Arbitrary Time Information Modeling via Polynomial Approximation for Temporal Knowledge Graph Embedding

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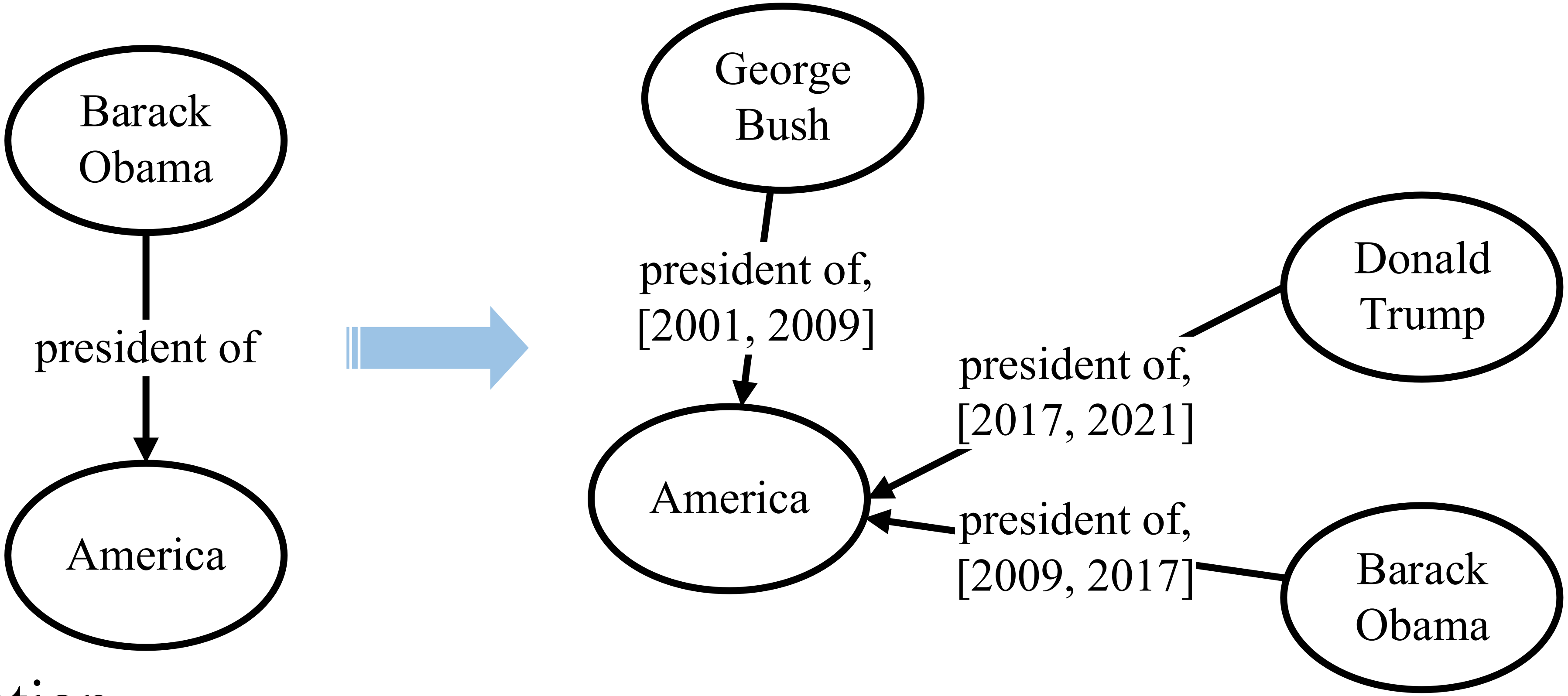
- # Background

➢ Knowledge Graph VS. Temporal Knowledge Graph



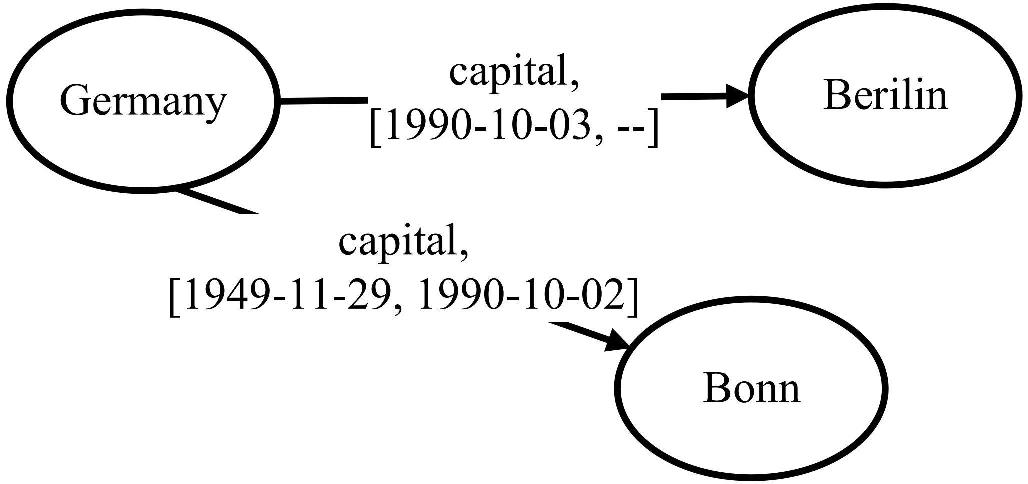
➢ Formalization

- A temporal knowledge graph is a *multi-relational graph* representation of a collection $\mathcal{F}$ of facts in quadruple form $(e_h, r, e_t, \tau) \in \mathcal{E} \times \mathcal{R} \times \mathcal{E} \times \mathcal{T}$. If $(e_h, r, e_t, \tau) \in \mathcal{F}$, then head entity e_h is related to tail entity e_t by relation r on timestamp τ.

Background

Main Challenges

- The limited capability to model arbitrary timestamps continuously.
- The lack of rich inference patterns under temporal constraints.



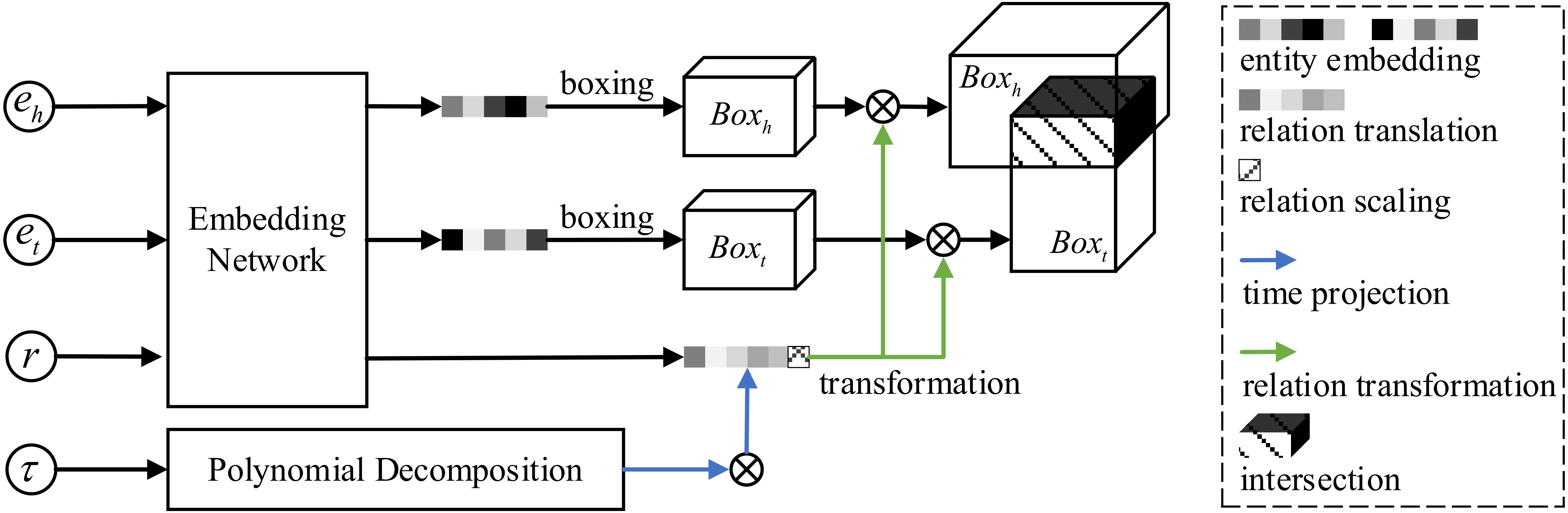
Query: (Germany, ?, Bonn, 1950)
(Germany, capital, ?, 2024)

Inference Pattern
Symmetry: $r_1(e_1, e_2 \vert \tau) \Rightarrow r_1(e_2, e_1 \vert \tau)$
Antisymmetry: $r_1(e_1, e_2 \vert \tau) \Rightarrow \neg r_1(e_2, e_1 \vert \tau)$
Inversion: $r_1(e_1, e_2 \vert \tau) \Leftrightarrow r_2(e_2, e_1 \vert \tau)$
Composition: $r_1(e_1, e_2 \vert \tau) \wedge r_2(e_2, e_3 \vert \tau) \Rightarrow r_3(e_1, e_3 \vert \tau)$
Hierarchy: $r_1(e_1, e_2 \vert \tau) \Rightarrow r_2(e_1, e_2 \vert \tau)$
Intersection: $r_1(e_1, e_2 \vert \tau) \wedge r_2(e_1, e_2 \vert \tau) \Rightarrow r_3(e_1, e_2 \vert \tau)$
Mutual exclusion: $r_1(e_1, e_2 \vert \tau) \wedge r_2(e_1, e_2 \vert \tau) \Rightarrow \perp$

• Methodology

➢ Motivation

- Polynomial decomposition-based temporal representation: flexibly represent arbitrary timestamp.
- Box embedding-based entity representation: learn rigid inference patterns.



- # Methodology

➢ Polynomial Decomposition based Temporal Representation

- Modeling the timestamp via polynomial decomposition-based representation (PTR).
- Weierstrass approximation theorem:

$$f \in C[a,b], \forall \epsilon > 0, \exists P_n \Rightarrow \forall x \in [a,b], |f - P_n| < \epsilon \tag{1}$$

- Temporal representation function of any given timestamp.

$$P_n(f_\tau, x) = \sum_{k=0}^{n} f(\frac{k}{n}) \binom{n}{k} x^k (1-x)^{n-k} \tag{2}$$

$$\mathcal{P}_\tau = P_n(f_\tau, x) = \boldsymbol{\alpha_\tau} \cdot \boldsymbol{X} \tag{3}$$

• Methodology

➢ Box Embedding based Entity Representation

- Modeling the entities via box embedding based entity representations (BER).
- The maximum and minimum coordinates of ***Gumbel boxes*** follow the Gumbel distribution, then the boxes can be formulated as:

$$\begin{aligned} Box(e) &= \prod_{i=1}^{d} [e_i^m, e_i^M], \\ e_i^m &\sim \mathrm{MaxGumbel}(\mu_i^m, \beta), \\ e_i^M &\sim \mathrm{MinGumbel}(\mu_i^M, \beta). \end{aligned} \tag{4}$$

- The approximation of ***volume in Gumbel boxes*** can be formulated as:

$$\mathbb{E}[Vol(Box(e))] \approx \prod_{i=1}^{d} \beta \log(1 + \exp(\frac{\mu_i^M - \mu_i^m}{\beta} - 2\gamma)) \tag{5}$$

- Methodology

➢ Modeling and Evaluation of Quadruples

- The ***evolutionary dynamics*** of entities and relations over time:

$$
\begin{aligned}
e_h' &= \mathcal{P}_\tau(e_h;W) = Box(e_h) + (W^T Box(e_h))W, \\
e_t' &= \mathcal{P}_\tau(e_t;W) = Box(e_t) + (W^T Box(e_t))W, \\
r_t' &= \mathcal{P}_\tau(r_t;W) = r_t + (W^T r_t)W.
\end{aligned} \tag{6}
$$

- Relation transformation $T_r \subseteq \mathbb{R}^{2\times d}$ for entity e:

$$
\begin{aligned}
e^t &= f_r^t(e|T_r) = Box(e) + T_r[0], \\
e^s &= f_r^s(e|T_r) = Box(e) \odot T_r[1].
\end{aligned} \tag{7}
$$

- Scoring function:

$$
\mathcal{S}(h,r,t,\tau) = \frac{\mathbb{E}[Vol(f_r^s \circ f_r^t(\mathcal{P}_\tau(e_h;W)) \cap f_r^s \circ f_r^t(\mathcal{P}_\tau(e_t;W)))]}{\mathbb{E}[Vol(f_r^s \circ f_r^t(\mathcal{P}_\tau(e_t;W)))]} \tag{8}
$$

• Methodology

➢ Analysis of Model Properties

- Local Identifiability:
  Assuming a set of parameters Ω is local identifiable if, for all $\theta \in \Omega$, there exists $N(\theta)$, a neighborhood of θ, such that for all $\theta' \in N(\theta), L(x|\theta') \neq L(x|\theta)$.

- Inference Patterns.

Inference Pattern	Setting
Symmetry: $r_1(e_1, e_2|\tau) \Rightarrow r_1(e_2, e_1|\tau)$	$P_{r_1}(e_1|e_2) = P_{r_1}(e_2|e_1) \neq 0$
Antisymmetry: $r_1(e_1, e_2|\tau) \Rightarrow \neg r_1(e_2, e_1|\tau)$	$P_{r_1}(e_1|e_2) \neq 0, P_{r_1}(e_2|e_1) = 0$
Inversion: $r_1(e_1, e_2|\tau) \Leftrightarrow r_2(e_2, e_1|\tau)$	$P_{r_1}(e_1|e_2) = P_{r_2}(e_2|e_1) \neq 0$
Composition: $r_1(e_1, e_2|\tau) \wedge r_2(e_2, e_3|\tau) \Rightarrow r_3(e_1, e_3|\tau)$	$P_{r_3}(e_1, e_2, e_3) \neq 0$
Hierarchy: $r_1(e_1, e_2|\tau) \Rightarrow r_2(e_1, e_2|\tau)$	$P_{r_1,r_2}(e_1|e_2) \geq P_{r_1}(e_1|e_2)P_{r_2}(e_1|e_2) \neq 0$
Intersection: $r_1(e_1, e_2|\tau) \wedge r_2(e_1, e_2|\tau) \Rightarrow r_3(e_1, e_2|\tau)$	$P_{r_3}(e_1|e_2) \geq P_{r_1,r_2}(e_1|e_2) \neq 0$
Mutual exclusion: $r_1(e_1, e_2|\tau) \wedge r_2(e_1, e_2|\tau) \Rightarrow \perp$	$P(\mathcal{B}(e_1^{r_1}) \cap \mathcal{B}(e_2^{r_1}), \mathcal{B}(e_1^{r_2}) \cap \mathcal{B}(e_2^{r_2})) = 0$

- Runtime and Space Complexity.
  time $O(d)$ and space $O((|E| + |R| + K)d)$

- # Experiments

➢ Comparing with SOTA

Model	YAGO11k MRR	YAGO11k Hits@3	YAGO11k Hits@10	WikiData MRR	WikiData Hits@3	WikiData Hits@10
TransE	0.100	0.138	0.244	0.178	0.192	0.339
DistMult	0.158	0.161	0.268	0.222	0.238	0.460
RotatE	0.167	0.167	0.305	0.116	0.236	0.461
QuatE	0.164	0.148	0.270	0.125	0.243	0.416
TTransE	0.108	0.150	0.251	0.172	0.184	0.329
HyTE	0.105	0.143	0.272	0.180	0.197	0.333
TA-DistMult	0.161	0.171	0.292	0.218	0.232	0.447
ATiSE	0.170	0.171	0.288	0.280	0.317	0.481
TeRo	<u>0.187</u>	0.197	0.319	**0.299**	<u>0.329</u>	<u>0.507</u>
RotateQVS	**0.189**	<u>0.199</u>	<u>0.323</u>	-	-	-
PTBox	0.162	**0.222**	**0.347**	<u>0.290</u>	**0.331**	**0.527**

Link prediction

Model	YAGO11k MR	YAGO11k Hits@1	WikiData MR	WikiData Hits@1
TransE	1.70	0.784	1.35	0.884
TransH	1.53	0.761	1.40	0.881
HolE	2.57	0.693	2.23	0.840
t-TransE	1.66	0.755	1.97	0.742
HyTE	1.23	0.812	1.13	0.926
PTBox	**1.12**	**0.896**	**1.12**	**0.934**

Relation prediction

- Experiments

➢ Ablation Study

PTR	BER	YAGO11k MRR	YAGO11k Hits@3	YAGO11k Hits@10	WikiData MRR	WikiData Hits@3	WikiData Hits@10
		0.105	0.143	0.272	0.180	0.197	0.333
✓		0.137	0.174	0.313	0.259	0.278	0.478
	✓	0.127	0.180	0.280	0.253	0.281	0.426
✓	✓	**0.162**	**0.222**	**0.347**	**0.290**	**0.331**	**0.527**

About proposed two modules

Mode	YAGO11k MRR	YAGO11k Hits@10	WikiData MRR	WikiData Hits@10
$\mathcal{P}_\tau(e)$	0.127	0.289	0.267	0.485
$\mathcal{P}_\tau(r)$	**0.162**	**0.347**	**0.290**	**0.527**
$\mathcal{P}_\tau(e,r)$	0.135	0.311	0.277	0.503

About different evolutionary patterns

- # Experiments

➢ Case Study

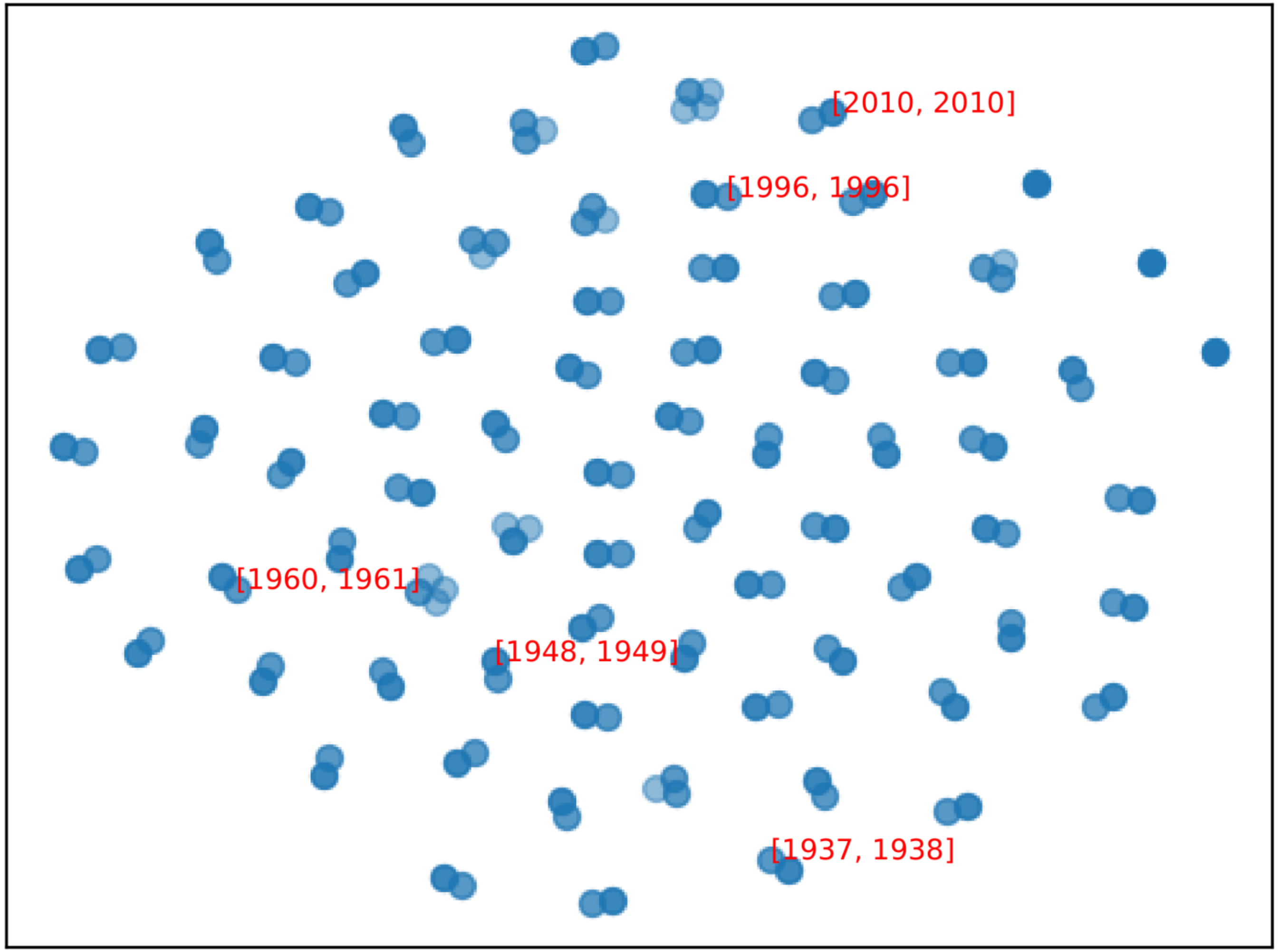
Case study of qualitative analysis on relation prediction. The order of prediction is in descending order. Correct one is in **bold**.

Test quadruples	HyTE	Ours
Katie_Holmes, ?, Tom_Cruise, [2006, 2012]	**isMarriedTo**, hasWonPrize	**isMarriedTo**, created
Tricia_Devereaux, ?, Illinois, [1975, 1975]	diedIn, **wasBornIn**	**wasBornIn**, diedIn
Jeremy_Lloyd, ?, London, [2014, 2014]	wasBornIn, **diedIn**	**diedIn**, wasBornIn
Will_Haining, ?, Fleetwood_Town_F.C., [2011, -]	isMarriedTo, **playsFor**	**playsFor**, isMarriedTo
Bob_Hope, ?, Toluca_Lake,_Los_Angeles, [2003, 2003]	isMarriedTo, hasWonPrize	isMarriedTo, **diedIn**

- Experiments

➢ Visualization

Visualization of polynomial decomposition based temporal representations on YAGO11k.



• Conclusion

- We propose an innovative temporal knowledge graph embedding method, namely PTBox. Experimental results verify the state-of-the-art performance of our method on two publicly available datasets.

- Proposing an interpretable time representation method that decomposes time information by polynomial approximation theory to flexibly represent arbitrary timestamp.

- Proposing a box-embedding-based entity representation method that effectively represents calibrated probability distributions and learns rigid inference patterns.

THANK YOU FOR LISTENING!