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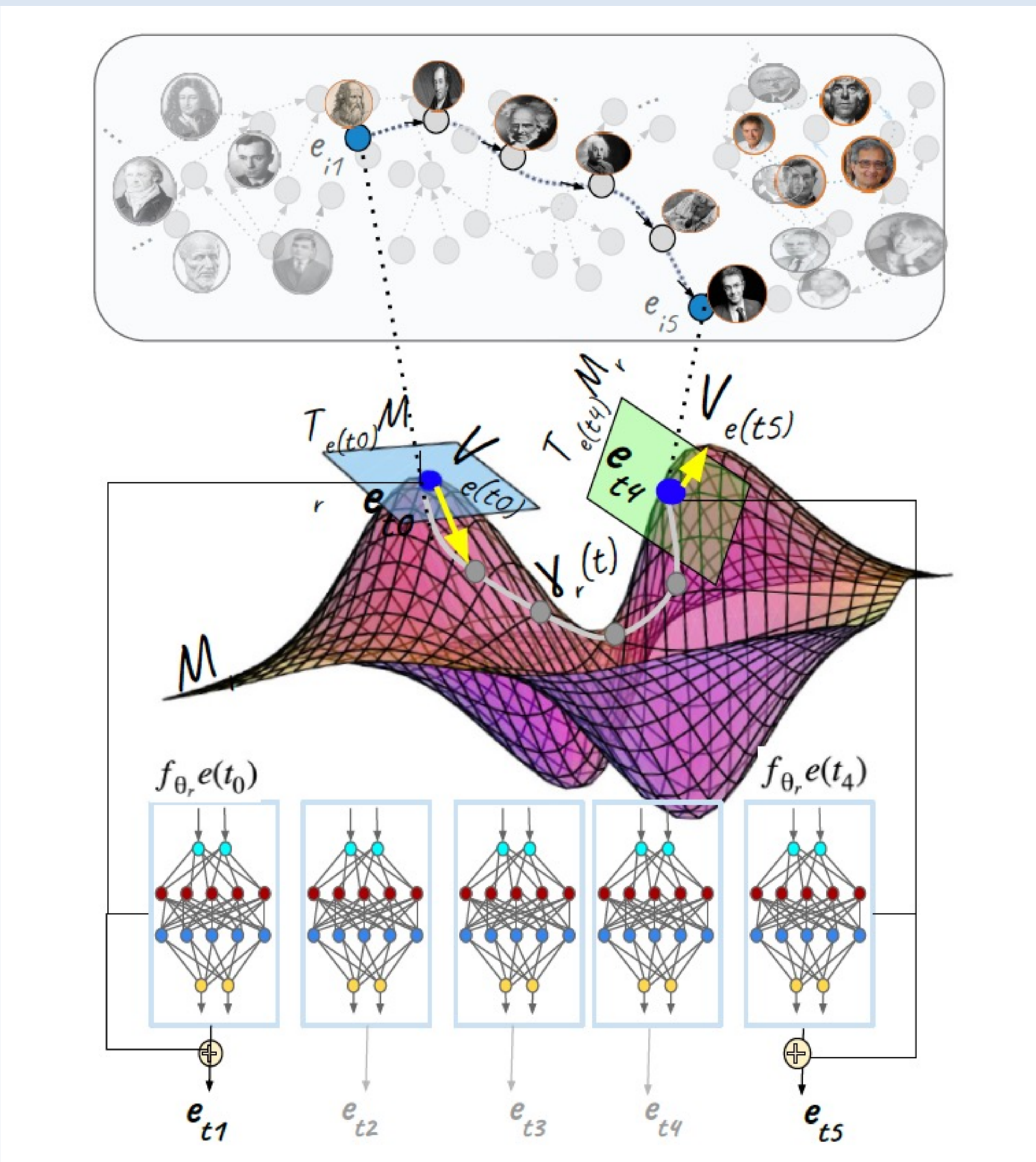
Temporo-relational Vector Field for Temporal Knowledge Graph Embedding

Introduction

Most real-world events evolve in time, which create the need to reasoning events' transition over time. To address this problem, many temporal knowledge graphs (TKGs), such as ICEWS and GDELT, which contain time information for each fact have been proposed. These datasets greatly facilitate the development of temporal knowledge graph embedding. However, most of current temporal knowledge graph embeddings embed time information as discrete timeslip and neglect the continuity of time information. To this end, we view entity representation transition between consecutive timeslips as timewise trajectories and relations between subject/object entities as relationwise trajectories. We represent each trajectories in a KG as a vector field on several manifolds. By specifically parameterizing ODEs with neural networks, the underlying embedding space is capable to represent various geometric forms for heterogeneous subgraphs and temporal information evolution.

Trajectory representation: vector field



- Given a smooth manifold $\mathcal{M}$:
- Its tangent space $\mathrm{T}_p\mathcal{M} \subset \mathbb{R}^n$ are all possible directions that a particle passing a given point may go. It is the set of all the vectors which are tangent to all the continuously differentiable curves passing through the given point p.
- For the given point p , its vector Field $f: \mathcal{M} \rightarrow \mathrm{T}\mathcal{M}$: defines trajectories $\gamma(t)$ via the ODE: $\frac{d\gamma(t)}{dt} = f(\gamma(t))$

Neuro-FieldE

Each trajectory (relation or timewise transition) can be seen as a vector field $f_\theta(e)$. It could be represented by differential of entity representation transition:

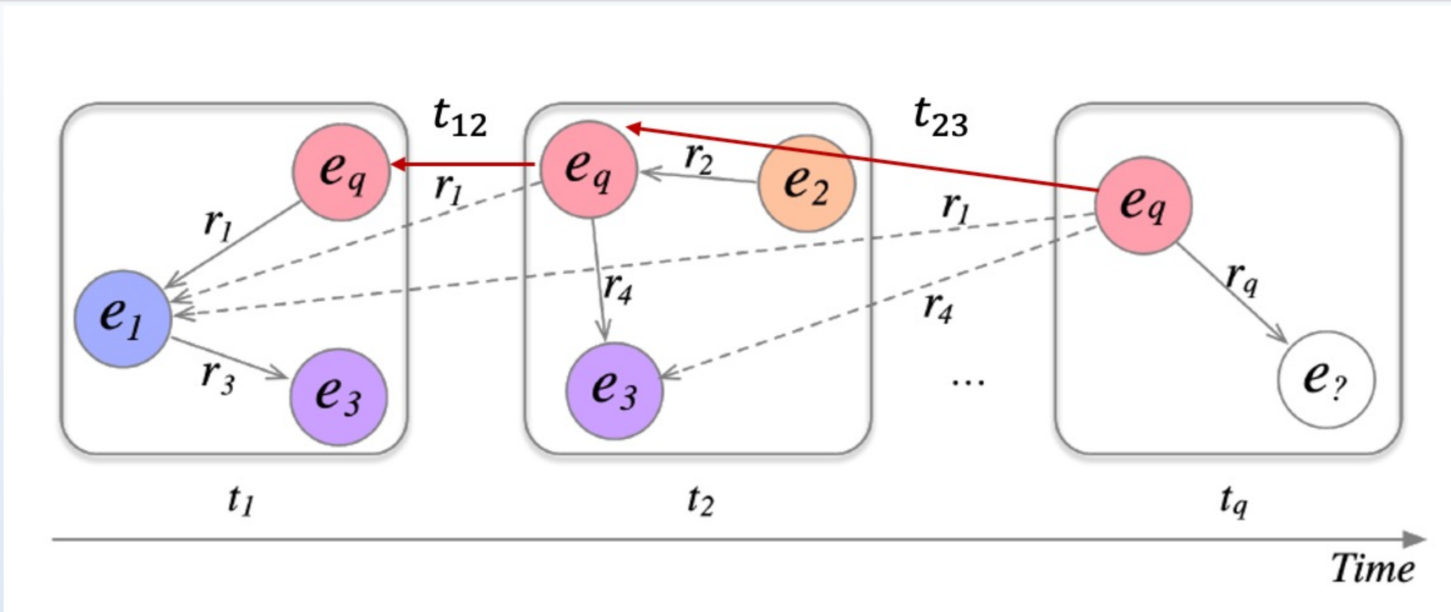
$$\frac{de(t)}{dt} = f_\theta(e(t)), e(t) \in \mathcal{M}$$

The vector field is parameterized by a multi-layer feedforward NN to approximate the underlying vector field.

$$f_{\theta_r}(e) = \sum w_i^o z\left(\sum w_{ij}^L z\left(\sum w_{jk}^{L-1} z\left(\cdots \sum w_{pq}^2 z(w_{qz}^1 e + b_z^1)\right)\right)\right)$$

Euclidean space: $e_2^{t_k} = e_1^{t_k} + f_{\theta_r}(e_1^{t_k}) \quad e_1^{t_{k+1}} = e_1^{t_k} + f_{\theta_t}(e_1^{t_k})$

Methodology



- A Temporal Knowledge Graph $\mathcal{K}$ consists of a set of quadruplet $(e_1, \boldsymbol{r}, e_2, \mathbf{t}) \in \mathcal{K}$ where $e_1, e_2 \in \boldsymbol{\mathcal{E}}, r \in \boldsymbol{\mathcal{R}}, \boldsymbol{t} \in \boldsymbol{T}$ denote the subject entity, the object entity, relation and time, respectively.

- **Entity Embedding from Timewise Rotation**: To relieve the memory cost of incursive entity representation computing, we introduce an additional Time Embedding T^{n*d}, where n is the number of timesteps and d is embedding space. The time-dependent entity representation is calculated by timewise rotation.
- $e_1^{t_{k-1}} = e_1 \circ t_{k-1}$
- $e_2^{t_{k-1}} = e_2 \circ t_{k-1}$

- **Entity Embedding from Time ODE**:
- $e_1^{t_k} = e_1^{t_{k-1}} + f_t(e_1^{t_{k-1}})$
- $e_2^{t_k} = e_2^{t_{k-1}} + f_t(e_2^{t_{k-1}})$

- **Score function from Relation ODE**:
- $f(e_1, r, e_2, t) = -\|e_1^{t_k} + f_r(e_1^{t_k}) - e_2^{t_k}\|$

- **Regularization between Time Rotation and Time ODE**:
- $\mathcal{R}_{1t_k} = \|e_1^{t_k} - e_1 \circ t_k\| \qquad \mathcal{R}_{2t_k} = \|e_2^{t_k} - e_2 \circ t_k\|$

- **Loss function**

$$\mathcal{L} = \log\sigma(f(e_1, r, e_2, t)) + \frac{1}{k}\sum_{i=1}^{k} \log\left(1 - \sigma(f(e_1, r, e_2, t))\right) + \alpha\mathcal{R}_{1t_k} + \beta\mathcal{R}_{2t_k}$$

Experiments

- **Link prediction results on ICEWS14**

Embedding Dimension	MRR	Hits@1	Hits@3	Hits@10
Dim = 50	0.426	0.332	0.469	0.609
Dim = 100	0.454	0.355	0.507	0.637
Dim = 200	0.493	0.397	0.549	0.675
Ablation Study	MRR	Hits@1	Hits@3	Hits@10
w/o Regularizer	0.287	0.170	0.343	0.513
w/o TimeODE	0.426	0.319	0.479	0.631
w/o RelODE	To be continued			

Next Step

- Extending from Euclidean Space to Hyperbolic Space as relevant paper[2] shows that embeddings under Hyperbolic Space have better performance
- Experimenting with new entity representation method
- Hyperparameter searching
- Adopting transition matrix to predict Time ODE parameters in future timesteps for future link prediction

References

1. Nayyeri M, Xu C, Hoffmann F, et al. Knowledge Graph Representation Learning using Ordinary Differential Equations[C]//Proceedings of the 2021 Conference on Empirical Methods in Natural Language Processing. 2021: 9529-9548.
2. Han Z, Ma Y, Chen P, et al. Dyernie: Dynamic evolution of riemannian manifold embeddings for temporal knowledge graph completion[J]. arXiv preprint arXiv:2011.03984, 2020.