Dihedron Algebraic Embeddings for Spatio-temporal Knowledge Graph Completion

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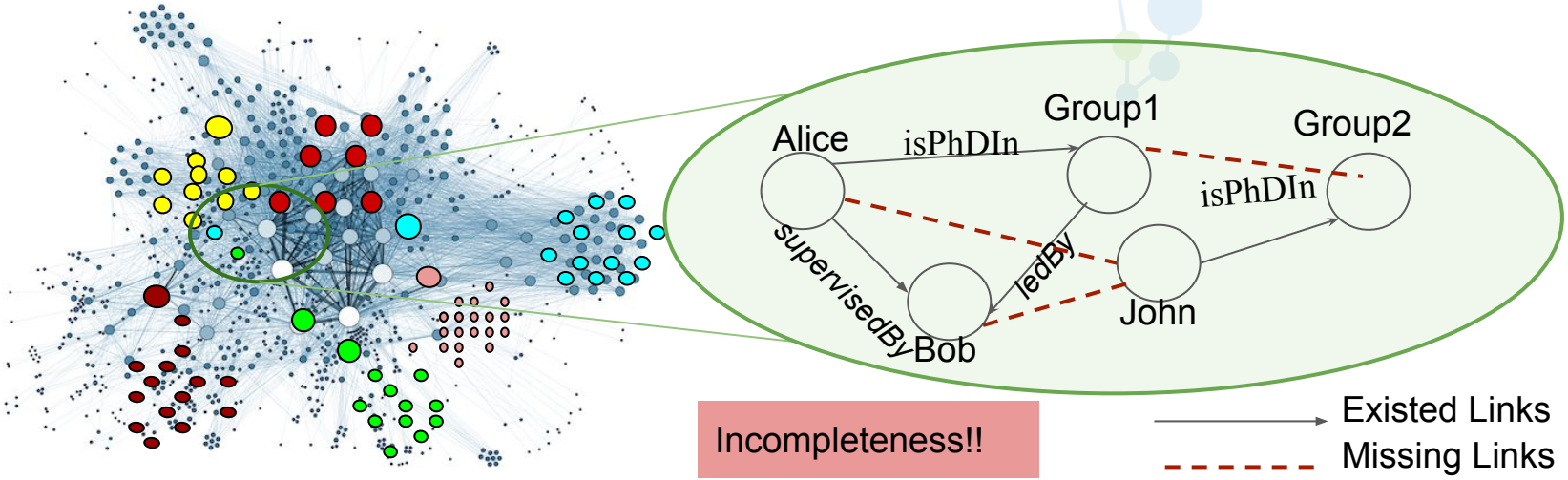
SMART DATA ANALYTICS
FROM DATA TO KNOWLEDGE

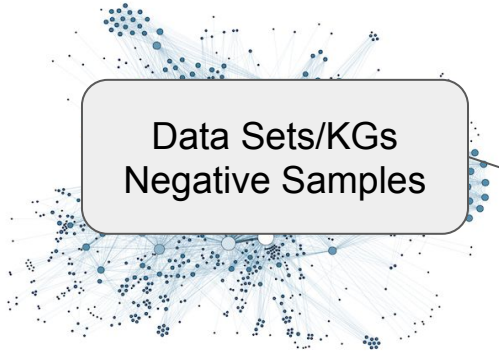
Knowledge Graph

- Symbolic information
- Relational and structured data
- Representation of facts in the form of triples: (Alice, *supervisedBy*, Bob)
- Represented in Graph

subject entity (s) | relation (r) | object entity (o)



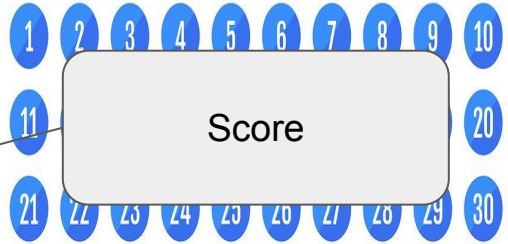
Knowledge Graph Embedding Models



Data Sets/KGs
Negative Samples

KGE

Score



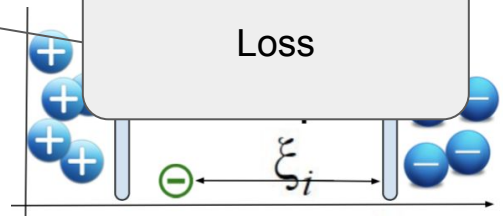
Embeddings

[0.1, -0.4, 1, ...]

Vectors, Matrix, ...

$$\begin{pmatrix} 2 & 5 & 7 & 8 \\ 1 & 2 & 3 & 1 \\ 4 & 5 & 0 & 1 \end{pmatrix}$$

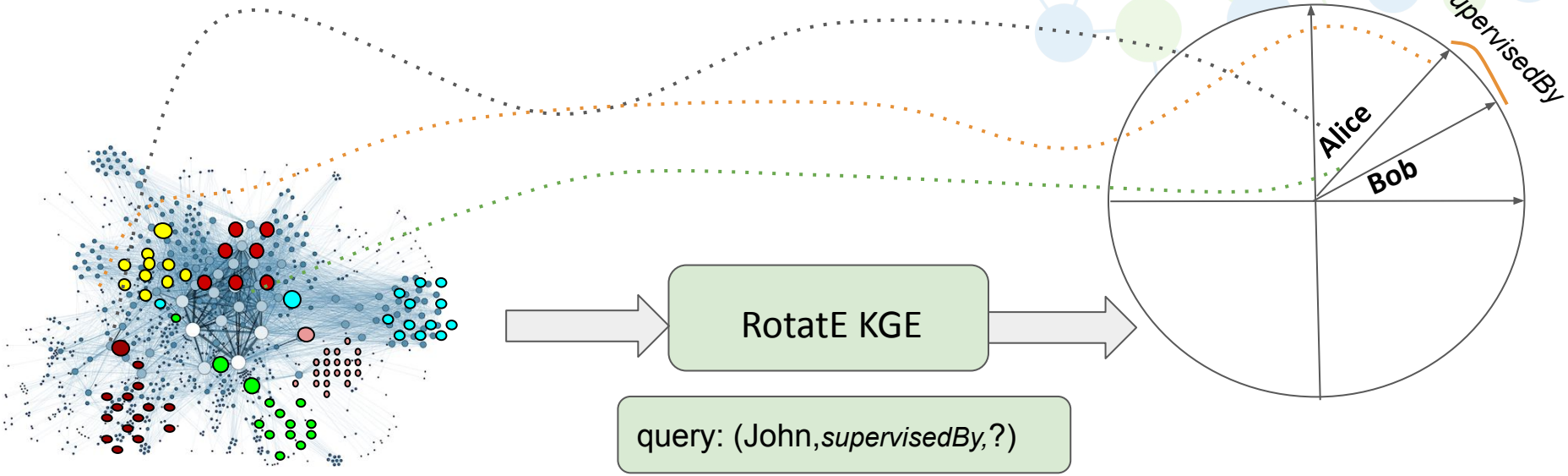
Loss



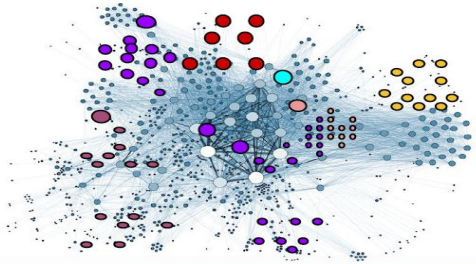
Score Function of Embedding Models

Vectors representation of entities and relations: (**s,r,o**)

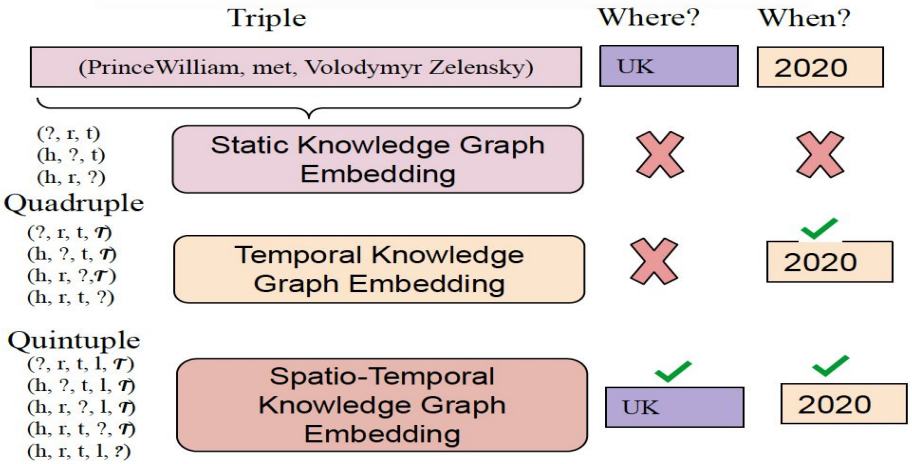
$\overrightarrow{subject} \circ \overrightarrow{relation} = \overrightarrow{object}$ (is an operator which applies rotation)



Spatio-Temporal Information in KG



PrinceWilliam met Volodymyr Zelensky in UK in 2020.



Query on Spatio-Temporal KGs

- Head query
- Relation Query
- Tail Query
- Location Query
- Time Query

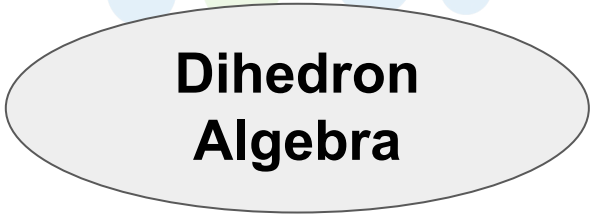
$(?, r, t, l, \tau)$	$(h, ?, t, l, \tau)$	$(h, r, ?, l, \tau)$	$(h, r, t, ?, \tau)$	$(h, r, t, l, ?)$
h	r	t	l	τ

- Who met Volodymyr Zelensky in UK in 2020. <?, r, t, l, R>?

- PrinceWilliam met whom in UK in 2020. <h, r, ?, l, R>?

Spatio-Temporal Query representation

- In each case, we have 4 elements:
- e.g., (?,r,t,l,τ)
- 4D algebra
- Hypercomplex space



Basic Elements of Dihedron Algebra

- Dihedron numbers $d = x_r\mathbf{1} + x_i\boldsymbol{i} + x_j\boldsymbol{j} + x_k\boldsymbol{k} \in \mathbb{D}$
- 4 elements: one real and three imaginary parts

$$\mathbf{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \boldsymbol{i} = \begin{bmatrix} 0 & 1 \\ \bar{1} & 0 \end{bmatrix}, \boldsymbol{j} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \boldsymbol{k} = \begin{bmatrix} 1 & 0 \\ 0 & \bar{1} \end{bmatrix}, \bar{a} = -a$$

$$\boldsymbol{i^2} = \bar{1},\ \boldsymbol{j^2} = 1,\ \boldsymbol{k^2} = 1, \boldsymbol{ij} = \boldsymbol{k},\ \boldsymbol{ij} = \boldsymbol{k},\ \boldsymbol{jk} = \bar{\boldsymbol{i}},\ \boldsymbol{ki} = \boldsymbol{j},\ \boldsymbol{ji} = \bar{\boldsymbol{k}},\ \boldsymbol{kj} = \boldsymbol{i}$$

$$\boldsymbol{ik} = \bar{\boldsymbol{j}}$$

Basic Elements of Dihedron Algebra

- Dihedron Matrix Representation

$$x_r\mathbf{1} + x_i\boldsymbol{i} + x_j\boldsymbol{j} + x_k\boldsymbol{k} = \begin{bmatrix} x_r + x_k & x_i + x_j \\ \bar{x}_i + x_j & x_r + \bar{x_k} \end{bmatrix}$$

$$\equiv (x_r, x_i, x_j, x_k)$$

$$\equiv \ x_r + v_q, \quad v_q = (x_i, x_j, x_k) \in \mathbb{R}^{3d} \, q \in \mathbb{D}$$

Basic Elements of Dihedron Algebra

- Dihedron Product between $q_x, q_y \in \mathbb{D}$

$$q_z = z_r\mathbf{1} + v_{q_z} = q_x \otimes q_y = (x_r\mathbf{1} + v_{q_x}) \otimes (y_r\mathbf{1} + v_{q_y})$$

$$= (x_r y_r - \langle v_{q_x}, v_{q_y} \rangle)\mathbf{1} + (x_r v_{q_y} + y_r v_{q_x}) + v_{q_x} \times v_{q_y}$$

$$\langle v_{q_x}, v_{q_y} \rangle = x_i y_i - x_j y_j - x_k y_k, \quad v_{q_x} \times v_{q_y} = \begin{bmatrix} -x_j y_k + x_k y_j \\ x_k y_i - x_i y_k \\ x_i y_j - x_y y_i \end{bmatrix}$$

Dihedron Representation of Spatio-Temporal Query

(h, r, t, l, τ)

$(h, r, ?, l, \tau)$ t

(t, r^{-1}, h, l, τ)

$(t, r^{-1}, ?, l, \tau)$ h

$$q = h\mathbf{1} + ri + lj + \tau k = \begin{bmatrix} h+\tau & r+l \\ \bar{r}+l & h+\bar{\tau} \end{bmatrix} \equiv h + v_q$$

$$v_q = (r, l, \tau) \in \mathbb{R}^{3d},\ q \in \mathbb{D}^d$$

$$t = e\mathbf{1} + v_t$$

$$v_t = t_x i + t_y j + t_z k$$

$$q = t\,\mathbf{1} + r^{-1} i + lj + \tau k = \begin{bmatrix} t+\tau & r^{-1}+l \\ \bar{r}^{-1}+l & t+\bar{\tau} \end{bmatrix} \equiv t + v_q$$

$$v_q = (r^{-1}, l, \tau) \in \mathbb{R}^{3d},\ q \in \mathbb{D}^d$$

$$h = e\mathbf{1} + v_h$$

$$v_h = h_x i + h_y j + h_z k$$

Score Function

$$S(q,t) = -\|s1 + v_s\|$$

$$s1 + v_s = q \otimes t \;\; = (h1 + v_q) \otimes (e1 + v_t)$$

$$s = h.e - v_q.v_t,\; v_s = hv_t + ev_q + v_q \times v_t$$

$$v_q.v_t = rt_x - lt_y - \tau t_z$$

$$v_q \times v_t = \begin{bmatrix} -lt_z + \tau t_y \\ \tau t_x - rt_z \\ rt_y - lt_x \end{bmatrix}$$

Advantage

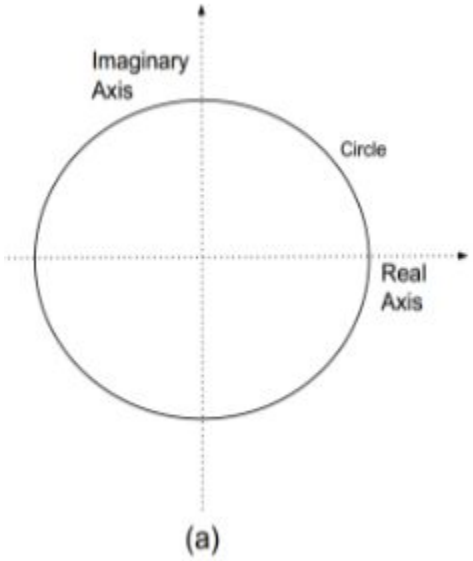
- **Efficiency** in memory and time
- No **mathematical operation** for query representation
- Simply **adaptable** to the query about location and time
- **Model several information** in different dimensionality
  - Entity is modeled in first dimension (1)
  - Relation is modeled in second dimension (i)
  - Location is modeled in third dimension (j)
  - Time is modeled in fourth dimension (k)

- **Capturing** spatio-temporal and relational correlation.
  - head entity-(relation, location, time) (hv_t)
  - tail entity-(relation, location,time) (ev_q)
  - head-tail entity (he)
  - relation-location rt_u
  - relation-time (rt_z)

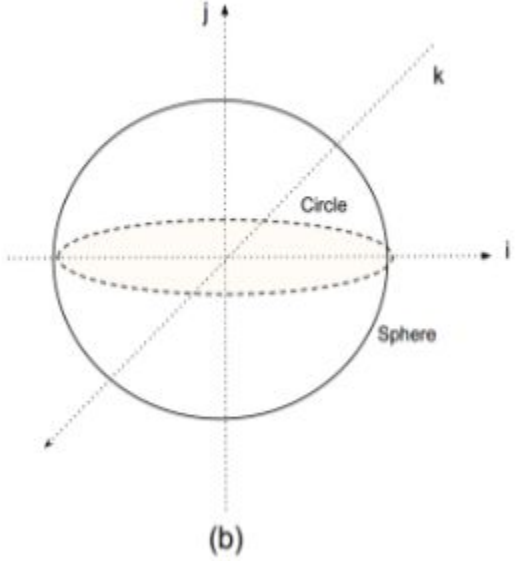
Model specifications

Model	(T-L)	Score function	Pattern	Embeddings
TransE [2]	(✗-✗)	$-\|\|q-t\|\|$	$q=h+r$	$q,h,r,t\in\mathbb{R}^d$
T-TransE (ours)	(✓-✗)	$-\|\|q-t\|\|$	$q=h+r+\tau$	$q,h,r,t,\tau\in\mathbb{R}^d$
ST-TransE (ours)	(✓-✓)	$-\|\|q-t\|\|$	$q=h+r+l+\tau$	$q,h,r,t,\tau,l\in\mathbb{R}^d$
RotatE [24]	(✗-✗)	$\|\|q-t\|\|$	$q=h\circ r$	$q,h,r,t\in\mathbb{C}^d$
T-RotatE (ours)	(✓-✗)	$-\|\|q-t\|\|$	$q=h\circ r\circ\tau$	$q,h,r,t,\tau\in\mathbb{C}^d$
ST-RotatE (ours)	(✓-✓)	$-\|\|q-t\|\|$	$q=h\circ r\circ l\circ\tau$	$q,h,r,t,\tau,l\in\mathbb{C}^d$
ComplEx [26]	(✗-✗)	$Re(q\times\bar{t})$	$q=h\times r$	$q,h,r,t\in\mathbb{C}^d$
T-ComplEx [12]	(✓-✗)	$Re(q\times\bar{t})$	$q=h\times r\times\tau$	$q,h,r,t,\tau\in\mathbb{C}^d$
ST-ComplEx	(✓-✓)	$Re(q\times\bar{t})$	$q=h\times r\times l\times\tau$	$q,h,r,t,l,\tau\in\mathbb{C}^d$
QuatE [33]	(✗-✗)	$Re(q\otimes_H\bar{t})$	$q=h\otimes_H r$	$q,h,r,t\in\mathbb{Q}^d$
T-QuatE (ours)	(✓-✗)	$Re(q\otimes_H\bar{t})$	$q=h\otimes_H r\otimes_H\tau$	$q,h,r,t,\tau\in\mathbb{Q}^d$
ST-QuatE (ours)	(✓-✓)	$Re(q\otimes_H\bar{t})$	$q=h\otimes_H r\otimes_H l\otimes_H\tau$	$q,h,r,t,l,\tau\in\mathbb{Q}^d$
DyHE (ours)	(✗-✗)	$-\|\|q-t\|\|$	$q=h\otimes_D r_{1,2}$	$q,h,r_{1,2},t\in\mathbb{D}^d$
T-DyHE (ours)	(✓-✗)	$-\|\|q-t\|\|$	$q=h\otimes_D r_{1,2}+\tau$	$q,h,r_{1,2},t,\tau\in\mathbb{D}^d$
ST-DyHE (ours)	(✓-✓)	$-\|\|q-t\|\|$	$q=h\otimes_D r_{1,2}+\tau+l$	$q,h,r_{1,2},t,l,\tau\in\mathbb{D}^d$

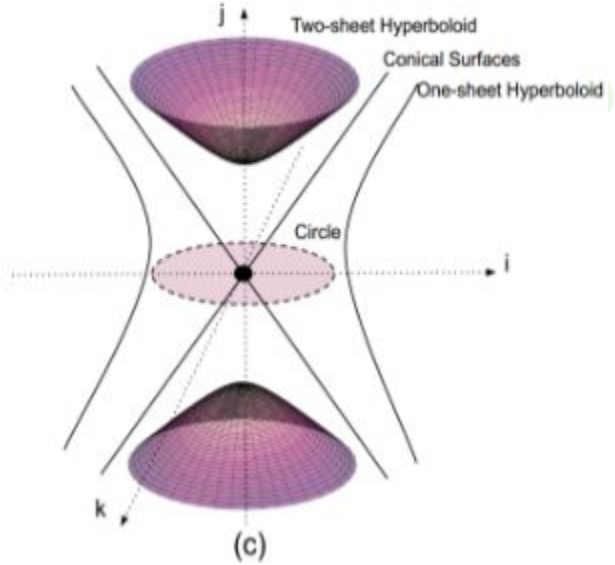
Geometric Interpretation



Complex



Quaternion



Dihedron

Evaluation Setup

Dataset Properties

Dataset	#Quintuple	#Enities	#Relations	#Time	#Locations
Yago3K	9734	3619	8	195	422
DBpedia34K	82,000	34604	7	5687	5687
WikiData53K	~103,000	53849	8	627	296

Evaluation Metrics

1. Mean Rank (MR)
2. Mean Reciprocal Rank (MRR)
3. Hit@1
4. Hit@10

The embedding dimension is set to be 100 and 200 negative sample are generated).

Link prediction Results (For h and t)

	YAGO3K			DBpedia34K			WikiData53K		
	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10
TransE	0.561	0.496	0.689	0.454	0.415	0.519	0.245	0.152	0.451
T-TransE	0.709	0.676	0.779	0.501	0.475	0.544	0.396	0.337	0.538
ST-TransE	0.705	0.670	0.775	0.500	0.451	0.577	0.565	0.546	0.599
RotatE	0.564	0.503	0.688	0.461	0.425	0.521	0.246	0.153	0.458
T-RotatE	0.700	0.679	0.736	0.505	0.487	0.534	0.356	0.283	0.525
ST-RotatE	0.682	0.668	0.702	0.428	0.412	0.455	0.523	0.486	0.588
ComplEx	0.562	0.501	0.686	0.462	0.427	0.523	0.250	0.154	0.464
T-ComplEx	0.702	0.674	0.753	0.500	0.482	0.529	0.376	0.306	0.539
ST-ComplEx	0.689	0.668	0.727	0.450	0.424	0.497	0.532	0.495	0.594
QuatE	0.564	0.503	0.685	0.460	0.425	0.519	0.249	0.156	0.459
T-QuatE	0.694	0.675	0.722	0.500	0.481	0.531	0.358	0.285	0.525
ST-QuatE	0.690	0.675	0.714	0.502	0.485	0.528	0.515	0.478	0.576
DyHE	0.563	0.503	0.684	0.460	0.426	0.518	0.243	0.152	0.448
T-DyHE	**0.715**	**0.684**	0.775	**0.516**	**0.487**	0.564	0.377	0.318	0.517
ST-DyHE	0.704	0.665	**0.779**	0.485	0.427	**0.583**	**0.568**	**0.550**	**0.599**
ST-NewDE	0.708	0.682	0.758	**0.536**	**0.500**	**0.598**	**0.572**	**0.556**	**0.603**

MRR and Hit@1 is increased from SOTA

outperforms in each metric on DB34K and WikiData53K dataset

Location and Time completion result

Performance increased in all metrics

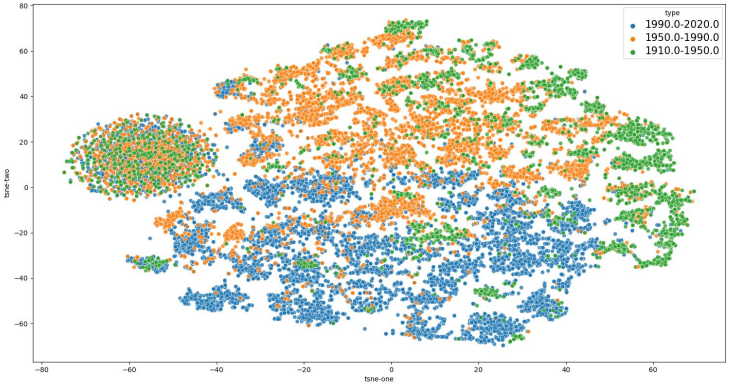
Performance increased in all metrics

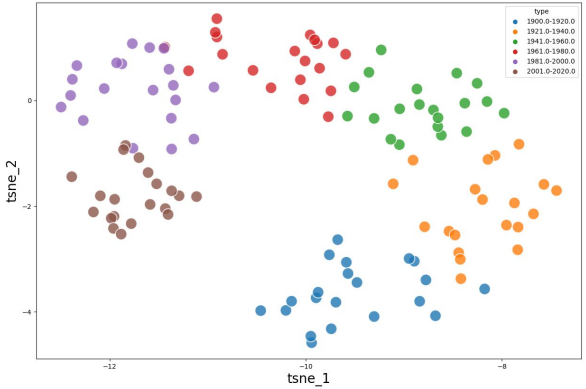
Location Completion $(h, r, t, ?, \tau)$									
	YAGO3K			DBpedia34K			WikiData53K		
	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10
ST-TransE	0.349	0.083	0.903	0.245	0.045	0.633	0.321	0.008	0.838
ST-NewDE	**0.352**	**0.114**	**0.920**	**0.354**	**0.094**	**0.797**	**0.582**	**0.231**	**0.970**

Time Completion $(h, r, t, l, ?)$									
	YAGO3K			DBpedia34K			WikiData53K		
	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10	MRR	Hits@1	Hits@10
ST-TransE	0.249	0.024	0.620	0.271	0.082	0.571	0.075	0.006	0.198
ST-NewDE	**0.580**	**0.241**	**0.958**	**0.432**	**0.151**	**0.792**	**0.162**	**0.020**	**0.514**

Analysis

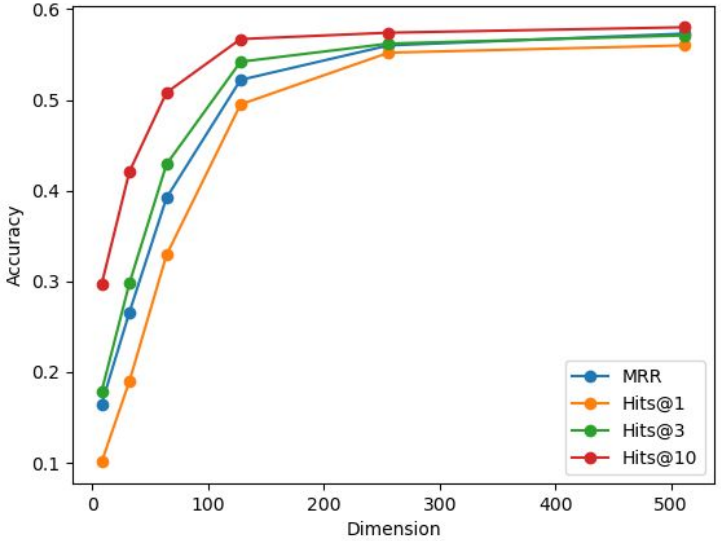
Entity embedding cluster w.r.t time and time clustering w.r.t. year.

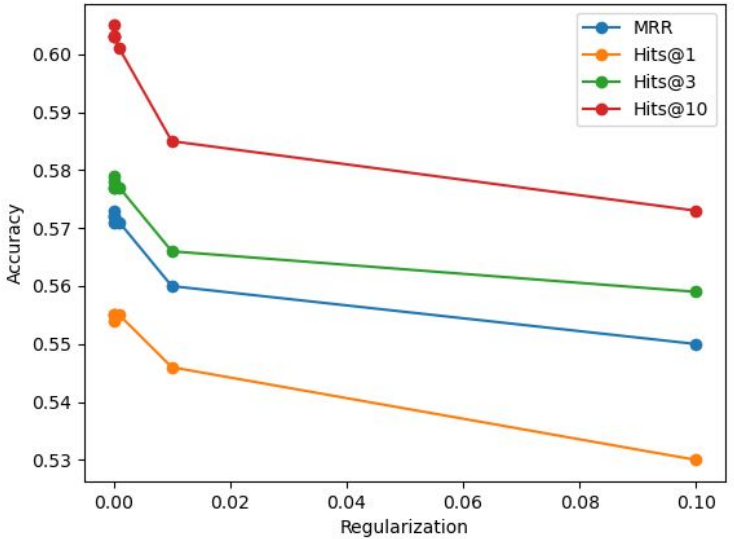




Analysis

Effect of embedding dimension and Regularization in performance metrics





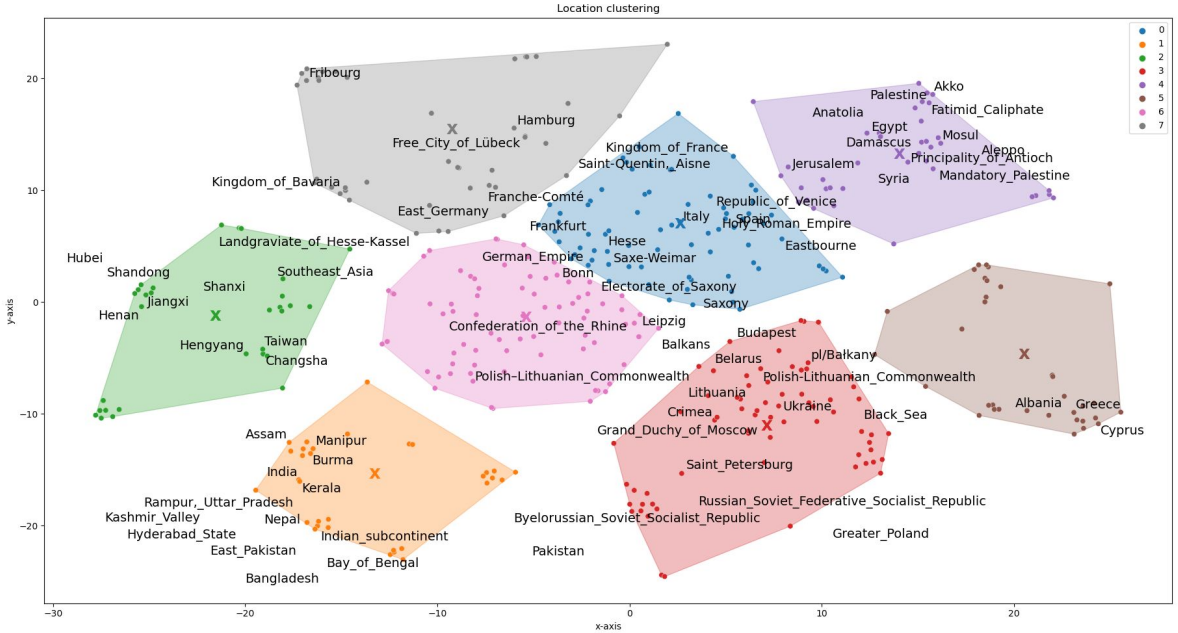
Analysis

Predicted answers on incomplete queries

Dataset	Query on head or tail parts	ST-NewDE	ComplEx
WikiData53K	(Philip_Guston, creatorOf, ?, United_States, 1972)	**Late_Afternoon**	Jules_Olitski
DBpedia34K	(Santiago_Calatrava, architectOf, ?, Maroussi, 1982)	**Olympic_Stadium_(Athens)**	SoFi_Stadium
YAGO3K	(?, created, Ulysses_(movie), Italy, 1955)	**Ennio_de_Concini**	Lasse_Hallstroem
Dataset	Query on location or time parts	ST-NewDE	ST-ComplEx
WikiData53K	(Edward_Witten, awardReceived, Alan_T._Waterman_Award, ?, 1982)	**United States**	Spain
DBpedia34K	(Nikolai_Nekrasov, authorOf, Korobeiniki_(poem), ?, 1861)	**Russia**	Serbia
YAGO3K	(Richard_Harvey, wroteMusicFor, Animal_Farm_(movie), United_States, ?)	**1999**	2010

Analysis

Results on clustering on the embedding of location



Conclusion and Future Work

- Presented embedding for spatio-temporal Knowledge Graphs
- Utilized Dihedron for modeling spatio-temporal queries.
- Measuring the plausibility of quintuple using Dihedron product
- Adapt existing KG embeddings to learn from spatio-temporal KG
- Design ablation models using spatio-temporal rotation and translation

Future work:

- Extend our model to capture granularity of time.
- Answering complex spatio-temporal queries.
- Using partial differential equation for modelling spatio-temporal KG