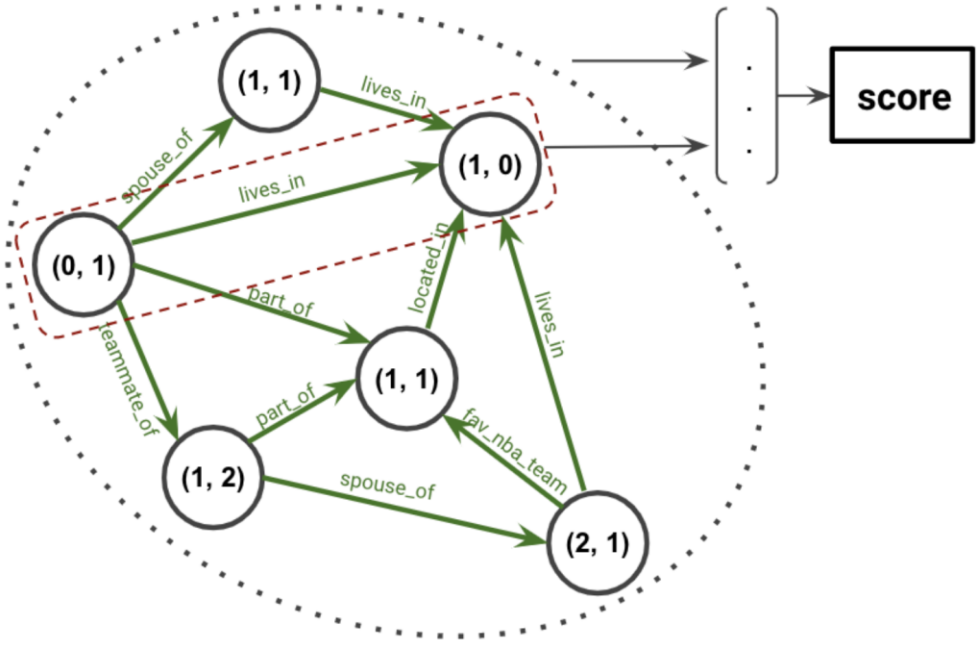
Enclosing subgraph



Entity labeling



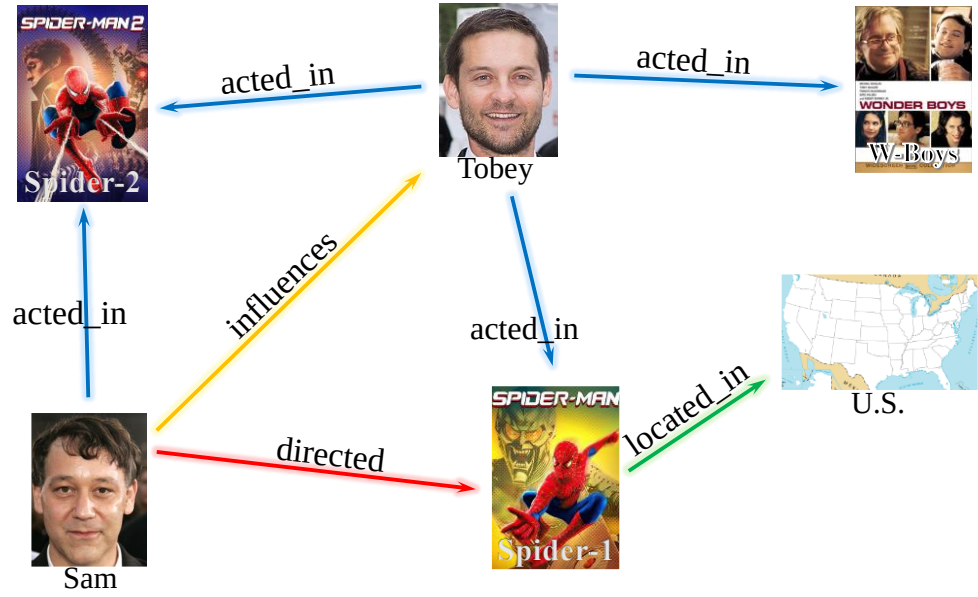
GNN scoring



Pros: inductive reasoning.

Cons: very expensive.

RED-GNN [Zhang et. al. 2022]



- Augment path to have the same length

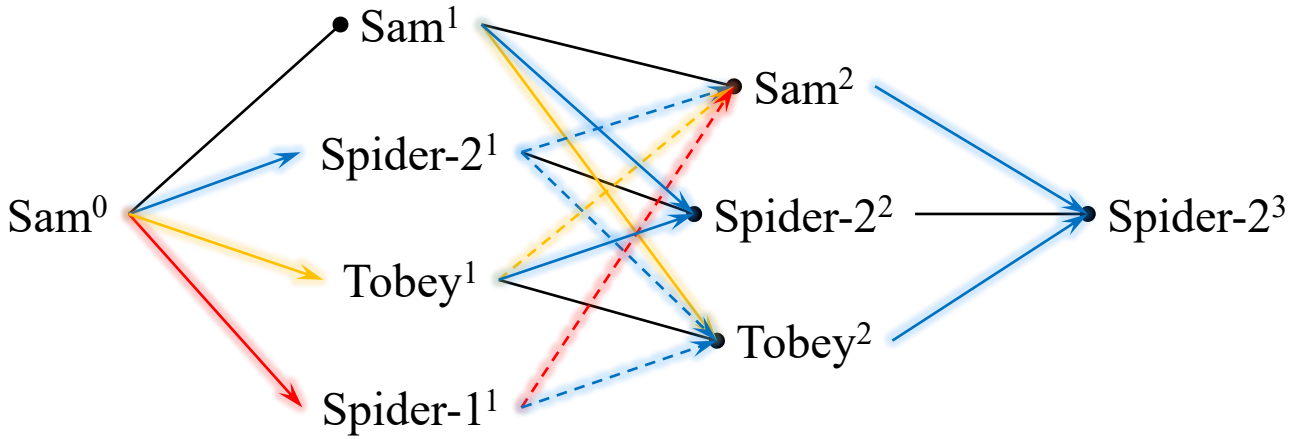
$$\text{Sam} \xrightarrow{directed} \text{Spider-1} \xrightarrow{acted\_in} \text{Tobey} \xrightarrow{acted\_in} \text{Spider-2}$$

$$\text{Sam} \xrightarrow{identity} \text{Sam} \xrightarrow{influences} \text{Tobey} \xrightarrow{acted\_in} \text{Spider-2}$$

$$\text{Sam} \xrightarrow{identity} \text{Sam} \xrightarrow{identity} \text{Sam} \xrightarrow{acted\_in} \text{Spider-2}$$

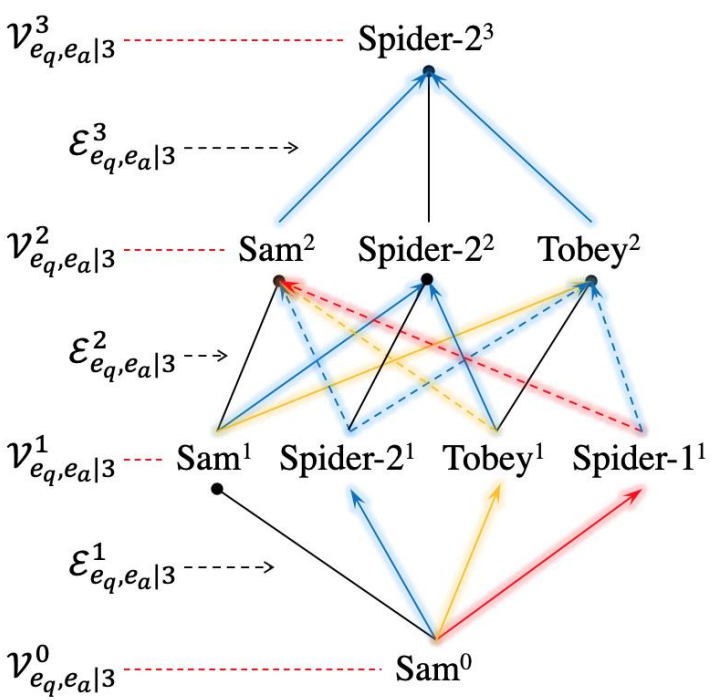
……

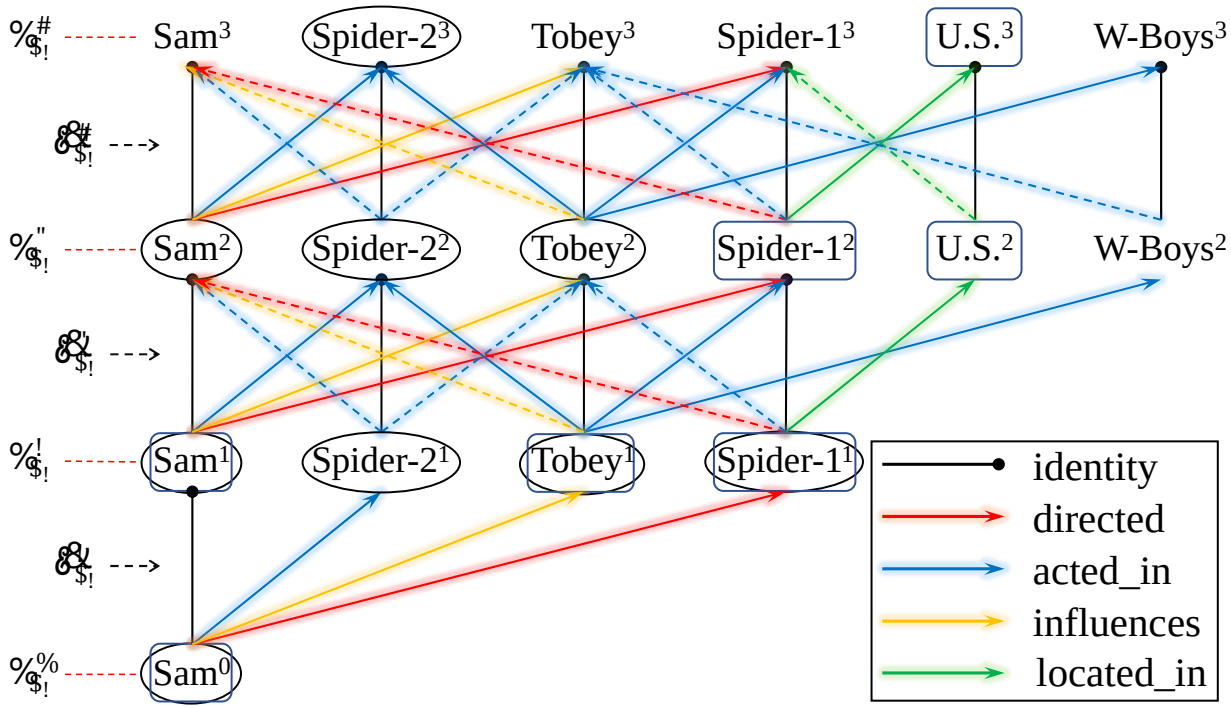
- R-Digraph: Stack the path to form relational digraph



RED-GNN [Zhang et. al. 2022]

$$\mathcal{G}_{e_q,e_o|\ell} = \cup_{(e_s,r,e_o)\in\hat{\mathcal{E}}^{\ell}_{eq}} \mathcal{G}_{e_q,e_s|\ell-1} \otimes \left\{(e_s,r,e_o) \in \hat{\mathcal{E}}^{\ell}_{e_q}\right\}.$$





individual computation

recursive/parallel computation

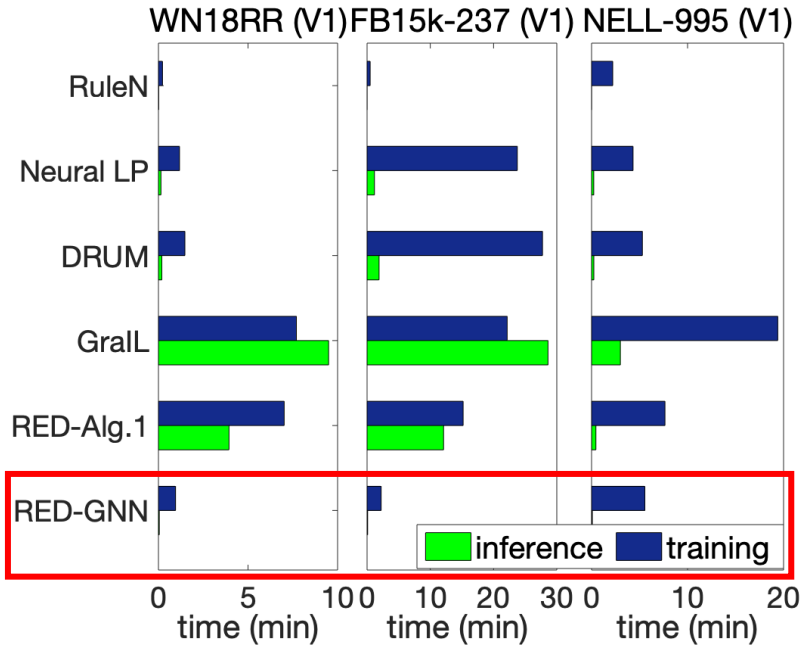
Results

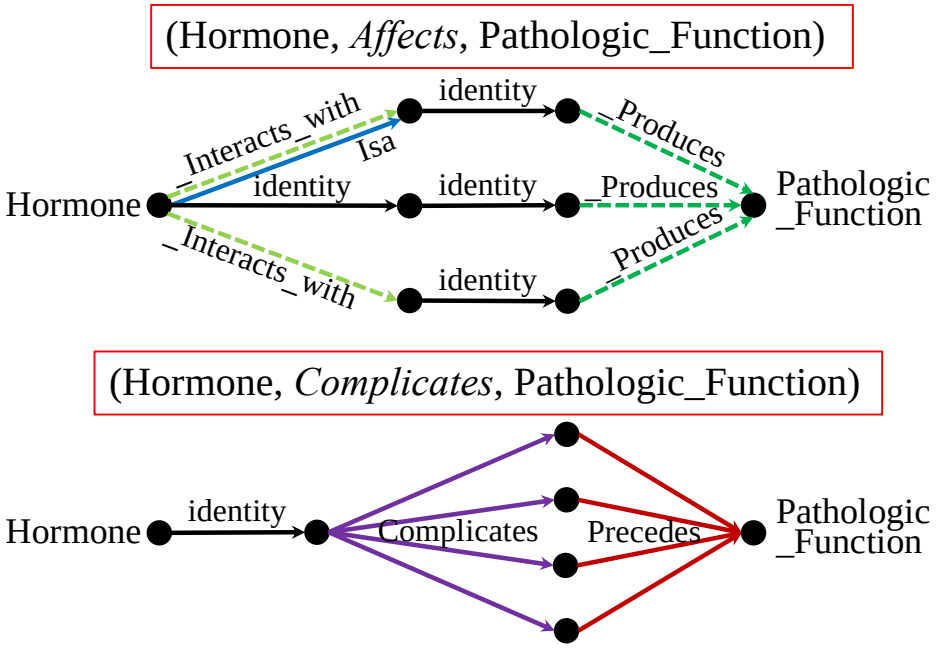
Table 1: Transductive reasoning. Best performance is indicated by the bold face numbers.

type	models	Family			UMLS			WN18RR			FB15k-237			NELL-995		
		MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10	MRR	H@1	H@10
triple	RotatE	.921	86.6	98.8	.925	86.3	99.3	.477	42.8	57.1	.337	24.1	53.3	.508	44.8	60.8
	QuatE	.941	89.6	99.1	.944	90.5	99.3	.480	44.0	55.1	.350	25.6	53.8	.533	46.6	64.3
path	MINERVA	.885	82.5	96.1	.825	72.8	96.8	.448	41.3	51.3	.293	21.7	45.6	.513	41.3	63.7
	Neural LP	.924	87.1	99.4	.745	62.7	91.8	.435	37.1	56.6	.252	18.9	37.5	out of memory		
	DRUM	.934	88.1	99.6	.813	67.4	97.6	.486	42.5	58.6	.343	25.5	51.6	out of memory		
	RNNLogic*	–	–	–	.842	77.2	96.5	.483	44.6	55.8	.344	25.2	53.0	–	–	–
GNN	CompGCN	.933	88.3	99.1	.927	86.7	**99.4**	.479	44.3	54.6	.355	26.4	53.5	out of memory		
	DPMPN	.981	97.4	98.1	.930	89.9	98.2	.482	44.4	55.8	**.369**	**28.6**	53.0	.513	45.2	61.5
	RED-GNN	**.992**	**98.8**	**99.7**	**.964**	**94.6**	99.0	**.533**	**48.5**	**62.4**	.364	27.3	**54.4**	**.543**	**47.6**	**65.1**

Table 2: Inductive reasoning. Best performance is indicated by the bold face numbers.

	WN18RR				FB15k-237				NELL-995			
	V1	V2	V3	V4	V1	V2	V3	V4	V1	V2	V3	V4
RuleN	.668	.645	.368	.624	.363	.433	.439	.429	.615	.385	.381	.333
Neural LP	.649	.635	.361	.628	.325	.389	.400	.396	.610	.361	.367	.261
DRUM	.666	.646	.380	.627	.333	.395	.402	.410	.628	.365	.375	.273
GraIL	.627	.625	.323	.553	.279	.276	.251	.227	.481	.297	.322	.262
RED-GNN	**.696**	**.690**	**.427**	**.651**	**.369**	**.469**	**.445**	**.442**	**.637**	**.419**	**.436**	**.363**





Outline

1. Background
   - Knowledge Graph (KG)
   - KG embedding
2. AutoML for model design
3. Scoring function design
   - Overview
   - AutoSF
4. Summary

Take away

	semantic	structure	interpretable	efficiency
Triplet-based	symmetric, inverse	×	×	fastest
Path-based	composition	sequential	logic rule	depends on # paths
Subgraph-based	high-order	topological	complex logic rule	depends on subgraph

AutoML for model design in KG reasoning can boost performance.
But the space/algorithm should seriously consider domain-specific knowledges.

Future work

- Automated GNN architecture design for KG.
- Efficient reasoning on large-scaled KGs, e.g., ogbl-wikikg.
- Reasoning on dynamic KGs.

Related papers

Knowledge Graph Embedding: A Survey of Approaches and Applications. Q. Wang, Z. Mao, B. Wang and L. Guo. TKDE 2017.

Taking the Human out of Learning Applications: A Survey on Automated Machine Learning. Q. Yao, M. Wang, Y. Chen et. al. 2019.

NSCaching: Simple and Efficient Negative Sampling for Knowledge Graph Embedding. **Y. Zhang**, Q. Yao, Y. Shao and L. Chen. ICDE 2019.

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Thank you!