KGTuner: Efficient Hyper-parameter Search for Knowledge Graph Learning

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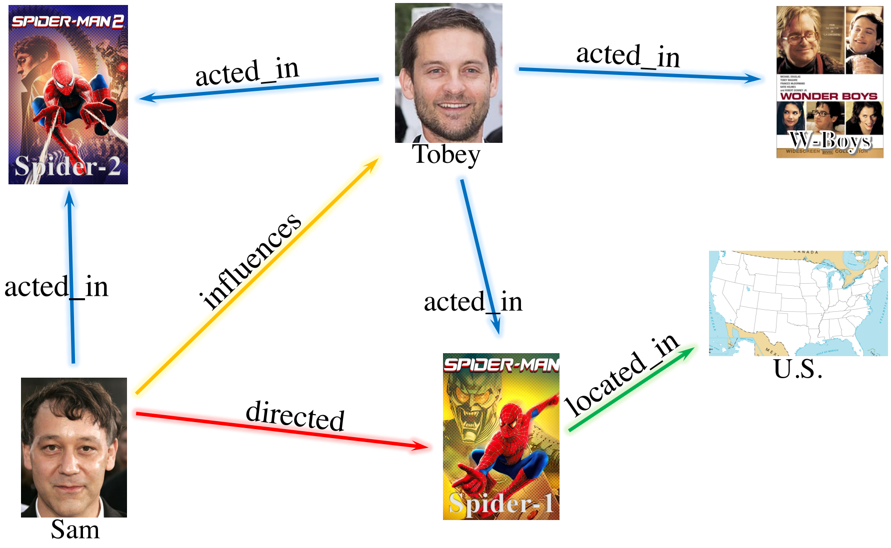
Outline

- Background
  - Review of knowledge graph learning
- A comprehensive understanding of HP in KG learning
- An efficient two-stage HP search algorithm
- Experiments
- Key takeaway and future directions

Background – 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).

KG is a semantic graph

- Semantic information
- Structural information

Google Knowledge Graph

WIKIDATA

Freebase

BIO2RDF

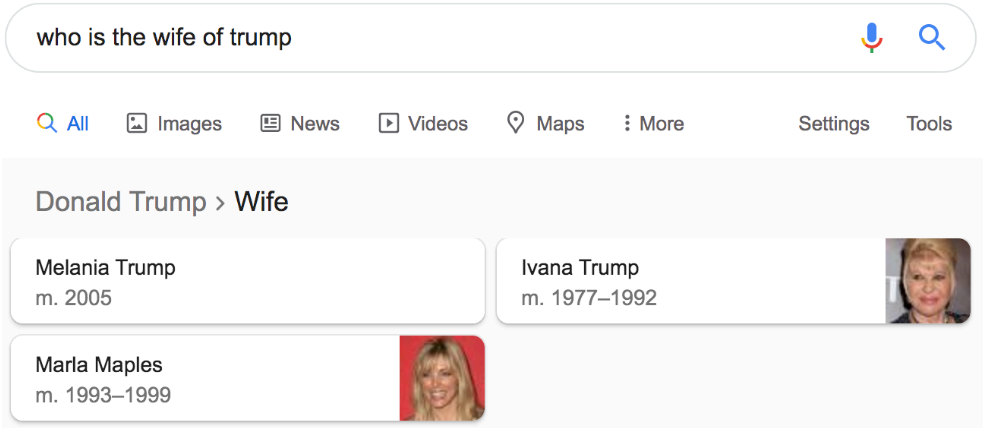
4Paradigm Sage Knowledge Base

低门槛、全流程知识图谱构建平台

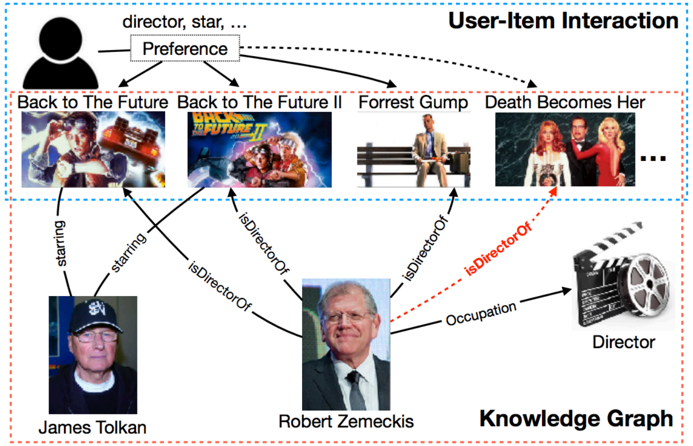
https://www.4paradigm.com/product/knowledge_base.html

Representative applications

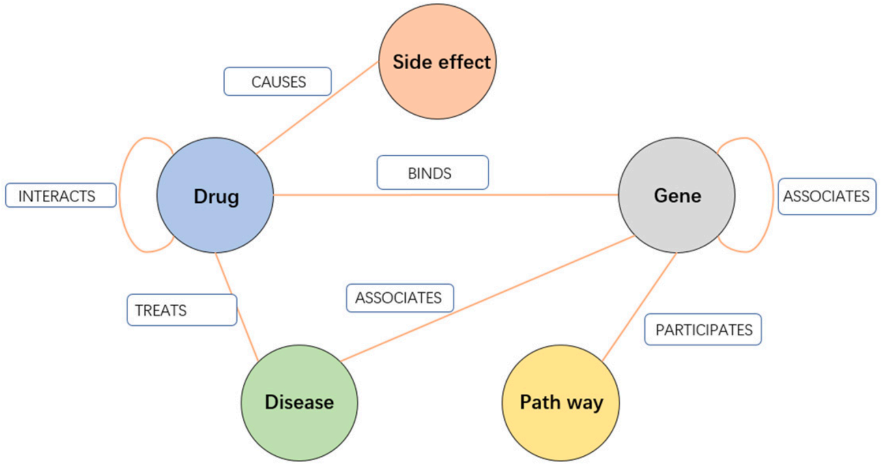
KGQA:



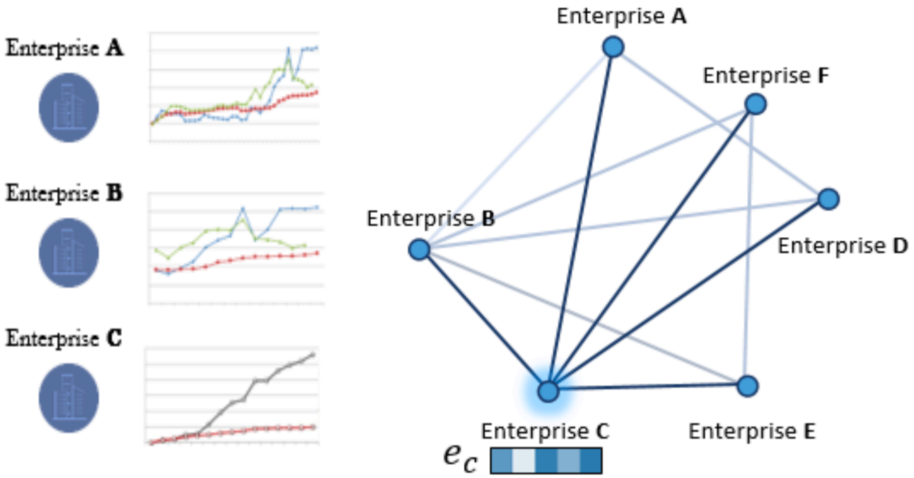
Recommendation:



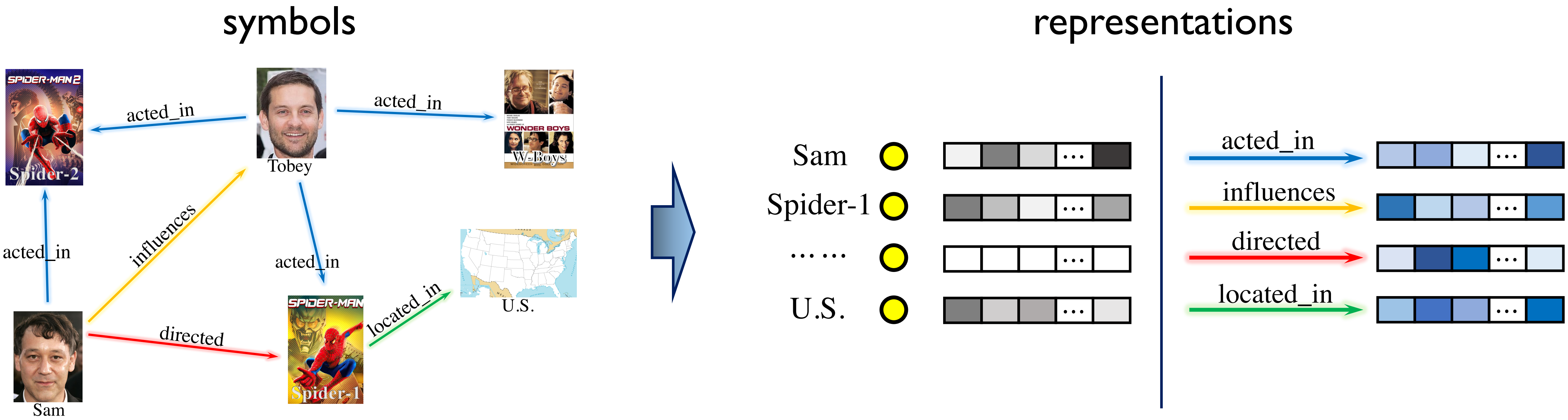
Drug discovery:



Stock prediction:



Background – Knowledge Graph Learning



Advantages:

- Continuous, ease of use in ML pipeline.
- Discover latent properties.
- Efficient similarity search.

Background – Machine learning on Knowledge Graph

For setting up a KG learning system, we need

- A **scoring function** $\boldsymbol{F}$ to measure the plausibility triplets
- A sampling scheme to generate **negative samples** $\boldsymbol{S}^{-}$
- A **loss function** $\boldsymbol{L}$ and **regularization** $\boldsymbol{r}$ to define the learning problem
- An **optimization** strategy for convergence procedure

We can formulate the learning framework as:

$$\underbrace{\min_{\boldsymbol{w}}}_{\text{optimization}} \overbrace{\mathcal{L}}^{\text{loss function}}\Big(\underbrace{F(\cdot,\boldsymbol{w})}_{\text{scoring function}},\ \mathcal{S}^{+}, \underbrace{\mathcal{S}^{-}}_{\text{negative sampling}}\Big) + \underbrace{r(\boldsymbol{w})}_{\text{regularization}}$$

Background – Machine learning on Knowledge Graph

Key components and related hyper-parameters (HPs)

$$\underbrace{\min_{\boldsymbol{w}}}_{\text{optimization}} \overbrace{\mathcal{L}}^{\text{loss function}}\Big(\underbrace{F(\cdot,\boldsymbol{w})}_{\text{scoring function[1]}},\ \mathcal{S}^+,\ \underbrace{\mathcal{S}^-}_{\text{negative sampling}}\Big) + \underbrace{r(\boldsymbol{w})}_{\text{regularization}}$$

component	name	type	range
negative sampling	# negative samples	cat	{32, 128, 512, 2048, 1VsAll, kVsAll}
loss function	loss function	cat	{MR, BCE_(mean, sum, adv), CE}
	gamma (MR)	float	[1, 24]
	adv. weight (BCE_adv)	float	[0.5, 2.0]
regularization	regularizer	cat	{FRO, NUC, DURA, None}
	reg. weight (not None)	float	$[10^{-12}, 10^{2}]$
	dropout rate	float	[0, 0.5]
optimization	optimizer	cat	{Adam, Adagrad, SGD}
	learning rate	float	$[10^{-5}, 10^{0}]$
	initializer	cat	{uniform, normal, xavier_uniform, xavier_norm}
	batch size	int	{128, 256, 512, 1024}
	dimension size	int	{100, 200, 500, 1000, 2000}
	inverse relation	bool	{True, False}

1: Note that HPs in SF are not covered here

Background – Machine learning on Knowledge Graph

Key components and related hyper-parameters

hyper-parameter

component	name	type	range
negative sampling	# negative samples	cat	{32, 128, 512, 2048, 1VsAll, kVsAll}
loss function	loss function gamma (MR) adv. weight (BCE_adv)	cat float float	{MR, BCE_(mean, sum, adv), CE} [1, 24] 0.00 [0.5, 2.0] 0.57
regularization	regularizer reg. weight (not None) dropout rate	cat float float	{FRO, NUC, DURA, None} $[10^{-12}, 10^{2}]$ 8.64 * 10^{-3} [0, 0.5] 0.25
optimization	optimizer learning rate initializer batch size dimension size inverse relation	cat float cat int int bool	{Adam, Adagrad, SGD} $[10^{-5}, 10^{0}]$ 1.77 * 10^{-2} {uniform, normal, xavier_uniform, xavier_norm} {128, 256, 512, 1024} {100, 200, 500, 1000, 2000} {True, False}

A configuration

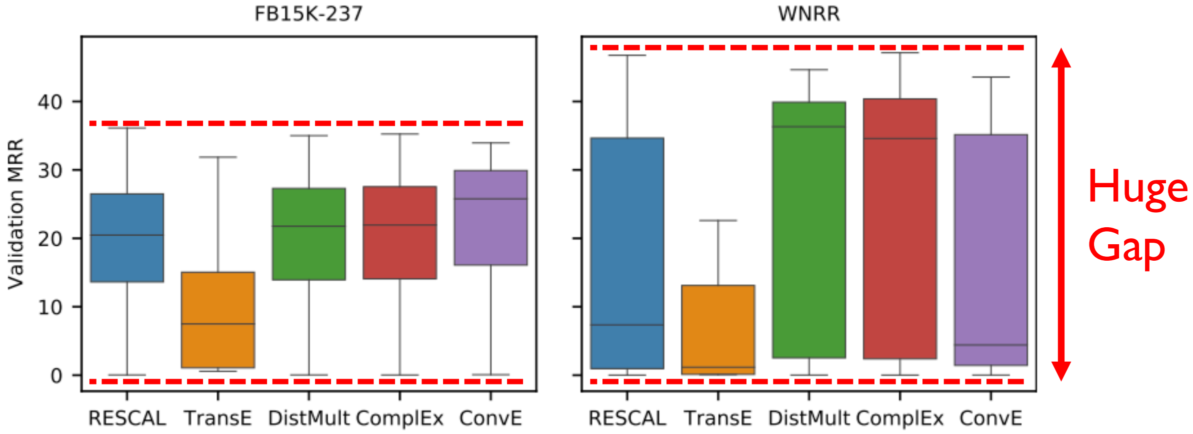
# negative samples	512
loss function	BCE_adv
gamma	0.00
adv. weight	0.57
regularizer	DURA
reg. weight	$8.64 * 10^{-3}$
dropout rate	0.25
optimizer	Adam
learning rate	$1.77 * 10^{-3}$
initializer	xavier_norm
batch size	512
dimension size	1000
inverse relation	False

Background – review of KGE models

		FB15k				WN18				FB15k-237				WN18RR				YAGO3-10			
		H@1	H@10	MR	MRR	H@1	H@10	MR	MRR	H@1	H@10	MR	MRR	H@1	H@10	MR	MRR	H@1	H@10	MR	MRR
Tensor Decomposition Models	DistMult	73.61	86.32	173	0.784	72.60	94.61	675	0.824	22.44	49.01	199	0.313	39.68	50.22	5913	0.433	41.26	66.12	1107	0.501
	ComplEx	81.56	90.53	34	0.848	94.53	95.50	3623	0.949	25.72	52.97	202	0.349	42.55	52.12	4907	0.458	50.48	70.35	1112	0.576
	ANALOGY	65.59	83.74	126	0.726	92.61	94.42	808	0.934	12.59	35.38	476	0.202	35.82	38.00	9266	0.366	19.21	45.65	2423	0.283
	SimplE	66.13	83.63	138	0.726	93.25	94.58	759	0.938	10.03	34.35	651	0.179	38.27	42.65	8764	0.398	35.76	63.16	2849	0.453
	HolE	75.85	86.78	211	0.800	93.11	94.94	650	0.938	21.37	47.64	186	0.303	40.28	48.79	8401	0.432	41.84	65.19	6489	0.502
	TuckER	72.89	88.88	39	0.788	94.64	95.80	510	0.951	25.90	53.61	162	0.352	42.95	51.40	6239	0.459	46.56	68.09	2417	0.544
Geometric Models	TransE	49.36	84.73	45	0.628	40.56	94.87	279	0.646	21.72	49.65	209	0.31	2.79	49.52	3936	0.206	40.57	67.39	1187	0.501
	STransE	39.77	79.60	69	0.543	43.12	93.45	208	0.656	22.48	49.56	357	0.315	10.13	42.21	5172	0.226	3.28	7.35	5797	0.049
	CrossE	60.08	86.23	136	0.702	73.28	95.03	441	0.834	21.21	47.05	227	0.298	38.07	44.99	5212	0.405	33.09	65.45	3839	0.446
	TorusE	68.85	83.98	143	0.746	94.33	95.44	525	0.947	19.62	44.71	211	0.281	42.68	53.35	4873	0.463	27.43	47.44	19455	0.342
	RotatE	73.93	88.10	42	0.791	94.30	96.02	274	0.949	23.83	53.06	178	0.336	42.60	57.35	3318	0.475	40.52	67.07	1827	0.498
Deep Learning Models	ConvE	59.46	84.94	51	0.688	93.89	95.68	413	0.945	21.90	47.62	281	0.305	38.99	50.75	4944	0.427	39.93	65.75	2429	0.488
	ConvKB	11.44	40.83	324	0.211	52.89	94.89	202	0.709	13.98	41.46	309	0.230	5.63	52.50	3429	0.249	32.16	60.47	1683	0.420
	ConvR	70.57	88.55	70	0.773	94.56	95.85	471	0.950	25.56	52.63	251	0.346	43.73	52.68	5646	0.467	44.62	67.33	2582	0.527
	CapsE	1.93	21.78	610	0.087	84.55	95.08	233	0.890	7.34	35.60	405	0.160	33.69	55.98	720	0.415	0.00	0.00	60676	0.000
	RSN	72.34	87.01	51	0.777	91.23	95.10	346	0.928	19.84	44.44	248	0.280	34.59	48.34	4210	0.395	42.65	66.43	1339	0.511
	AnyBURL	81.09	87.86	288	0.835	94.63	95.96	233	0.951	24.03	48.93	480	0.324	44.93	55.97	2530	0.485	45.83	66.07	815	0.528

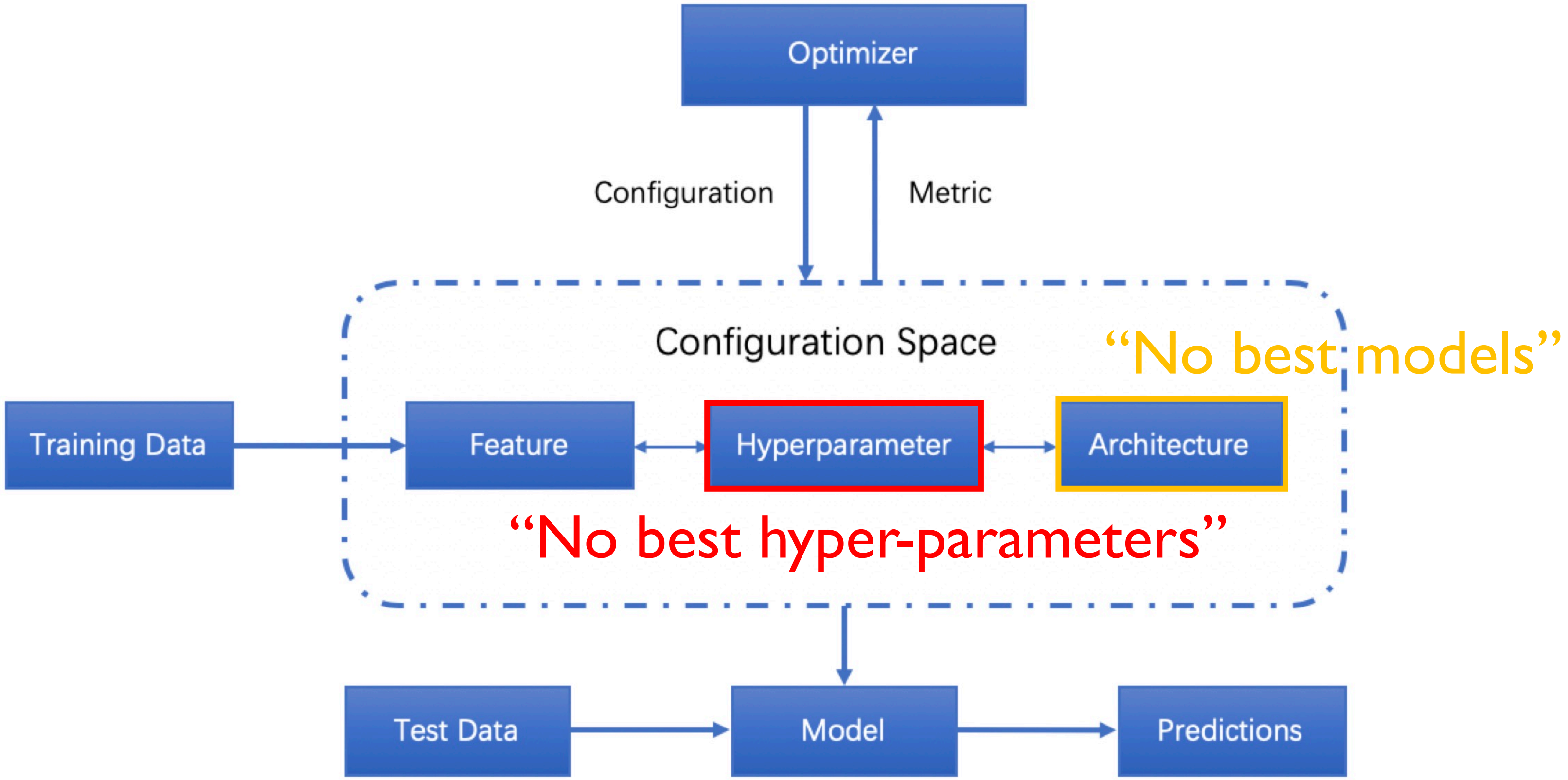
No best models

		RESCAL	TransE	DistMult	ComplEx	ConvE
FB15K-237	Valid. MRR	*36.1*	*31.5*	*35.0*	*35.3*	*34.3*
	Emb. size	128 *(-0.5)*	512 *(-3.7)*	256 *(-0.2)*	256 *(-0.3)*	256 *(-0.4)*
	Batch size	512 *(-0.5)*	128 *(-7.1)*	1024 *(-0.2)*	1024 *(-0.3)*	1024 *(-0.4)*
	Train type	1vsAll *(-0.8)*	NegSamp –	NegSamp *(-0.2)*	NegSamp *(-0.3)*	1vsAll *(-0.4)*
	Loss	CE *(-0.9)*	CE *(-7.1)*	CE *(-3.1)*	CE *(-3.8)*	CE *(-0.4)*
	Optimizer	Adam *(-0.5)*	Adagrad *(-3.7)*	Adagrad *(-0.2)*	Adagrad *(-0.5)*	Adagrad *(-1.5)*
	Initializer	Normal *(-0.8)*	XvNorm *(-3.7)*	Unif. *(-0.2)*	Unif. *(-0.5)*	XvNorm *(-0.4)*
	Regularizer	None *(-0.5)*	L2 *(-3.7)*	L3 *(-0.2)*	L3 *(-0.3)*	L3 *(-0.4)*
	Reciprocal	No *(-0.5)*	Yes *(-9.5)*	Yes *(-0.3)*	Yes *(-0.3)*	Yes –
WNRR	Valid. MRR	*46.8*	*22.6*	*45.4*	*47.6*	*44.3*
	Emb. size	128 *(-1.0)*	512 *(-5.1)*	512 *(-1.1)*	128 *(-1.0)*	512 *(-1.2)*
	Batch size	128 *(-1.0)*	128 *(-5.1)*	1024 *(-1.1)*	512 *(-1.0)*	1024 *(-1.3)*
	Train type	KvsAll *(-1.0)*	NegSamp –	KvsAll *(-1.1)*	1vsAll *(-1.0)*	KvsAll *(-1.2)*
	Loss	CE *(-2.0)*	CE *(-5.1)*	CE *(-2.4)*	CE *(-3.5)*	CE *(-1.4)*
	Optimizer	Adam *(-1.2)*	Adagrad *(-5.8)*	Adagrad *(-1.5)*	Adagrad *(-1.5)*	Adam *(-1.4)*
	Initializer	Unif. *(-1.0)*	XvNorm *(-5.1)*	Unif. *(-1.3)*	Unif. *(-1.5)*	XvNorm *(-1.4)*
	Regularizer	L3 *(-1.2)*	L2 *(-5.1)*	L3 *(-1.1)*	L2 *(-1.0)*	L1 *(-1.2)*
	Reciprocal	Yes *(-1.0)*	Yes *(-5.9)*	Yes *(-1.1)*	No *(-1.0)*	Yes –



No best hyper-parameters 🤔

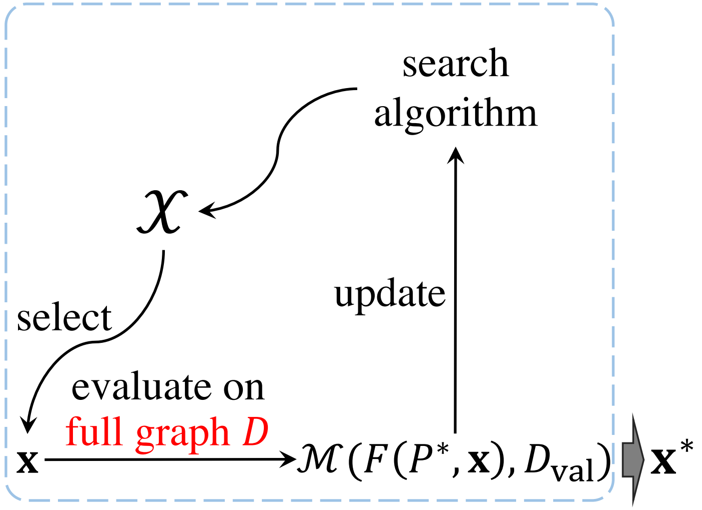
Background – from the AutoML scope

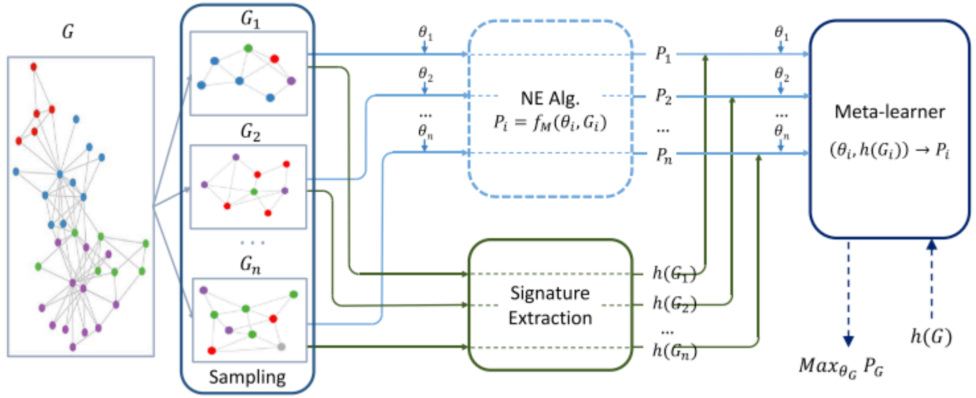


https://awesomeopensource.com/project/hibayesian/awesome-automl-papers

Background – review of HPO methods

Taxonomy	Examples	Cons
Sampled-based	Grid search	Low efficiency Can not learn from historical records
	Random search	
Bayesian optimization	Hyperopt (TPE) [1]	Slow feedback from the original KG
	SMAC (RF) [2]	
	Ax (GP) [3]	
	AutoNE [4]	(Subgraph-based) No specialized designs for KGE
	e-AutoGR [5]	
	$\phi(HP\ configuration) \rightarrow Performance$	





[1] Hyperopt: A python library for optimizing the hyperparameters of machine learning algorithms.
[2] Sequential model-based optimization for general algorithm configuration.
[3] https://github.com/facebook/Ax
[4] Autone: Hyperparameter optimization for massive network embedding.
[5] Explainable automated graph representation learning with hyperparameter importance.

Motivation and Objective

Weakness of existing works

Low efficiency in searching for HP configuration

- usually in a time-consuming trial-and-error way
- interaction, importance, and tunability of HPs are unclear
- lacking understanding of KGE components

Objective of KGbench:

- *Design a searching algorithm,*
- *for any given dataset and embedding model with limited budget,*
- *to* ***efficiently*** *search for the hyper-parameter configuration.*

Outline

- Background
- A comprehensive understanding of HP in KGE
  - search space
  - validation curvature
  - evaluation cost
- An efficient two-stage HP search algorithm
- Experiments
- Key takeaway and future directions

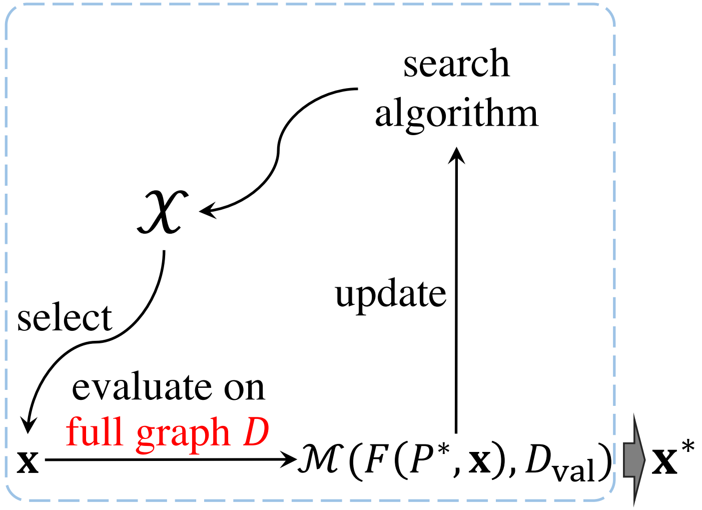
Motivation and Objective

HP searching problem setup

Definition 1 (Hyper-parameter search for KG embedding). *The problem of HP search for KG embedding model is formulated as*

$$\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathcal{X}} \mathcal{M}\big(F(\boldsymbol{P}^*, \mathbf{x}), D_{val}\big), \quad (2)$$

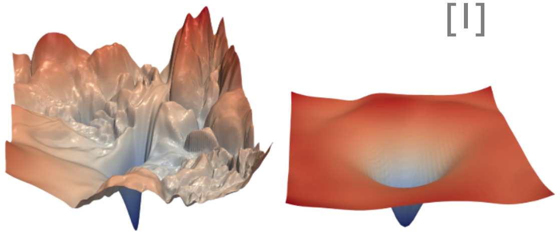
$$\boldsymbol{P}^* = \arg\min_{\boldsymbol{P}} \mathcal{L}\big(F(\boldsymbol{P}, \mathbf{x}), D_{tra}\big). \quad (3)$$



Three major aspects for efficiency in Def. 1

1. the **size** of search space χ
2. the validation **curvature** of $\mathcal{M}$
3. the evaluation **cost** in solving $argmin_{\mathcal{P}}$

[1]



[1] Visualizing the loss landscape of neural nets

Understanding the HP in KGE

Three major aspects for efficiency in Def. 1
1. the size of search space χ
2. the validation curvature of $\mathcal{M}$
3. the evaluation cost in solving $argmin_{\mathcal{P}}$

Recall the search space

name	type	range
# negative samples	cat	{32, 128, 512, 2048, 1VsAll, kVsAll}
loss function	cat	{MR, BCE_(mean, sum, adv), CE}
gamma (MR)	float	[1, 24]
adv. weight (BCE_adv)	float	[0.5, 2.0]
regularizer	cat	{FRO, NUC, DURA, None}
reg. weight (not None)	float	$[10^{-12}, 10^{2}]$
dropout rate	float	[0, 0.5]
optimizer	cat	{Adam, Adagrad, SGD}
learning rate	float	$[10^{-5}, 10^{0}]$
initializer	cat	{uniform, normal, xavier_uniform, xavier_norm}
batch size	int	{128, 256, 512, 1024}
dimension size	int	{100, 200, 500, 1000, 2000}
inverse relation	bool	{True, False}

Questions to be answered
- What are the properties of each HP?
  - ranking distribution
  - consistency
  - computing cost
- Can we decrease the range for each HP?
- Can we decouple some HPs?

Understanding the HP in KGE

Excavating properties of HPs

name	type	range
# negative samples	cat	{32, 128, 512, 2048, 1VsAll, kVsAll}
loss function	cat	{MR, BCE_(mean, sum, adv), CE}
gamma (MR)	float	[1, 24]
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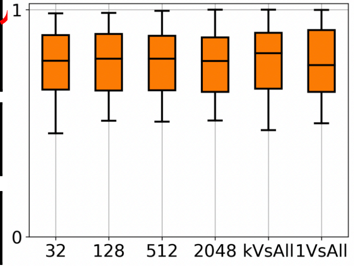
inverse relation	bool	{True, False}

enumerating

sampling anchors [1]

# negs.	32	128	512	2048	1VsAll	kVsAll
anchor-1	0.21	0.32	0.19	0.41	0.43	0.44
anchor-2	0.33	0.29	0.34	0.36	0.40	0.38
anchors	…	…	…	…	…	…
anchor-n	0.15	0.19	0.14	0.19	0.28	0.25

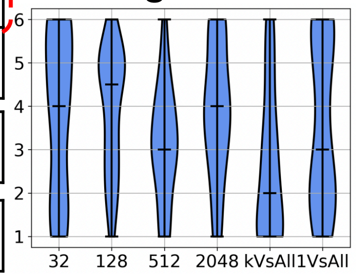
Performance dist.



option ranking

anchor-1	5	4	6	3	2	1
anchor-2	5	6	4	3	1	2
anchors	…	…	…	…	…	…
anchor-n	5	4	6	4	1	2

Ranking dist.



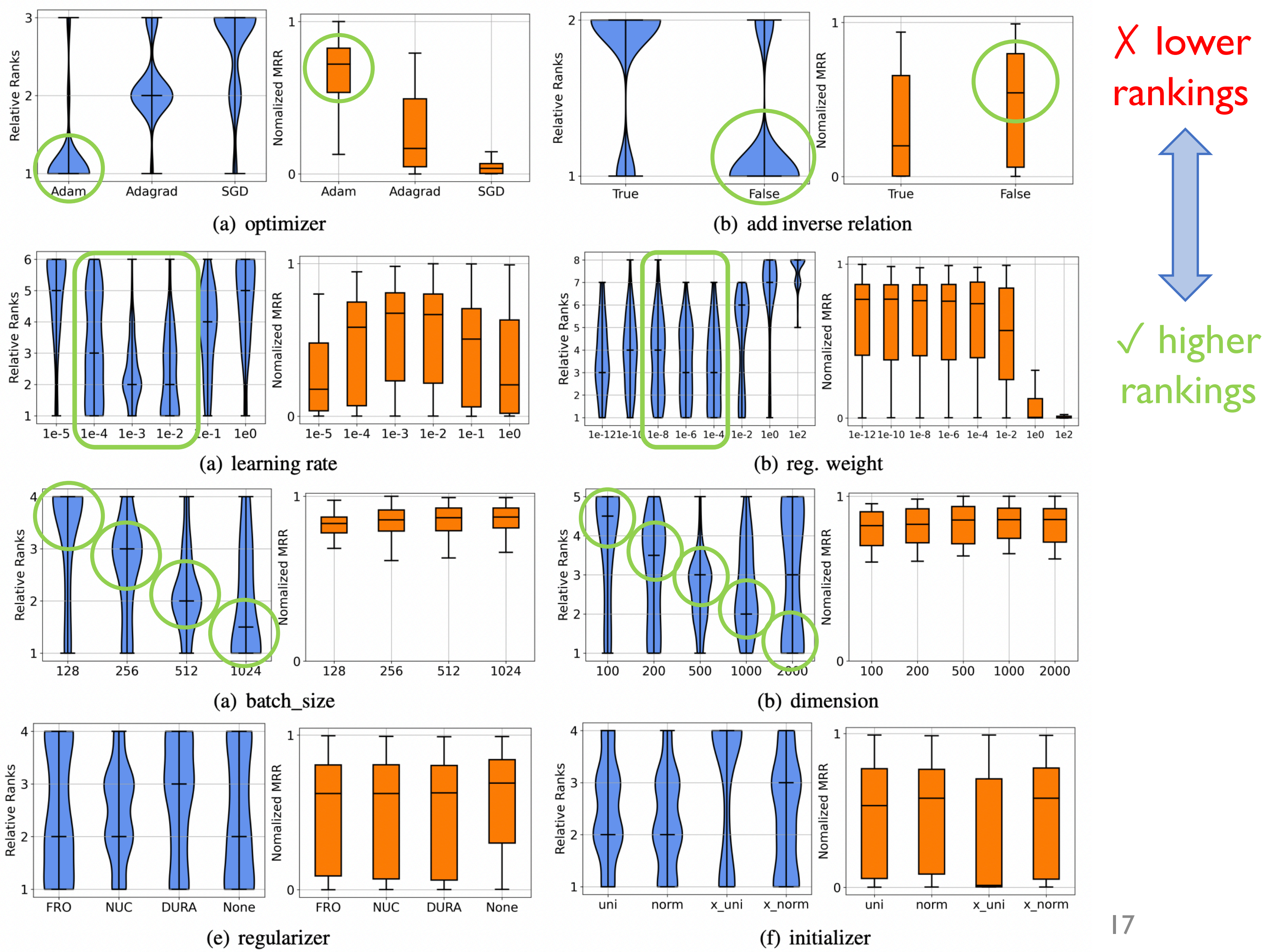
[1] Design Space for Graph Neural Networks

Understanding the HP in KGE

Excavating properties of HPs | Ranking/Performance distribution

The HPs can be classified into 4 groups

1. reduced options
2. shrunken range
3. monotonously related
4. no obvious patterns



(a) optimizer (b) add inverse relation

(a) learning rate (b) reg. weight

(a) batch_size (b) dimension

(e) regularizer (f) initializer

Understanding the HP in KGE

Excavating properties of HPs

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# negative samples	cat	{32, 128, 512, 2048, 1VsAll, kVsAll}
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enumerating

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anchors	…	…	…	…	…	…
anchor-n	0.15	0.19	0.14	0.19	0.28	0.25

anchor ranking

anchor-1					2	1	1	✓
anchor-2					5	5	0	
anchors	…	…	…	…	…	…		
anchor-n					25	48	23	✗

$|\text{rank}(\theta_1)-\text{rank}(\theta_2)|$

SRCC $$1-\frac{\sum_{\mathbf{x}\in\mathcal{X}_i}|r(\mathbf{x},\theta_1)-r(\mathbf{x},\theta_2)|^2}{|\mathcal{X}_i|\cdot(|\mathcal{X}_i|^2-1)}$$

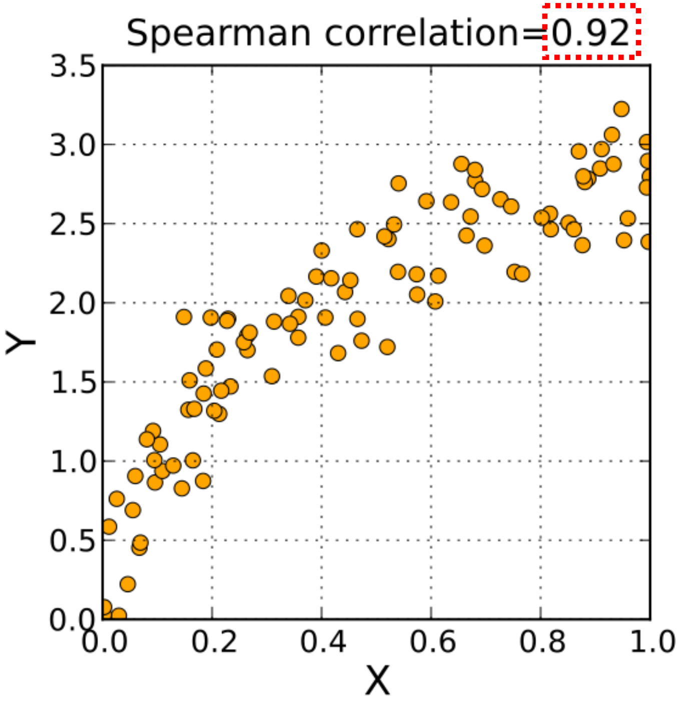
[1] Design Space for Graph Neural Networks

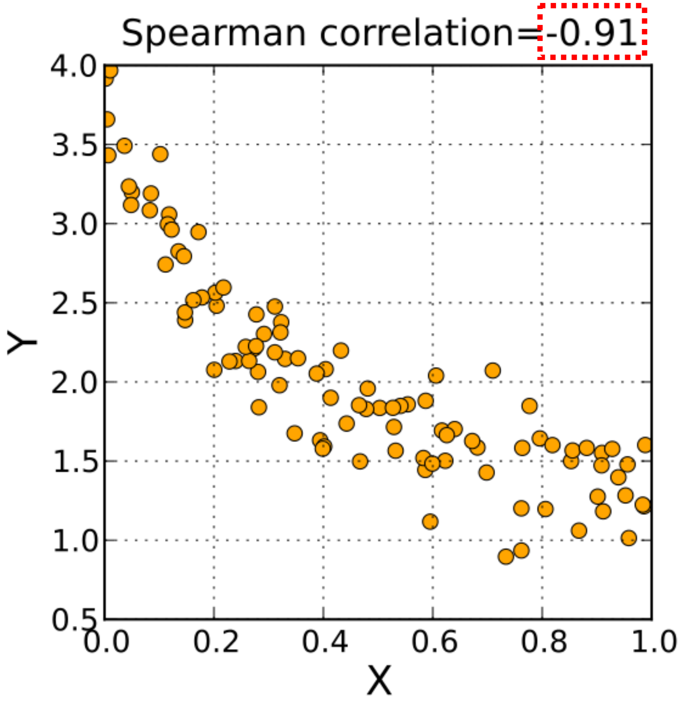
Understanding the HP in KGE

Positive and negative Spearman rank correlations

$$1 - \frac{\sum_{\mathbf{x} \in \mathcal{X}_i} |r(\mathbf{x}, \theta_1) - r(\mathbf{x}, \theta_2)|^2}{|\mathcal{X}_i| \cdot (|\mathcal{X}_i|^2 - 1)}$$

Positive





negative

https://en.wikipedia.org/wiki/Spearman%27s_rank_correlation_coefficient

Understanding the HP in KGE

Excavating properties of HPs

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enumerating

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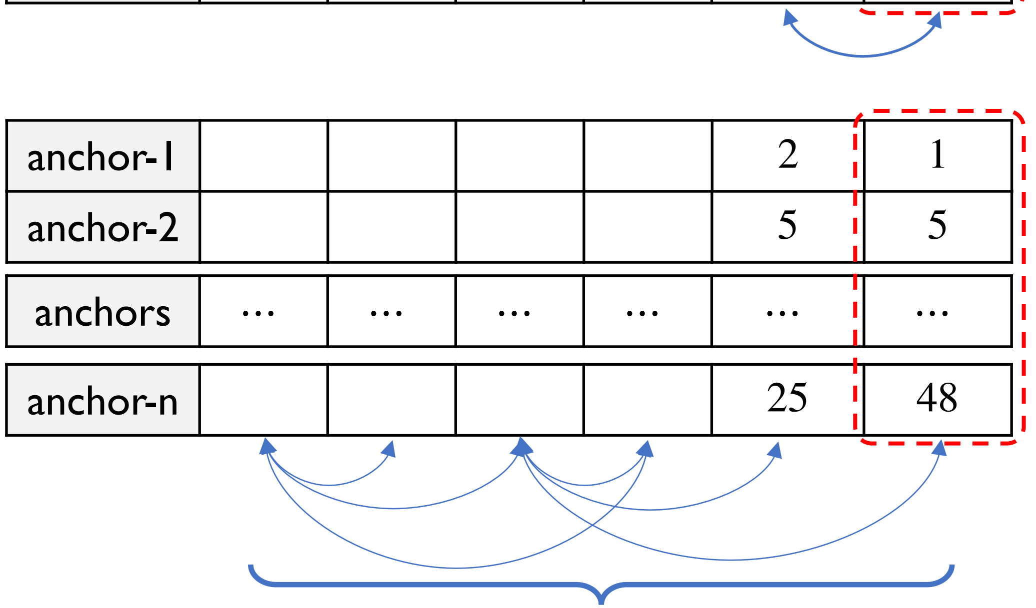
anchors	…	…	…	…	…	…
anchor-n	0.15	0.19	0.14	0.19	0.28	0.25

anchor ranking

anchor-1					2	1
anchor-2					5	5
anchors	…	…	…	…	…	…
anchor-n					25	48



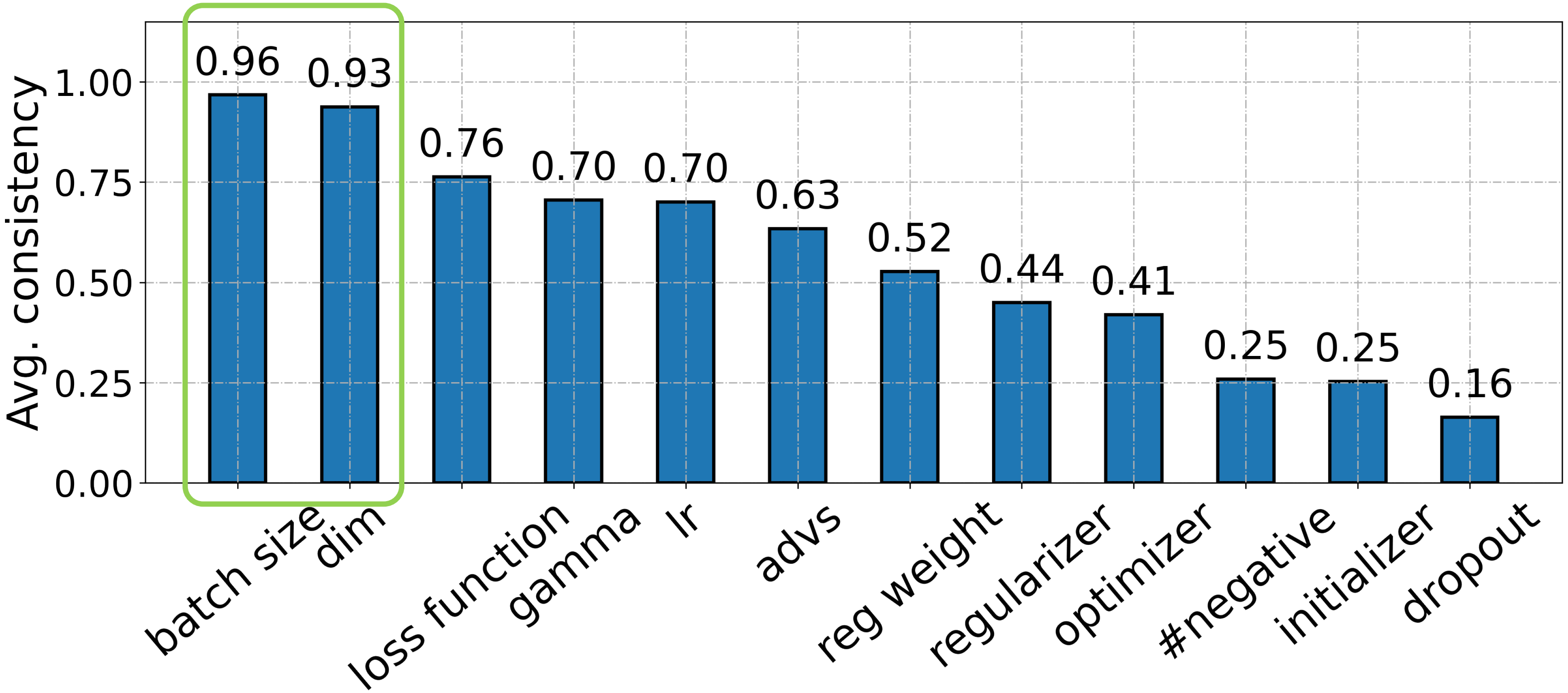
Consistency = Average pairwise SRCC

[1] Design Space for Graph Neural Networks

Understanding the HP in KGE

Excavating properties of HPs | Consistency

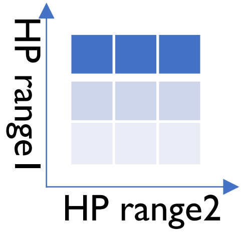
> **Observation:**
> the batch size and dimension size show higher consistency than the other HPs.



Outline

- Background
- A comprehensive understanding of HP in KGE
  - search space
  - validation curvature
  - evaluation cost
- An efficient two-stage HP search algorithm
- Experiments
- Key takeaway and future directions

Understanding the HP in KGE



Excavating properties of HPs | from the aspect of predictor

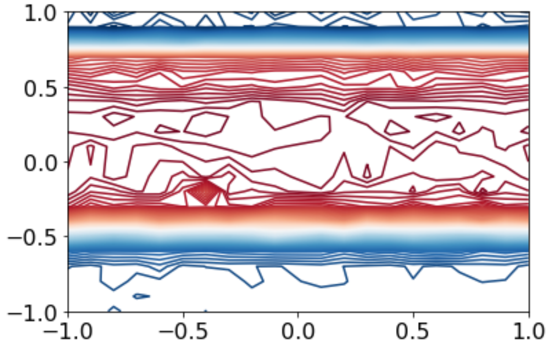
Predictors
- Gaussian process (GP)
- Multi layer perceptron (MLP)
- Random forest (RF)

Observation:
RF is better in approximating the curvature

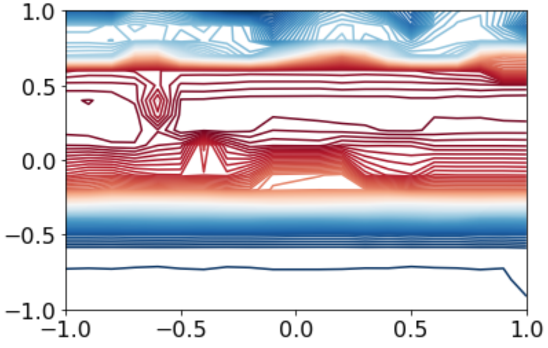
# train configurations	10	20	30
GP	0.0693±0.02	0.029±0.01	0.019±0.01
MLP	2.121±0.4	2.052±0.3	0.584±0.1
RF	**0.003±0.002**	**0.002±0.001**	**0.001±0.001**

MSE results

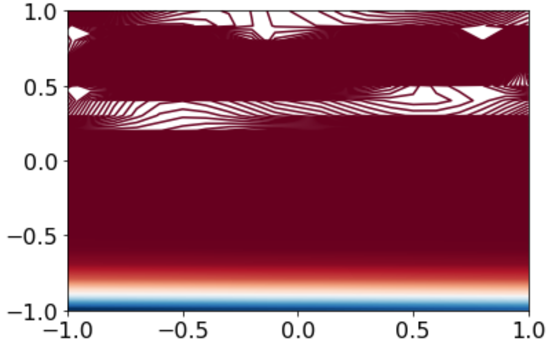
Validation curvature



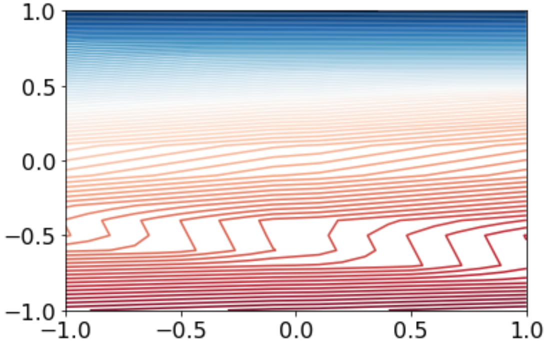
Ground truth



RF prediction



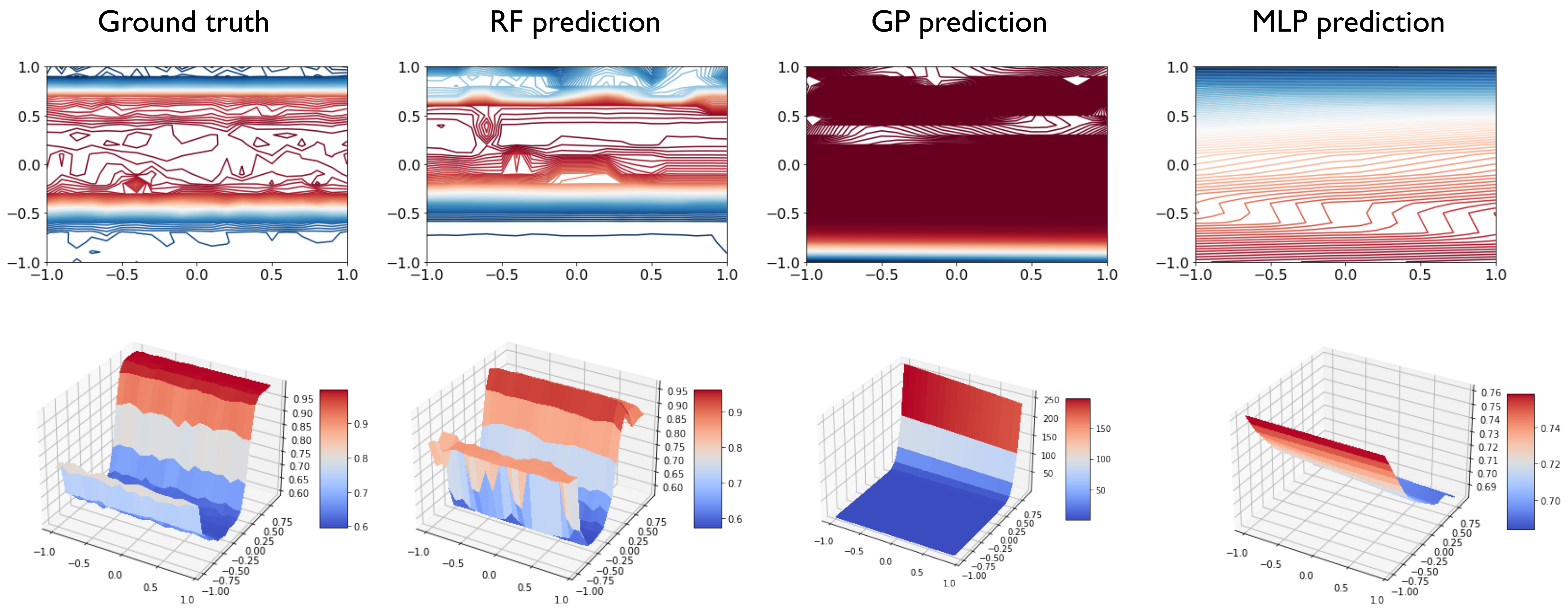
GP prediction



MLP prediction

Understanding the HP in KGE

Excavating properties of HPs | from the aspect of predictor



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Understanding the HP in KGE

Excavating properties of HPs | Time cost

Three major aspects for efficiency in Def. 1

1. the size of search space χ
2. the validation curvature of $\mathcal{M}$
3. the evaluation cost in solving $argmin_{\mathcal{P}}$

dataset	#entity	#relation	#train	#validate	#test
WN18RR (Dettmers et al., 2017)	41k	11	87k	3k	3k
FB15k-237 (Toutanova and Chen, 2015)	15k	237	272k	18k	20k
ogbl-biokg (Hu et al., 2020)	94k	51	4,763k	163k	163k
ogbl-wikikg2 (Hu et al., 2020)	2,500k	535	16,109k	429k	598k

Average evaluation time cost:

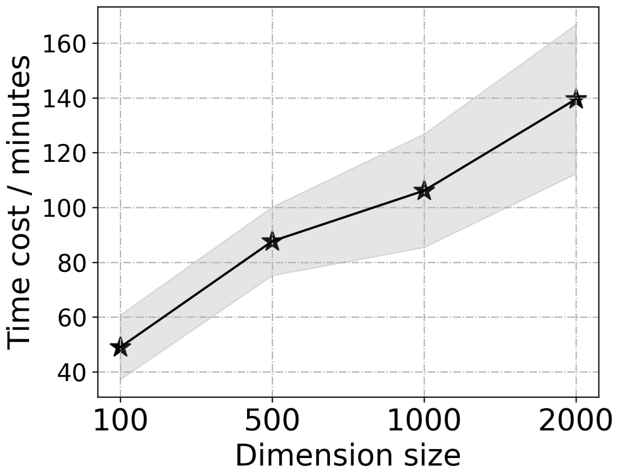
~2.1h
~3.5h
~17.3h
~21.7h

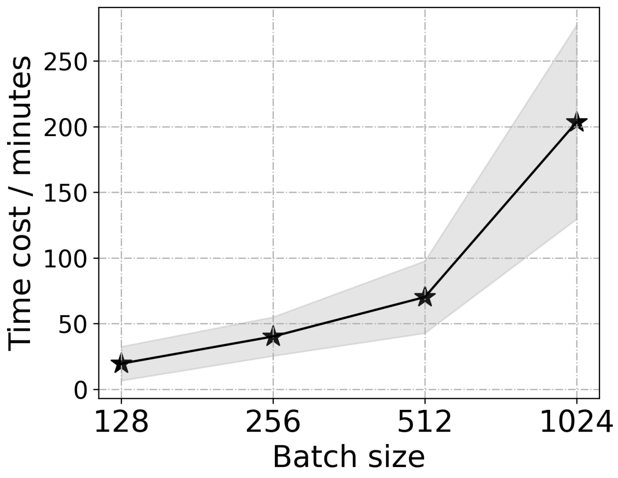
Understanding the HP in KGE

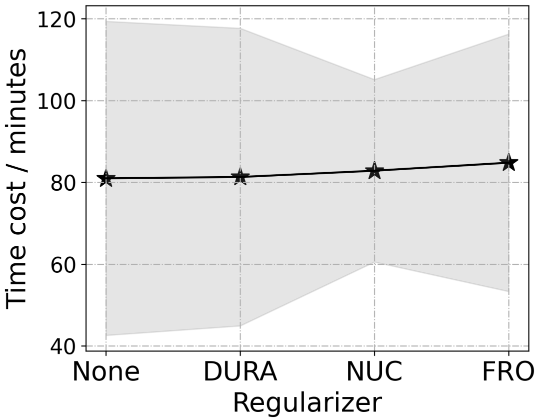
Excavating properties of HPs | Time cost[1]

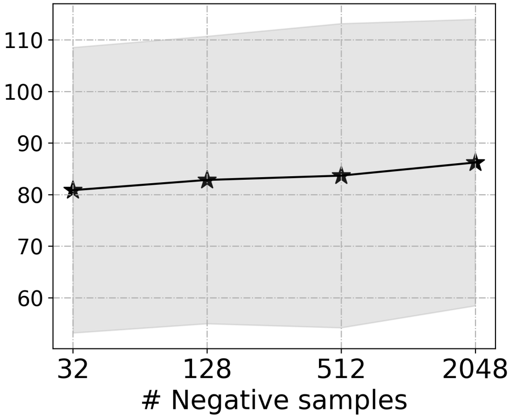
Three major aspects for efficiency in Def. 1
1. the size of search space χ
2. the validation curvature of $\mathcal{M}$
3. the evaluation cost in solving $argmin_{\mathcal{P}}$

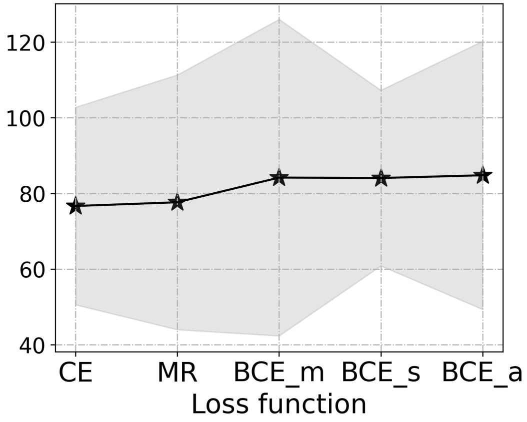
Observation:
batchsize↑ or dimension↑
⇒ time cost↑







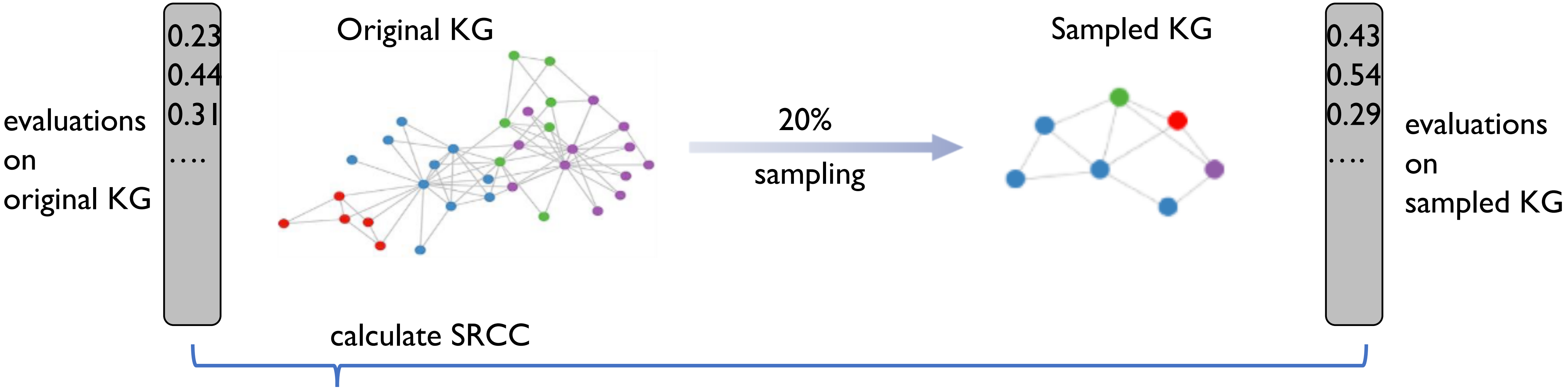


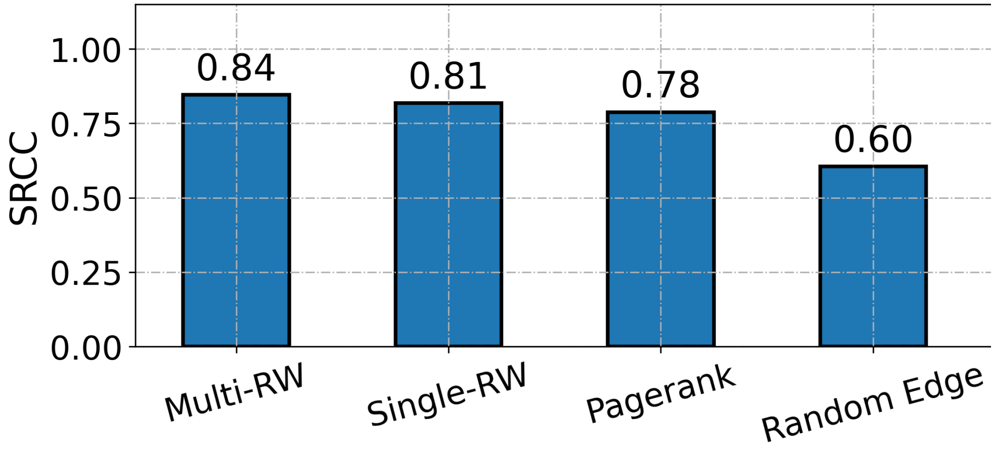


1: The experiments are implemented with PyTorch framework,
on a machine with Intel Xeon 6230R CPUs, 754 GB memory and RTX 3090 GPUs with 24 GB.

Understanding the HP in KGE

Excavating properties of HPs | Transferability of subgraphs





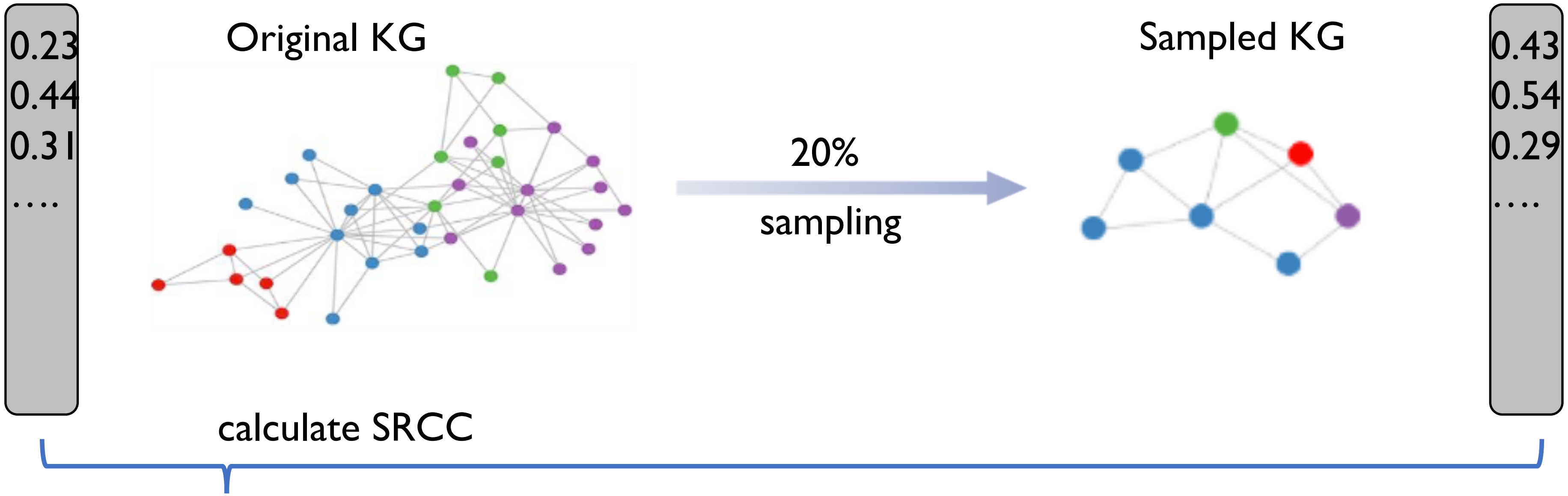
Observation:

- Good correlation between subgraph and original graph
- Multi-start random walk is the best choice

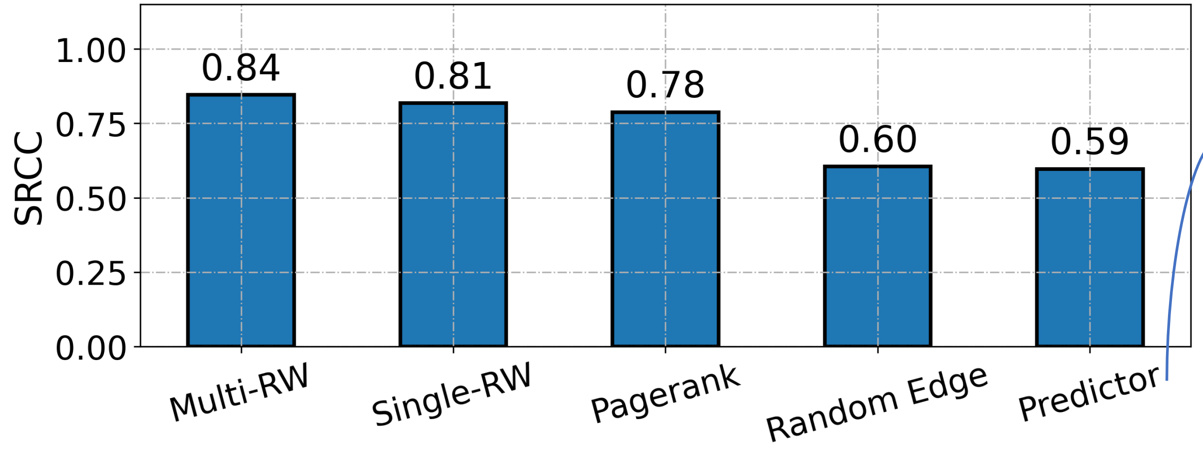
Understanding the HP in KGE

Excavating properties of HPs | Transferability of subgraphs

evaluations on original KG



evaluations on sampled KG

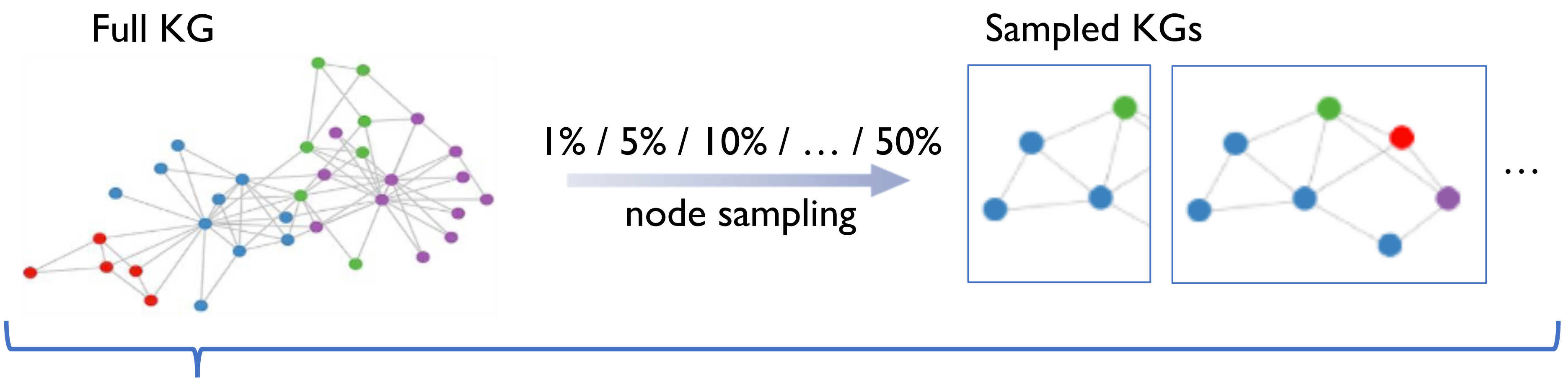


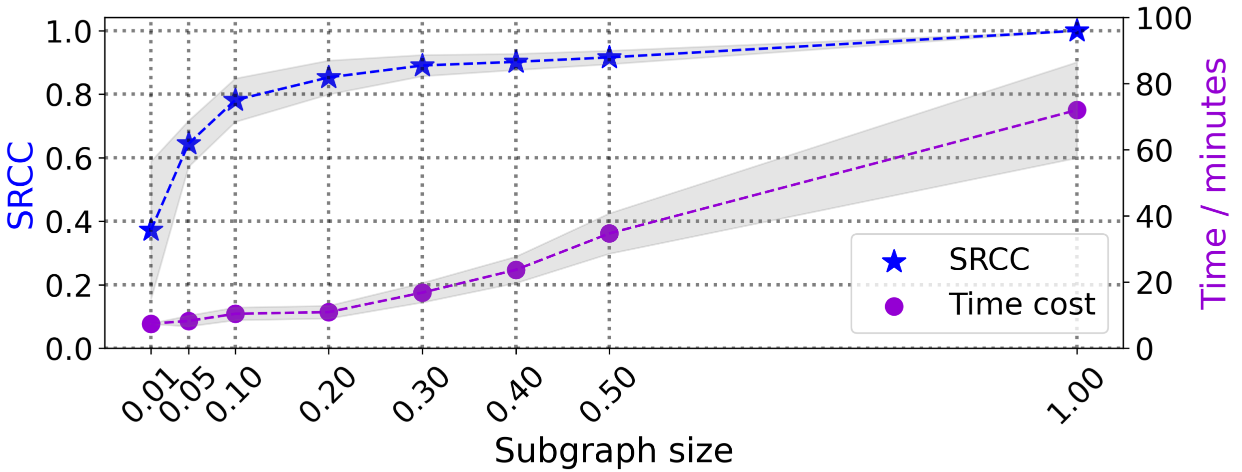
Predictor

- train with sampled KG + original KG
- lower SRCC compared with direct transfer
- similar cases for GP/MLP/RF

Understanding the HP in KGE

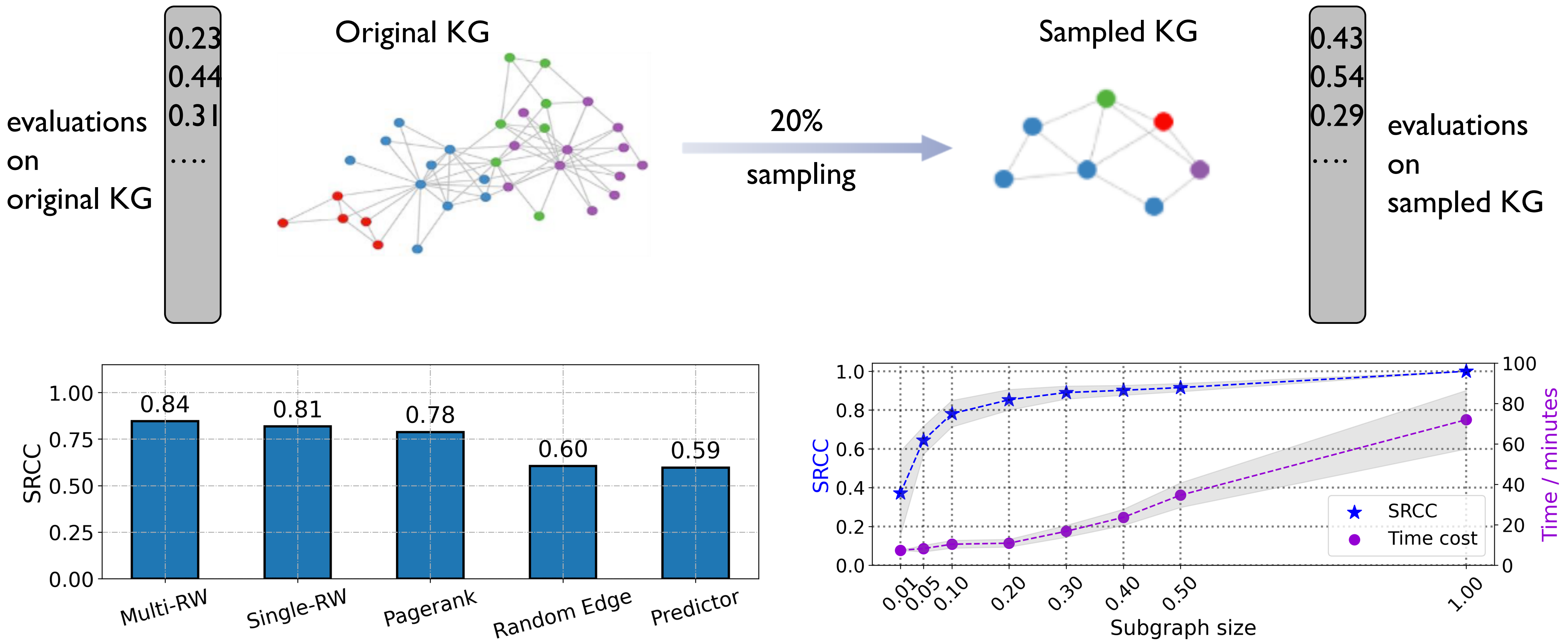
Excavating properties of HPs | Transferability of subgraphs





Observation:

- When the subgraph size↑, the consistency↑ and the cost↑
- To balance the consistency and cost, the subgraphs with 20% nodes are the better choices



evaluations
on
original KG
0.23
0.44
0.31
....
Original KG
20%
sampling
Sampled KG
0.43
0.54
0.29
....
evaluations
on
sampled KG
SRCC
1.00
0.75
0.50
0.25
0.00
0.84
0.81
0.78
0.60
0.59
Multi-RW
Single-RW
Pagerank
Random Edge
Predictor
SRCC
1.0
0.8
0.6
0.4
0.2
0.0
Time / minutes
100
80
60
40
20
0
0.01
0.05
0.10
0.20
0.30
0.40
0.50
1.00
Subgraph size
SRCC
Time cost

Understanding the HP in KGE

Summary of the observations

- Ranking distribution/consistency for each HP's values
  - dimension/batch size
- Full HP range can be shrunken and decoupled

- The validation curvature is pretty complex
- RF is better than GP/MLP as the predictor

- Sampling with multi-start random walk can reduce cost while possessing high performance consistency

Three major aspects for efficiency in Def. 1

1. the size of search space χ
2. the validation curvature of $\mathcal{M}$
3. the evaluation cost in solving $argmin_{\mathcal{P}}$

$$\mathbf{x}^* = \arg\max_{\mathbf{x}\in\mathcal{X}} \mathcal{M}\big(F(\boldsymbol{P}^*, \mathbf{x}), D_{val}\big),$$
$$\boldsymbol{P}^* = \arg\min_{\boldsymbol{P}} \mathcal{L}\big(F(\boldsymbol{P}, \mathbf{x}), D_{tra}\big).$$

How to design algorithm based on the above observations? 🤔

Outline

- Background
- A comprehensive understanding of HP in KGE
- An efficient two-stage HP search algorithm
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Efficient two-stage HP search algorithm

Reducing the search space

name	ranges in the whole space	revised ranges
optimizer	{Adam, Adagrad, SGD}	Adam
learning rate	$[10^{-5}, 10^{0}]$	$[10^{-4}, 10^{-1}]$
reg. weight	$[10^{-12}, 10^{2}]$	$[10^{-8}, 10^{-2}]$
dropout rate	[0, 0.5]	[0, 0.3]
inverse relation	{True, False}	{False}
batch size	{128, 256, 512, 1024}	128
dimension size	{100, 200, 500, 1000, 2000}	100

shrunken range HPs :
can be searched more exactly

decoupled HPs:
can be directly tuned
apart from other HPs

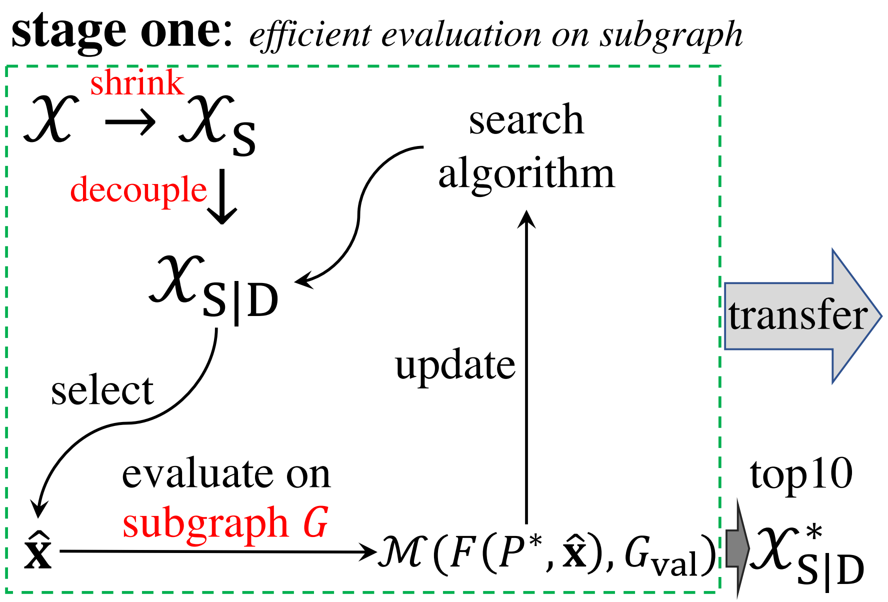
Reduced space = shrinkage range HPs + decoupled HPs
The reduced space is about **700 times smaller** than the full space

Efficient two-stage HP search algorithm

TwO-Stage Search algorithm (KGTuner)

Stage1: exploration on reduced space

- quickly search HP on sampled KG
- with predictor RF and acquisition BORE



Algorithm 1 KGTuner: two-stage search algorithm

Require: KG embedding model F, dataset D, and budget B;
shrink the search space $\mathcal{X}$ to $\mathcal{X}_{\text{S}}$ and decouple $\mathcal{X}_{\text{S}}$ to $\mathcal{X}_{\text{S|D}}$;
 # state one: *efficient evaluation on subgraph*
sample a subgraph (with 20% entities) G from D_{tra} by multi-start random walk;
repeat
  sample a configuration $\hat{\mathbf{x}}$ from $\mathcal{X}_{S|D}$ by RF+BORE;
  evaluate $\hat{\mathbf{x}}$ on the subgraph G to get the performance;
  update the RF with record $\left(\hat{\mathbf{x}}, \mathcal{M}(F(P^*, \hat{\mathbf{x}}), G_{\text{val}})\right)$;
until $B/2$ budget exhausted;
save the *top10* configurations in $\mathcal{X}^*_{\text{S|D}}$;
 # state two: *fine-tune the top configurations*
increase the batch/dimension size in $\mathcal{X}^*_{\text{S|D}}$ to get $\tilde{\mathcal{X}}^*$;
set $y^* = 0$ and re-initialize the RF surrogate;
repeat
  select a configuration $\tilde{\mathbf{x}}^*$ from $\tilde{\mathcal{X}}^*$ by RF+BORE;
  evaluate on full graph G to get the performance;
  update the RF with record $\left(\tilde{\mathbf{x}}^*, \mathcal{M}(F(P^*, \tilde{\mathbf{x}}^*), D_{\text{val}})\right)$;
  if $\mathcal{M}(F(P^*, \tilde{\mathbf{x}}^*), D_{\text{val}}) > y^*$ **then**
  $y^* \leftarrow \mathcal{M}(F(P^*, \tilde{\mathbf{x}}^*), D_{\text{val}})$ and $\mathbf{x}^* \leftarrow \tilde{\mathbf{x}}^*$; **end if**
until the remaining $B/2$ budget exhausted;
return $\mathbf{x}^*$.

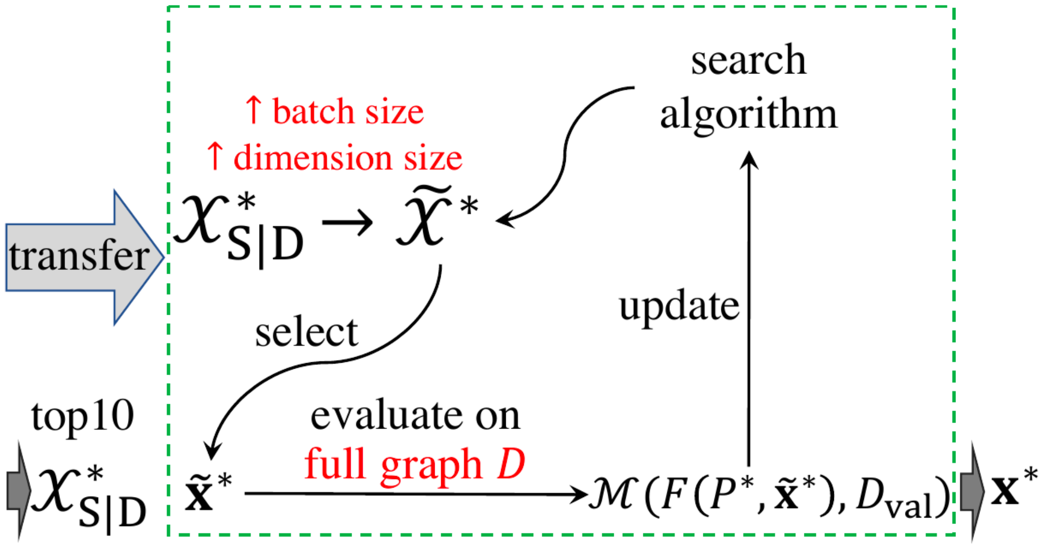
Efficient two-stage HP search algorithm

TwO-Stage Search algorithm (KGTuner)

Stage2: exploitation with fine-tuning

- transfer top10 configurations from stage 1
- finetune configuration on original KG
  - with higher dimension and batchsize

stage two: *fine-tune the top configurations*



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  evaluate $\hat{\mathbf{x}}$ on the subgraph G to get the performance;

  update the RF with record $\left(\hat{\mathbf{x}}, \mathcal{M}(F(P^*, \hat{\mathbf{x}}), G_{\text{val}})\right)$;

until $B/2$ budget exhausted;

save the *top10* configurations in $\mathcal{X}^*_{S|D}$;

 # state two: *fine-tune the top configurations*

increase the batch/dimension size in $\mathcal{X}^*_{S|D}$ to get $\tilde{\mathcal{X}}^*$;

set $y^* = 0$ and re-initialize the RF surrogate;

repeat

  select a configuration $\tilde{\mathbf{x}}^*$ from $\tilde{\mathcal{X}}^*$ by RF+BORE;

  evaluate on full graph G to get the performance;

  update the RF with record $\left(\tilde{\mathbf{x}}^*, \mathcal{M}(F(P^*, \tilde{\mathbf{x}}^*), D_{\text{val}})\right)$;

  if $\mathcal{M}(F(P^*, \tilde{\mathbf{x}}^*), D_{\text{val}}) > y^*$ **then**

  $y^* \leftarrow \mathcal{M}(F(P^*, \tilde{\mathbf{x}}^*), D_{\text{val}})$ and $\mathbf{x}^* \leftarrow \tilde{\mathbf{x}}^*$; **end if**

until the remaining $B/2$ budget exhausted;

return $\mathbf{x}^*$.

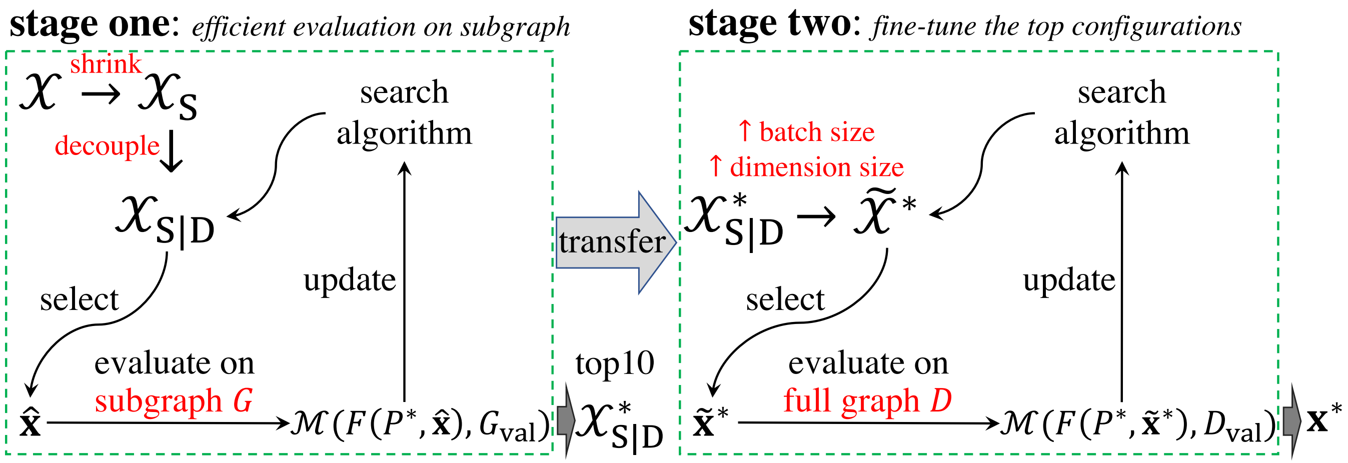
Efficient two-stage HP search algorithm

Stage1: exploration on reduced space

- quickly search HP on sampled KG
- with predictor RF and acquisition BORE

Stage2: exploitation with fine-tuning

- transfer top10 configurations from stage 1
- finetune configuration on original KG



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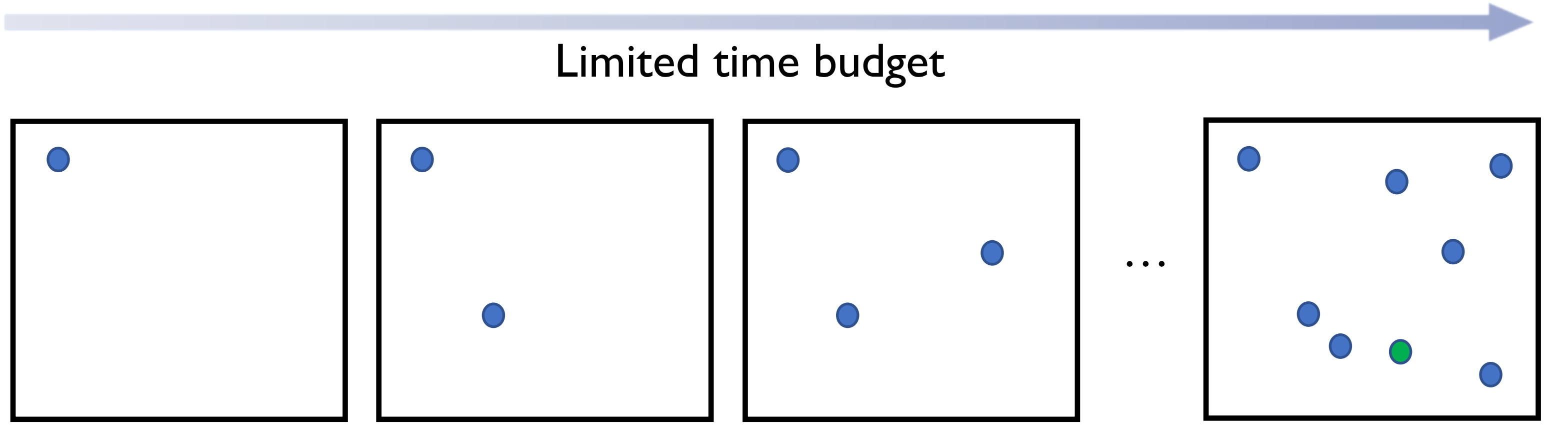
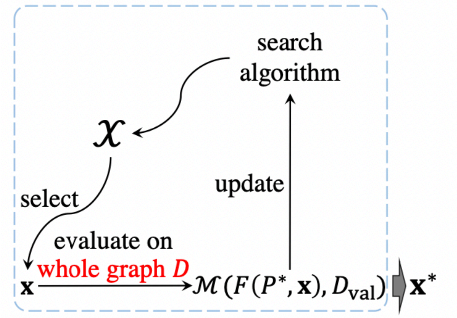
until the remaining $^{B}/_{2}$ budget exhausted;
return $\mathbf{x}^*$.

Efficient two-stage HP search algorithm

Searching process diagram



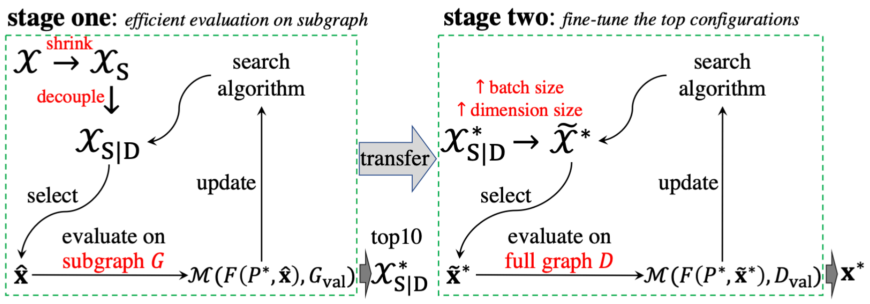
One-stage method



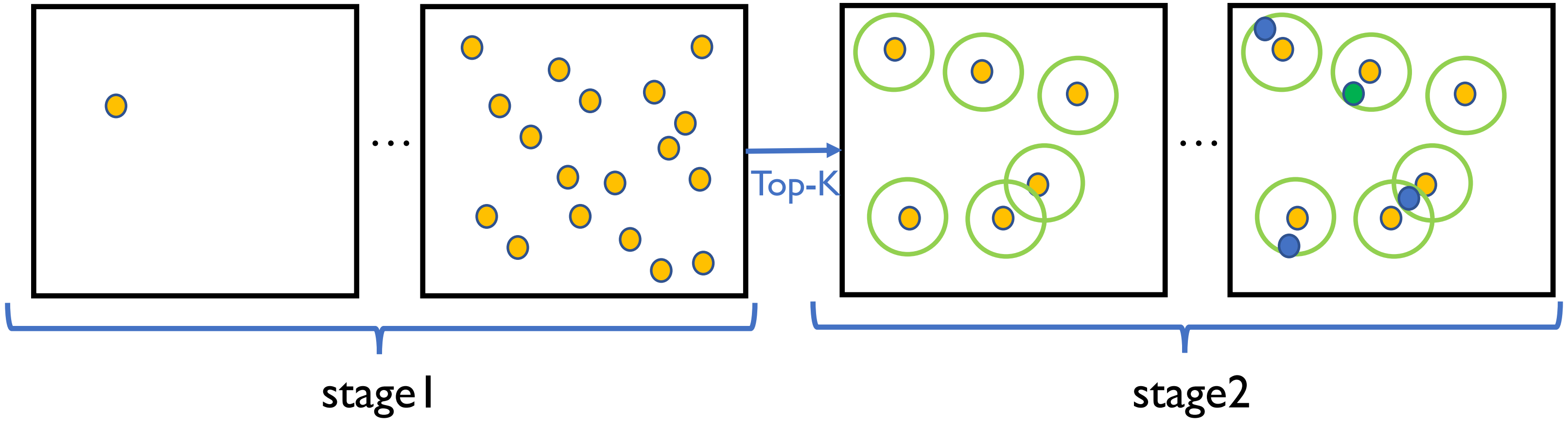
(a) Conventional methods.

evaluation on original KG / sampled KG optimal configuration

Two-stage method (ours)



(b) KGTuner



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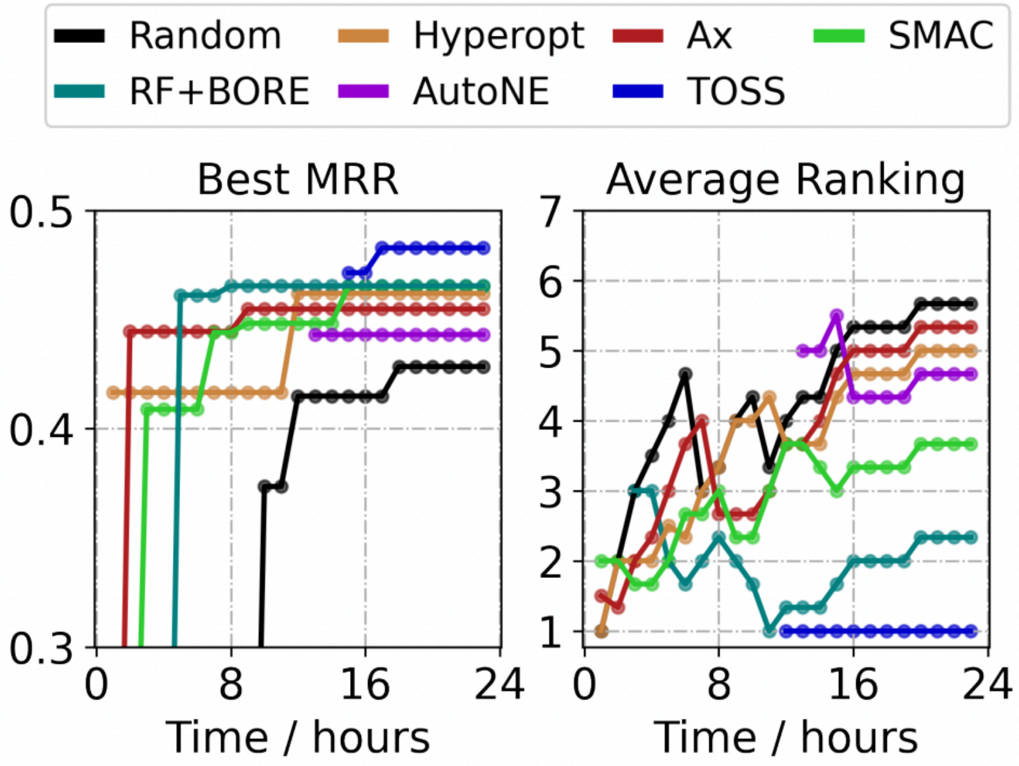
Experiment

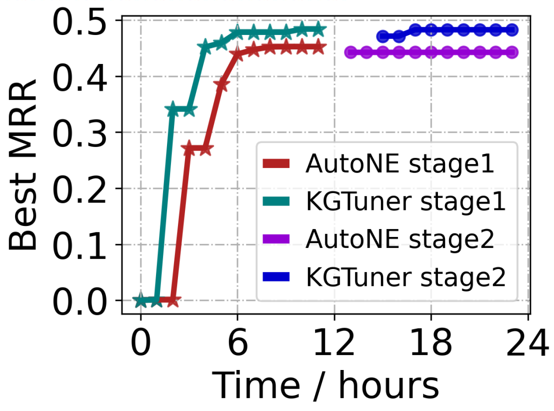
Search algorithm comparison

Observations

- Random search is the worst due to the full randomness.
- SMAC and RF+BORE achieve better performance than Hyperopt and Ax since RF can fit the space better than TPE and GP.
- Due to the weak approximation and transferability, AutoNE also performs bad.
- KGTuner is much better than all the baselines



	search space reduce	search space decouple	surrogate model	fast evaluation
Random	×	×	×	×
Hyperopt	×	×	TPE	×
Ax	×	×	GP	×
SMAC	×	×	RF	×
RF+BORE	×	×	RF	×
AutoNE	×	×	GP	√
TOSS	√	√	RF	√



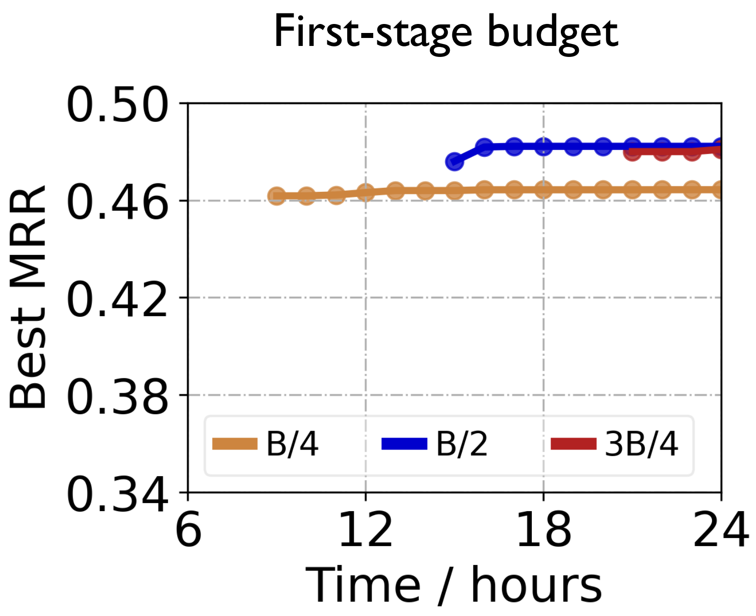
Experiment

Searched configuration performance

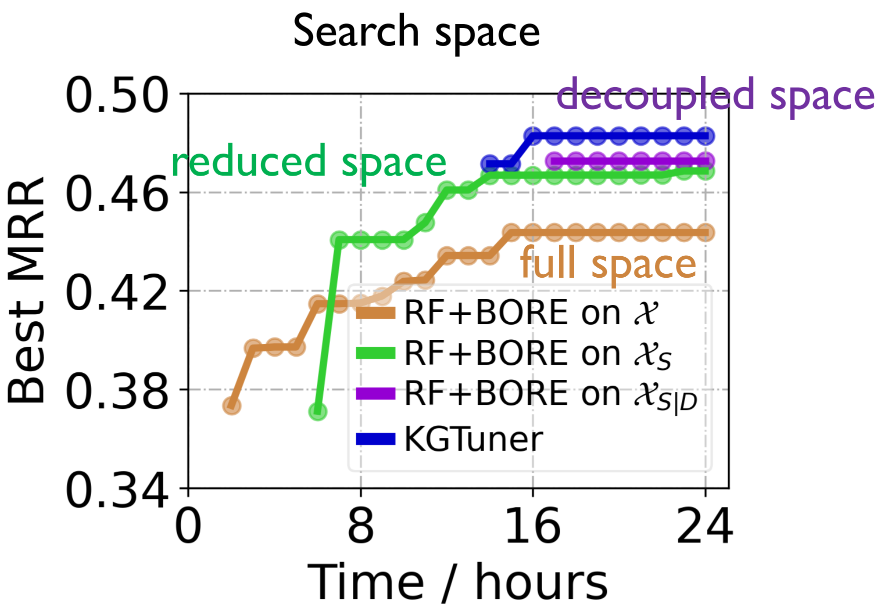
	models	ogbl-biokg	ogbl-wikikg2
original	TransE	0.7452	0.4256
	RotatE	0.7989	0.2530
	DistMult	0.8043	0.3729
	ComplEx	0.8095	0.4027
	AutoSF	0.8320	0.5186
KGTuner	TransE	0.7781 (4.41%↑)	0.4739 (11.34%↑)
	RotatE	0.8013 (0.30%↑)	0.2944 (16.36%↑)
	DistMult	0.8241 (2.46%↑)	0.4837 (29.71%↑)
	ComplEx	0.8385 (3.58%↑)	0.4942 (22.72%↑)
	AutoSF	0.8354 (0.41%↑)	0.5222 (0.69%↑)
average improvement		2.23%	16.16%

		WN18RR				FB15k-237			
		MRR	Hit@1	Hit@3	Hit@10	MRR	Hit@1	Hit@3	Hit@10
Original	ComplEx	0.440	0.410	0.460	0.510	0.247	0.158	0.275	0.428
	DistMult	0.430	0.390	0.440	0.490	0.241	0.155	0.263	0.419
	RESCAL	0.420	-	-	0.447	0.270	-	-	0.427
	ConvE	0.430	0.400	0.440	**0.520**	0.325	0.237	0.356	0.501
	TransE	0.226	-	-	0.501	0.294	-	-	0.465
	RotatE	0.476	**0.428**	0.492	0.571	**0.338**	0.241	**0.375**	**0.533**
	TuckER	0.470	**0.443**	0.482	0.526	**0.358**	**0.266**	**0.394**	**0.544**
LibKGE (Ruffinelli et al., 2019)	ComplEx	0.475	0.438	0.490	0.547	0.348	0.253	0.384	**0.536**
	DistMult	0.452	**0.413**	0.466	0.530	0.343	0.250	**0.378**	**0.531**
	RESCAL	0.467	**0.439**	0.480	0.517	0.356	0.263	**0.393**	**0.541**
	ConvE	**0.442**	**0.411**	**0.451**	0.504	**0.339**	**0.248**	**0.369**	0.521
	TransE	0.228	**0.053**	0.368	0.520	0.313	0.221	0.347	0.497
KGTuner (ours)	ComplEx	**0.484**	**0.440**	**0.506**	**0.562**	**0.352**	**0.263**	**0.387**	0.530
	DistMult	**0.453**	0.407	**0.468**	**0.548**	**0.345**	**0.254**	0.377	0.527
	RESCAL	**0.479**	0.436	**0.496**	**0.557**	**0.357**	**0.268**	0.390	0.535
	ConvE	0.437	0.399	0.449	0.515	0.335	0.242	0.368	**0.523**
	TransE	**0.233**	0.032	**0.399**	**0.542**	**0.327**	**0.228**	**0.369**	**0.522**
	RotatE	**0.480**	0.427	**0.501**	**0.582**	**0.338**	**0.243**	0.373	0.527
	TuckER	**0.480**	0.437	**0.500**	**0.557**	0.347	0.255	0.382	0.534

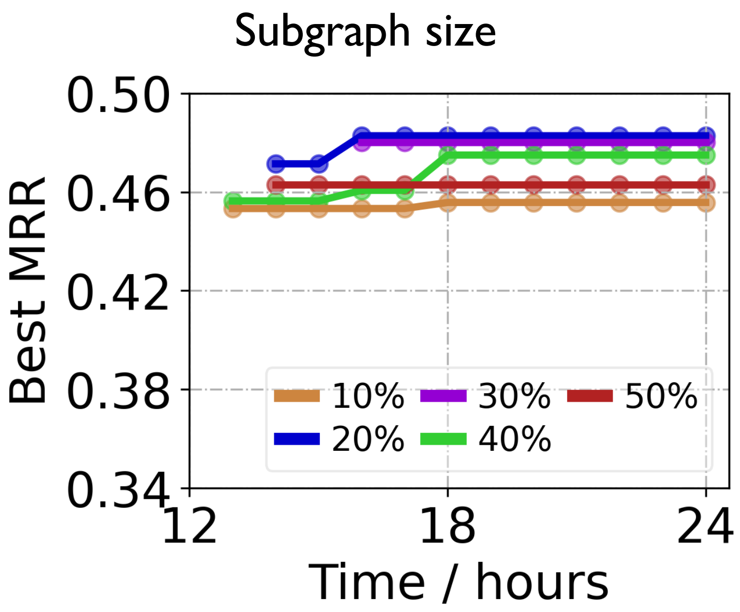
Experiment | Ablation study



budget = B/2 👍



Subgraph + Decouple 👍



Subgraph size = 20%/30% 👍

Experiment

Searched optimal configurations

Table 9: Searched optimal hyperparameters for the WN18RR dataset.

HP/Model	ComplEx	DistMult	RESCAL	ConvE	TransE	RotatE	TuckER
# negative samples	512	128	128	1VsAll	128	2048	128
loss function	BCE_adv	BCE_adv	BCE_mean	BCE_sum	CE	BCE_adv	CE
gamma	0.00	0.00	0.00	0.00	6.00	3.10	0.00
adv. weight	0.57	1.41	0.00	0.00	0.00	1.93	0.00
regularizer	DURA	NUC	DURA	FRO	FRO	FRO	DURA
reg. weight	$8.64 * 10^{-3}$	$9.58 * 10^{-3}$	$1.76 * 10^{-3}$	$1.00 * 10^{-4}$	$1.00 * 10^{-4}$	$6.51 * 10^{-6}$	$1.42 * 10^{-3}$
dropout rate	0.25	0.29	0.00	0.00	0.20	0.00	0.00
optimizer	Adam	Adam	Adam	Adam	Adam	Adam	Adam
learning rate	$1.77 * 10^{-3}$	$4.58 * 10^{-3}$	$1.73 * 10^{-3}$	$1.00 * 10^{-3}$	$1.00 * 10^{-3}$	$6.43 * 10^{-4}$	$1.37 * 10^{-3}$
initializer	xavier_norm	norm	uniform	uniform	uniform	norm	uniform
batch size	512	1024	512	1024	512	512	512
dimension size	1000	2000	1000	2000	1000	1000	200
inverse relation	False	False	False	False	False	False	False

Limited range

Monotonously

Table 10: Searched optimal hyperparameters for the FB15k-237 dataset.

HP/Model	ComplEx	DistMult	RESCAL	ConvE	TransE	RotatE	TuckER
# negative samples	512	kVsAll	2048	512	512	2048	2048
loss function	BCE_adv	CE	CE	BCE_sum	BCE_adv	BCE_adv	BCE_adv
gamma	0.00	0.00	0.00	0.00	6.76	7.58	0.00
adv. weight	1.93	0.00	0.00	0.00	1.99	1.57	1.94
regularizer	DURA	FRO	DURA	DURA	FRO	DURA	DURA
reg. weight	$9.75 * 10^{-3}$	$1.00 * 10^{-4}$	$9.01 * 10^{-3}$	$6.42 * 10^{-3}$	$2.16 * 10^{-3}$	$5.12 * 10^{-3}$	$1.47 * 10^{-4}$
dropout rate	0.22	0.30	0.00	0.08	0.03	0.02	0.02
optimizer	Adam	Adam	Adam	Adam	Adam	Adam	Adam
learning rate	$9.70 * 10^{-4}$	$1.00 * 10^{-3}$	$1.19 * 10^{-3}$	$2.09 * 10^{-3}$	$2.66 * 10^{-4}$	$2.98 * 10^{-4}$	$3.19 * 10^{-4}$
initializer	uniform	normal	xavier_norm	normal	xavier_norm	uniform	normal
batch size	1024	1024	512	1024	512	512	512
dimension size	2000	2000	500	500	1000	1000	500
inverse relation	False	False	False	False	False	False	False

Reduced options

Outline

- Background
- A comprehensive understanding of HP in KGE
- An efficient two-stage HP search algorithm
- Experiments
- Key takeaway and future directions

Key takeaways

Recall the difficulties

Lacking understanding of KGE components

Low efficiency in searching for hyperparameter

KGTuner

A comprehensive understanding of HPs

An efficient two-stage HP search algorithm

Code: https://github.com/AutoML-Research/KGTuner

Email: zhangyongqi@4paradigm.com

Limitation and future directions

Limitation

- Limited to pure embedding models
- Not considering HPs inside the SF model
- Lacking of theoretical analysis and guarantees

Potential directions

- apply with GNN to solve the scaling problem
- combine HPO with NAS
- transferability across datasets/models/tasks