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Improving Temporal Knowledge Graph Forecasting via Multi-Rewards Mechanism and Confidence-Guided Tensor Decomposition Reinforcement Learning

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Outline

Introduction

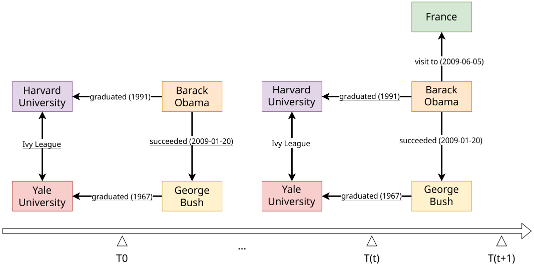


Figure: Example of Part of Temporal Knowledge Graph.

- In practice, data change over time.
- Reasoning problem on Temporal Knowledge Graph (TKG) can viewed in two settings:
  - Interpolation which focusing on completing the missing links at past timestamps.
  - Extrapolation which focusing on forecasting future facts.

$\Rightarrow$ We mainly focus on extrapolation setting.

Static & Temporal Knowledge Graph Reasoning

Table: Path-based Reasoning models for Static & Temporal Knowledge Graph

Method	Future timestamps	Unseen entities	Efficient	Explanatory	Reward Flexible	Action Selection	Open Source
MINERVA [20]	x	x	✓	x	x	x	✓
Multi-hop KG [19]	x	✓	✓	x	x	x	✓
RE-NET [16]	✓	x	x	x	x	x	✓
CyGNett [9]	✓	x	✓	x	x	x	✓
TANGO [6]	✓	x	x	x	x	x	✓
TAgent [8]	✓	x	x	x	x	x	x
TITer [7]	✓	✓	✓	✓	x	x	✓
TPath [3]	✓	x	✓	x	x	x	x
DREAM [2]	✓	x	x	x	✓	x	x
RLAT [1]	✓	x	x	x	x	x	x

Challenges in RL for TKG Reasoning

General, when compared to interpolation, extrapolation setting is more difficult and challenging. Recently, path-based reasoning methods are potential solutions for this setting and face two challenges:

- The reward function is a critical component for the agent. Most current works focus on constructing a binary global reward function, which makes the agent's learning process inflexible.
- The action space for the agent is too large, and there is limited research on how to select appropriate actions for the agent.

Our contributions

- Proposing a new multi-reward function, incorporating various reward criteria for the agent.
- Incorporating Tensor decomposition architectures such as TuckER, ComplEx, and LowFER with MLP and KAN-Policy Network to generate reliability scores for actions.
- Performing experiments and ablation study on standard datasets for the future link prediction task with improvements on metrics.

Outline

Basic Notations

- Let $\mathcal{E}$, $\mathcal{R}$, $\mathcal{T}$, and $\mathcal{Q}$ denote the sets of entities, relations, timestamps and quadruples.
- Each quadruplet in TKG can be defined as a tuple (e_s, r, e_o, t).

Problem Statement

Considering TKG as $\mathcal{G}_{(1,T)} = \{\mathcal{G}_1, \mathcal{G}_2, ..., \mathcal{G}_T\}$, where $\mathcal{G}_t = \{\mathcal{E}_t, \mathcal{R}, \mathcal{Q}_t\}$ is a static multi-relational graph, and $\mathcal{E}_t$ and $\mathcal{Q}_t$ denote entities and facts that exist at time t.

- Input: with given a query $(e_q, r_q, ?, t_q)$ or $(?, r_q, e_q, t_q)$, and a set of known facts $\{(e_{s_i}, r_i, e_{o_i}, t_i) | t_i < t_q\}$
- Output: potential candidates which can replace the missing object or subject entity in the input query.

RL Framework for TKG reasoning

Mains components in framework are:

- States: Let $\mathcal{S}$ as state space, each state can represent as $s_\ell = (e_{(\ell)}, t_{(\ell)}, e_q, t_q, r_q) \in \mathcal{S}$.
- Actions: Let $\mathcal{A}$ be the action space. Set of actions for step ℓ is $\mathcal{A}_\ell = \{(r', e', t') | (e_l, r', e', t') \in \mathcal{Q}, t' \leq t_l, t' < t_q\}$ which implies outgoing edges of the current node of agent.
- Transition function $\xi : \mathcal{S} \times \mathcal{A} \rightarrow \mathcal{S}$ defined by:

$$(s_\ell, \mathcal{A}_\ell) \mapsto (e_{\ell+1}, t_{\ell+1}, e_q, t_q, r_q) = s_{\ell+1} \tag{1}$$

  which transfer the environment state to a new node through edge selected by agent.
- Reward function: Commonly, binary global reward function is defined by:

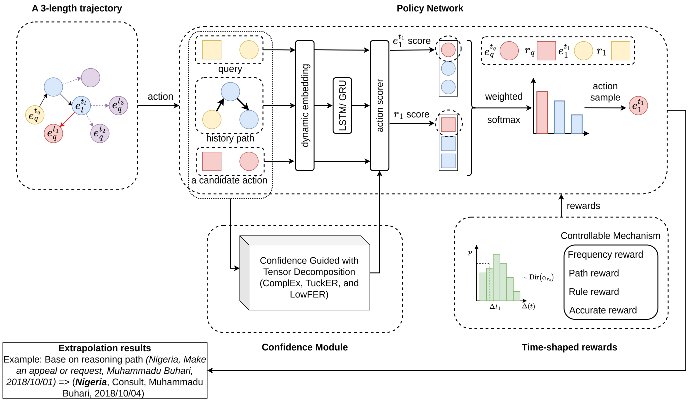
$$R_{bin}(s_L) = \mathbb{I}(e_l == e_{gt}), \tag{2}$$

  where $\mathbb{I}(.)$ is a function that return 1 or 0.

Outline

Overview of our proposed model CATTer

Inspired by path-based methods for static & temporal KGs, we propose new temporal path-based reinforcement learning for extrapolated TKG reasoning with two advances: 1) multi-reward function and 2) confidence-guided policy network.



Overview of our proposed model CATTer

Following TITer, there is no edge between snapshots, so we add three types of edges:

1. Reversed edges
2. Self-loop edges
3. Temporal Edges

Multi-reward Mechanism with Rule Enhancing

We proposed new multi-reward function:

$$\mathsf{R} = (1 + \alpha_1 \mathsf{R}_{\mathsf{gt}})(1 + \alpha_2 \mathsf{R}_{\mathsf{rule}})(\mathsf{R}_{\mathsf{bin}} + \alpha_3 \mathsf{R}_{\mathsf{path}}), \tag{3}$$

where $\mathsf{R}_{\mathsf{bin}}$ is binary reward, R_{gt} is (adjusted) ground truth frequency reward, $\mathsf{R}_{\mathsf{rule}}$ is high-frequency rule reward, $\mathsf{R}_{\mathsf{path}}$ is (adjusted) path length reward, and $\alpha_1 \in (0, 1)$, $\alpha_2 \in (0, 1)$, and $\alpha_3 \in (0, 1)$ are weights.

Binary global reward

The *binary global reward* that is defined by:

$$\mathsf{R}_{bin}(s_L) = \mathbb{I}(e_\ell == e_{gt}). \tag{4}$$

Adjusted ground truth frequency reward

With given (e_q, r_q, e_{gt}, t_q), $N_{\text{gt}} = \{n_1, n_2, \ldots, n_m\}$ denote the number of times that the e_{gt} occur in m snapshot $\{G_{t_q-1}, G_{t_q-2}, \ldots, G_{t_q-m}\}$, i.e., $n_i, (i = 1, \ldots, m)$ is the number of times that e_{gt} occurs in subgraph G_{t_q-i}. We expect the e_{gt} should occur maximum as possible

We define the ground truth frequency reward as follows:

$$\mathsf{R}_{\text{gt}}(s_L) = \begin{cases} f_i, & \text{if } t_{q-m} \le t_i \le t_q, \\ 0, & \end{cases} \tag{5}$$

where

$$f_i = \frac{n_i}{\max(N_{\text{gt}}) - \min(N_{\text{gt}})}. \quad \text{(normalized by max and min)}$$

Adjusted path length reward

We expect the path length to e_{gt} should be minimum as possible. So, we proposed *adjusted path length reward* which can be defined as:

$$\mathsf{R}_{\mathsf{path}}(s_L) = \frac{w_{\mathsf{path}}}{p_\ell - 1} \tag{6}$$

where $p_\ell \leq p_{\max}$ denotes the length of the path taken by the agent to capture the target entity from the source node at step ℓ, $p_{\max}$ is the maximum path length which agent can reach a node, and $w_{\mathsf{path}} \in (0, 1)$ is the weight for current path length which is taken.

Note that: minus one in denominator means to accelerate our expectations.

High-frequency rule reward

In our observations, knowledge graphs usually contain a pair entity relation, frequently appearing in the timelines.

Formally, given a common pair entity-relation set, which is denoted as $\mathsf{ER} = \{(e_i, r_i)\}_{i=1}^{k}$. Each pair in ER has a frequency of occurrence greater than or equal to a threshold ϑ depending on the dataset. Then, we define a *high-frequency rule reward* for our agent as follows:

$$\mathsf{R}_{\mathsf{rule}}(s_L) = \begin{cases} w_{\mathsf{rule}}, & \text{if } (e_\ell, r_\ell) \in \mathsf{ER}, \\ 0, & \text{otherwise} \end{cases} \tag{7}$$

where w_{rule} is reward value for matching rule.

Multi-reward reshaping

Based on the training set, we estime a Dirichlet Distribution for each relation. Then, we reshape the original multi-reward with this distribution:

$$\begin{aligned} \widetilde{R}(s_L) &= (1 + p_{\Delta t_L} R(s_L) \\ \Delta t_L &= t_q - t_L \\ (p_1, \ldots, p_k) &\sim \text{Dirichlet}(\boldsymbol{\alpha}_{r_q}), \boldsymbol{\alpha}_{r_q} \in \mathbb{R}^K \end{aligned} \tag{8}$$

Policy Network

- Dynamic Embedding. Relative time encoding function to represent time information.

$$\mathbf{\Phi}(t_q - t) = \sigma(\mathbf{w}\Delta t + \mathbf{b}) = \mathbf{\Phi}(\Delta t); \tag{9}$$

$$\mathbf{e}_i^t = [\mathbf{e}_i; \mathbf{\Phi}(\Delta t)] \tag{10}$$

- Historical Path Encoding. We use LSTM/ GRU to encode the search history which is the sequence of actions taken.

$$\begin{aligned} \mathbf{h}_\ell^{\mathsf{gru}} &= \mathsf{GRU}([\mathbf{r}_{\ell-1}; \mathbf{e}_{\ell-1}^{t_{\ell-1}}], \mathbf{h}_{\ell-1}), \\ \mathbf{h}_0^{\mathsf{gru}} &= \mathsf{GRU}([\mathbf{r}_0; \mathbf{e}_q^{t_q}, \mathbf{0}]). \end{aligned} \tag{11}$$

with $\mathbf{r}_0$ is dummy relation for initialization. Similar if we use LSTM.

Policy Network

- Action scoring. We use a weighted action scoring to help agent pay more attention to attributes of destination nodes.

$$\phi(a_n, s_\ell) = \beta_n \left\langle \widetilde{\mathbf{e}}, \mathbf{e}_n^{t_n} \right\rangle + (1-\beta_n) \left\langle \widetilde{\mathbf{r}}, \mathbf{r}_n \right\rangle, \tag{12}$$

with

$$\begin{aligned}
\widetilde{\mathbf{e}} &= \mathbf{W}_e \mathsf{ReLU}(\mathbf{W}_1[\mathbf{h}_\ell^{\mathsf{lstm/gru}}; \mathbf{e}_q^{t_q}; \mathbf{r}_q]),\\
\widetilde{\mathbf{r}} &= \mathbf{W}_r \mathsf{ReLU}(\mathbf{W}_1[\mathbf{h}_\ell^{\mathsf{lstm/gru}}; \mathbf{e}_q^{t_q}; \mathbf{r}_q]),\\
\beta_n &= \mathsf{sigmoid}(\mathbf{W}_\beta[\mathbf{h}_\ell^{\mathsf{lstm/gru}}; \mathbf{e}_q^{t_q}; \mathbf{r}_q; \mathbf{e}_n^{t_n}; \mathbf{r}_n]),
\end{aligned}$$

where $\mathbf{W}_1$, $\mathbf{W}_e$, $\mathbf{W}_r$ and $\mathbf{W}_\beta$ are trainable parameters for MLP or KAN.

Policy Network

- Confidence Rate Action Calculation. We calculate the confidence rate $c_{a_n|q}$ of each $a_n \in \mathcal{A}_\ell$ via softmax function which receive the input vector from tensor decomposition such as TuckER [15], ComplEx [22], and LowFER [11] as follow:

$$c_{a_n|q} = \frac{\exp(\psi_{a_n|q})}{\sum_{a'_\ell \in A_\ell} \exp(\psi_{a'_\ell|q})}, \tag{13}$$

where

$$\psi_{a_n|q} = \mathcal{W} \times_1 \mathbf{e}_q^{t_q} \times_2 \mathbf{r}_q \times_3 \mathbf{e}_n^{t_n}, \text{ if use TuckER,}$$
$$\psi_{a_n|q} = \mathrm{Re}\left(\left\langle \mathbf{e}_q^{t_q}, \mathbf{r}_q, \overline{\mathbf{e}_n^{t_n}} \right\rangle\right) \text{ if use ComplEx,}$$
$$\psi_{a_n|q} = (\mathbf{S}^k \mathrm{diag}(\mathbf{U}^\top \mathbf{e}_q^{t_q}) \mathbf{V}^\top \mathbf{r}_q)^\top \mathbf{e}_n^{t_n}, \text{if use LowFER,}$$

Policy Network

- The policy $\pi_\theta(a_\ell \mid s_\ell)$ at step ℓ is defined as:

$$\pi_\theta(a_\ell \mid s_\ell) = \frac{\exp(\phi(a_\ell, s_\ell) * c_{a_\ell|q})}{\sum_{a'_\ell \in \mathcal{A}_\ell} \exp(\phi(a'_\ell, s_\ell) * c_{a'_\ell|q})} \tag{14}$$

Optimization

We apply REINFORCE algorithm [27] that will iterate through all quadruple in $\mathcal{Q}_{train}$ and update θ with the following stochastic gradient method such as SGD [21], Adam [21, 24] or AdaGrad [26]:

$$\nabla_\theta J(\theta) \approx \nabla_\theta \sum_{m \in [1,L]} \widetilde{R}(s_L | e_s, r, t) \log \pi_\theta(a_\ell | s_\ell) \tag{15}$$

Outline

Datasets and Baselines

- Baselines.
  1. Interpolation-based models: TTransE [18], TA-DistMult [17], DE-SimplE [12], and TNTComplEx [14].
  2. Extrapolation-based models: RE-NET [13], CyGNet [10], TANGO [4], xERTE [5], and TITer [7].
- Datasets. ICEWS14 and ICEWS18 [23], WIKI [18] and YAGO [25].

Performance and efficiency comparison

Method	ICEWS14				ICEWS18			
	MRR ↑	Hit@1 ↑	Hit@3 ↑	Hit@10	MRR ↑	Hit@1 ↑	Hit@3 ↑	Hit@10 ↑
TTransE	13.43	3.11	17.32	34.55	8.31	1.92	8.56	21.89
TA-DistMult	26.47	17.09	30.22	45.41	16.75	8.61	18.41	33.59
DE-SimplE	32.67	24.43	35.69	49.11	19.30	11.53	21.86	34.80
TNTComplEx	32.12	23.35	36.03	49.13	27.54	19.52	30.80	42.86
CyGNet	32.73	23.69	36.31	50.67	24.93	15.90	28.28	42.61
RE-NET	38.28	28.68	41.34	54.52	28.81	19.05	32.44	**47.51**
xERTE	40.79	32.70	45.67	57.30	29.31	21.03	**33.51**	46.48
TANGO-Tucker	–	–	–	–	28.68	19.35	32.17	47.04
TANGO-DistMult	–	–	–	–	26.75	17.92	30.08	44.09
TITer	**41.73**	**32.74**	**46.46**	**58.44**	**29.98**	**22.05**	33.46	44.83
TITer*	40.33	31.00	45.30	57.71	29.42	21.63	32.83	43.96
CATTer-MLP	41.21	32.47	45.75	57.37	29.54	21.60	32.99	44.51
CATTer-KAN	40.13	31.04	44.80	57.19	29.11	21.37	32.46	43.60
APG (%) ↑ (MLP)	**0.62**	**0.54**	**0.61**	**0.64**	**-0.22**	**-0.39**	**-0.02**	**0.03**
RPG (%) ↑ (MLP)	**2.18**	**4.74**	**0.99**	**-0.59**	**0.41**	**-0.14**	**0.49**	**1.25**
APG (%) ↑ (KAN)	**0.65**	**0.48**	**0.77**	**0.92**	**-0.61**	**-0.68**	**-0.54**	**-0.53**
RPG (%) ↑ (KAN)	**-0.49**	**0.13**	**-1.10**	**-0.90**	**-1.05**	**-1.20**	**-1.13**	**-0.82**

Performance and efficiency comparison

Method	WIKI				YAGO			
	MRR ↑	Hit@1 ↑	Hit@3 ↑	Hit@10	MRR ↑	Hit@1 ↑	Hit@3 ↑	Hit@10 ↑
TTransE	29.27	21.67	34.43	42.39	31.19	18.12	40.91	51.21
TA-DistMult	44.53	39.92	48.73	51.71	54.92	48.15	59.61	66.71
DE-SimplE	45.43	42.6	47.71	49.55	54.91	51.64	57.30	60.17
TNTComplEx	45.03	40.04	49.31	52.03	57.98	52.92	61.33	66.69
CyGNet	33.89	29.06	36.10	41.86	52.07	45.36	56.12	63.77
RE-NET	49.66	46.88	51.19	53.48	58.02	53.06	61.08	66.29
xERTE	71.14	68.05	76.11	79.01	84.19	80.09	88.02	89.78
TANGO-Tucker	50.43	48.52	51.47	53.58	57.83	53.05	60.78	65.85
TANGO-DistMult	51.15	49.66	52.16	53.35	62.70	59.18	60.31	67.90
TITer	**75.50**	**72.96**	**77.49**	**79.02**	87.47	84.89	**89.96**	90.27
TITer*	73.56	71.48	74.86	76.40	87.80	85.52	89.92	90.31
CATTer-MLP	74.18	72.02	75.47	77.04	**87.58**	**85.13**	89.90	**90.34**
CATTer-KAN	74.21	71.96	75.63	77.32	87.19	84.84	89.38	89.78
APG (%) ↑ (MLP)	**0.88**	**1.47**	**0.45**	**-0.34**	**0.12**	**-0.03**	**0.16**	**0.55**
RPG (%) ↑ (MLP)	**0.84**	**0.76**	**0.81**	**0.83**	**-0.25**	**-0.46**	**-0.02**	**0.03**
APG (%) ↑ (KAN)	**-0.2**	**0.04**	**-0.5**	**-0.52**	**-0.31**	**-0.26**	**-0.37**	**-0.36**
RPG (%) ↑ (KAN)	**0.88**	**0.67**	**1.03**	**1.20**	**-0.69**	**-0.80**	**-0.60**	**-0.59**

Performance and efficiency comparison

Table: Number of trainable parameters and calculation of our proposed models and baselines. MACs stand for Multi-Adds operations, and M stand for million.

Method	# Params	# MACs
RE-NET	5.459M	4.370M
CyGNet	8.568M	8.554M
xERTE	2.927M	225.895M
TITer	1.455M	0.225M
CATTer	1.425M	0.220M

Convergence Study

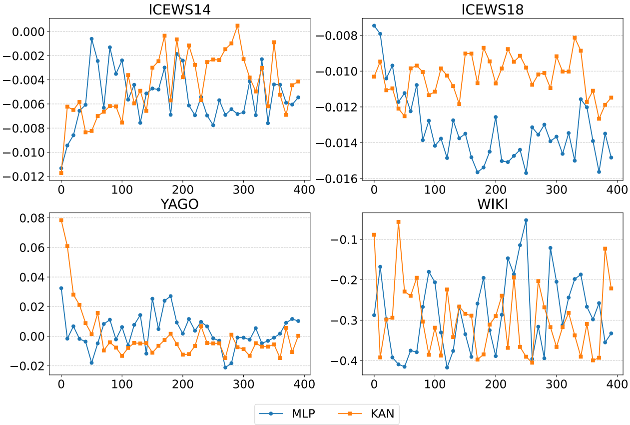


Figure: The change of the loss function over each epoch with MLP and KAN Policy Network.

Convergence Study

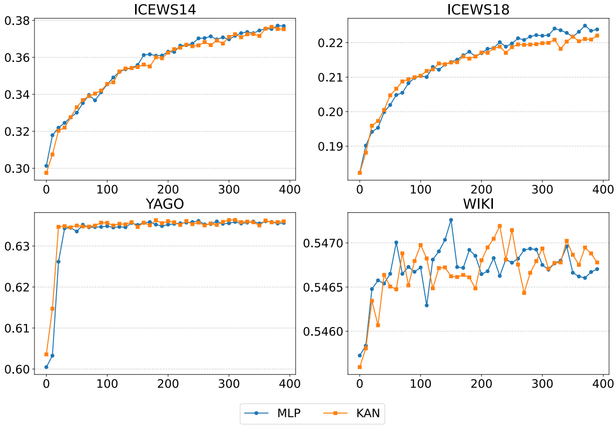
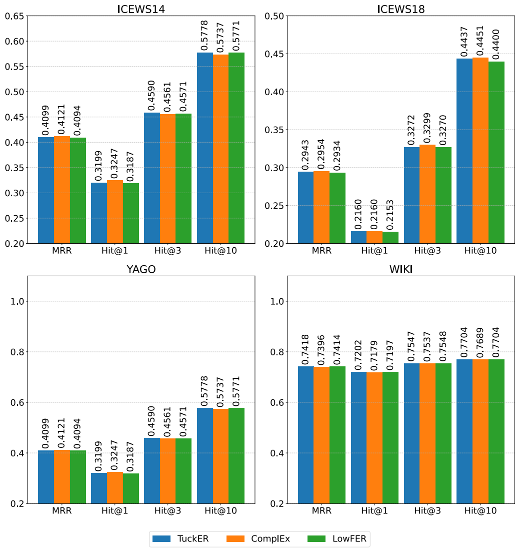


Figure: The change of the multi-reward function over each epoch with MLP and KAN Policy Network.

The Effect of Tensor decomposition methods for action confidence



The effect of multi-rewards

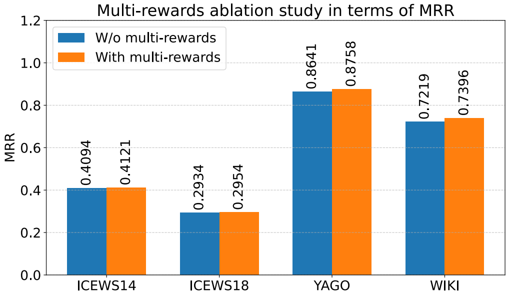


Figure: The effect of multi-reward mechanism for agent learning on ICEWS14, ICEWS18, YAGO and WIKI dataset.

Outline

Conclusion

- Introduces CATTer, an improved temporal-path-based RL model based on TimeTraveler.
- Integrates confidence probability into MLP and KAN layers.
- Designs a flexible Policy Network for better action selection.
- Employs a multi-reward function for improved adaptability in TKGs.
- Experimental results show enhanced future link prediction.
- Future work: Incorporating sub-graph patterns and temporal rules.

Thanks for your attention

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