APPTeK: Agent-Based Predicate Prediction in Temporal Knowledge Graphs

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Abstract

In temporal Knowledge Graphs (tKGs), the temporal dimension is attached to facts in a knowledge base resulting in quadruples between entities such as (Nintendo, released, Super Mario, Sep-13-1985), where the predicate holds within a time interval or at a timestamp. We propose a reinforcement learning agent gathering temporal relevant information about the query entities’ neighborhoods, simultaneously. We refer to the encodings of the explored graph structures as fingerprints which are used as input to a Q-network. Our agent decides sequentially which relation type needs to be explored next to expand the local subgraphs of the query entities. Our evaluation shows that the proposed method yields competitive results compared to state-of-the-art embedding algorithms for tKGs, and we additionally gain information about the relevant structures between subjects and objects.

1 Introduction

The task of Knowledge Graph Completion (KGC) is about adding missing facts, and a plethora of methods have been proposed for this task (Wang et al., 2014; Lao et al., 2011; Lin et al., 2018; Shen et al., 2018; Das et al., 2017; Xiong et al., 2017; Chen et al., 2018). In general, there are two ways to complete a knowledge graph. The entity prediction task aims at retrieving all entities w.r.t a query predicate. In contrast, the predicate prediction task is: given two entities, predict the type of relationship holding between these entities (Onuki et al., 2019; Guo et al., 2019; Teru et al., 2020).

A property of most knowledge bases is that facts change over time. For example, the triples (Barack Obama, is_president_of, USA) and (Donald Trump, is_president_of, USA) both held in the past but are now invalid. To be able to represent changing facts over time correctly, KGs have been extended to temporal Knowledge Graphs (tKGs). In particular, each fact in a tKG is complemented by the time the fact was valid. In recent research, it has been shown that methods for static KGs are not always feasible for tKGs (Leblay and Chekol, 2018; García-Durán et al., 2018; Dasgupta et al., 2018), and thus, new methods are needed for completion.

In this paper, we propose a novel technique for predicate prediction on tKGs, i.e., queries have the form (subject, ?, object, timestamp). The idea of our method is to train a reinforcement learning (RL) agent that actively gathers information about the relation of subject and object at a given time. This information is represented as a so-called topology and technically corresponds to a subgraph of the tKG. Topologies can be used in a downstream task as input to a classifier for predicting the relation types holding between entities. Furthermore, in contrast to embedding models yielding low-dimensional vector representations, topologies can be visually analyzed to give human users an insight into how two entities are connected.

Though there exist several methods for completing static knowledge graphs based on RL (Das et al., 2018; Lin et al., 2018; Shen et al., 2018; Fu et al., 2019), our method shows significant differences. First, previous RL approaches rely on finding paths between subject and object. In contrast, our agent is based on topologies that generalizes in the sense that several paths between entities can be found at once. The agent’s training procedure employs Q-Learning where encodings (fingerprints) of the explored topologies are used as input. Furthermore, our agent employs a bidirectional search that simultaneously gathers information about both query entities. Finally, as we focus on predicate prediction instead of entity prediction, we only need to train a single agent for all relation types, whereas previous RL methods need to train a dedicated agent for each relation type (Xiong et al., 2017). We compare our method, called APPTeK, with KGC techniques for tKGs on three open benchmark datasets in our experiments.
and demonstrate its benefits. The contributions of this paper are:

- A predicate prediction method for tKGs that is based on topologies instead of paths.
- An RL agent that is trained to find these topologies for a given pair of query entities.
- An empirical evaluation of the advantages of our approach on three benchmark tKGs.

2 Related Work

We provide an overview of related works in the field of i) Reasoning on Static Knowledge Graphs, and ii) Reasoning on Temporal Knowledge Graphs.

i) In DeepPath (Xiong et al., 2017), the authors merged ideas from path-based and embedding-based reasoning with deep RL. In (Chen et al., 2018), the authors introduced DIVA that bridges path finding and reasoning with variational inference. For fact prediction, MINERVA (Das et al., 2018) takes path walking to the correct answer entity as a sequential optimization problem by maximizing the expected reward. In order to tackle the sparsity reward problem, the authors of (Lin et al., 2018) propose a soft reward mechanism instead of using a binary reward function. In M-Walk (Shen et al., 2018), the model applies a RNN controller to capture the historical trajectory and uses Monte Carlo Tree Search (MCTS) for effective path generation. MemoryPath (Li et al., 2021a) has been proposed as another RL-motivated approach leveraging LSTMs and graph attention mechanisms to form memory components.

All of the proposed RL approaches for static KGs aim at the entity prediction task and are not applicable to predicate prediction. Additionally, all of the methods listed above disregard the temporal aspect.

ii) Reasoning on tKGs are categorized into interpolation and extrapolation methods (Jin et al., 2020). Whereas the former tries to infer missing historical facts (Wu et al., 2020; Xu et al., 2020; Jung et al., 2021; Bai et al., 2021b; Xu et al., 2021), the latter tries to predict facts that will hold in the future (Han et al., 2020; Jin et al., 2020; Zhu et al., 2021; Deng et al., 2020; Sun et al., 2021; Li et al., 2021b; Bai et al., 2021a). CyGNet (Zhu et al., 2021) and RE-NET (Jin et al., 2020) proposed methods for the entity prediction task by encoding historical facts related to the subject entity into the query. In (Li et al., 2021c), an RE-GCN embedding model is proposed that incorporates an evolution unit, enabling both, entity and predicate prediction. Some approaches are built upon formerly introduced heuristics on static KGs, like TTransE (Leblay and Chekol, 2018), TA-TransE (García-Durán et al., 2018), and HyTE (Dasgupta et al., 2018), which are based on the translation-based method TransE (Bordes et al., 2013). Extensions of DistMult (Yang et al., 2015) are defined by the models like TA-DistMult proposed in (García-Durán et al., 2018) or Know-Evolve (Trivedi et al., 2017). Also, the SimplE model (Kazemi and Poole, 2018) has been extended in (Goel et al., 2020) to DE-SimplE, which incorporates a dyachronic transformation function for including the temporal information in the latent embedding space. The same technique is also applied on TransE (Bordes et al., 2013) and DistMulti (Yang et al., 2015), resulting in the models DE-TransE, resp., DE-DistMulti.

Even though most of these methods have been introduced to solve the entity prediction task, we adopt several methods which currently represent the state-of-the-art in tKG completion to predicate prediction. Thus, we can compare our new agent-based approach to the most promising methods for KGC in temporal KGs. Details about the modifications are described in more detail in Sec. 4.

3 APPTeK - tKGR Agent

3.1 Preliminaries

A temporal Knowledge Graph (tKG) can be represented by a set of time-dependent facts \( \mathcal{G} = \{(u, r, v, t) | u, v \in \mathcal{E}, r \in \mathcal{R}, t \in \mathcal{T}\} \), where \( \mathcal{E} \) is a set of entities, \( \mathcal{R} \) is a set of relations and \( \mathcal{T} \) denotes the temporal domain. The components of a quadruple are denoted by a subject and an object entity \( u, v \in \mathcal{E} \) being linked by a semantic predicate \( r \in \mathcal{R} \) at a specific time \( t \in \mathcal{T} \). The latter can either describe a particular point in time or a time interval.

Next, we define the (interpolated) predicate prediction task in temporal Knowledge Graph Reasoning (tKGR) for knowledge graph completion (KGC).

**Definition 1** ((Interp.) Predicate Pred. in tKG)

Given a tKG and a query quadruple \( (u_q, ?, v_q, t_q) \), where \( ? \) is the unknown predicate, in a (interpolated) predicate prediction problem, we try to infer the relation types \( r_q \in \mathcal{R} \) holding between \( u_q \) and \( v_q \) at time \( t_q \) given the already known quadruples in the tKG.
3.2 MDP Formulation

In the following, we define the Markov Decision Process (MDP) for our setting. An MDP is defined by the tuple \((S, A, R, P)\), where \(S\) is the set of states, \(A\) is the set of actions, \(R\) is the reward function and \(P\) is the state transition function.

For the sake of brevity, we will use \(x\) to substitute \(\{u_q, v_q\}\) but emphasize that the single agent queries topologies always from both entities, simultaneously.

3.2.1 State Space \(S\)

The state comprises the topologies visited by the agent, i.e., the known part of the graph. Likewise to traditional graph expansion techniques, we distinguish between already visited entities and entities that can be explored next. We refer to them as the core and periphery information.

Considering the query entities \(x \in \{u_q, v_q\}\), we denote the core information of a topology as \(c^i_x\) and the periphery information as \(p^i_x\) in step \(i\).

Core Information. The core \(c^i_x\) comprises information about quadruples which have been visited by the agent. Technically, it is defined as a subgraph of the input tKG, i.e., \(c^i_x \subseteq G\).

Periphery Information. The periphery information \(p^i_x\) consists of quadruples \((u_p, r_p, v_p, t_p)\) where \(u_p\) is found in \(c^i_x\) but \(v_p\) is not. In addition, we also have to consider the temporal proximity of the fact time \(t_p\) to the query time \(t_q\).

Formally, the periphery is defined as follows: Let \(G = \{(u, r, v, t) | u, v \in \mathcal{E}, r \in \mathcal{R}, t \in \mathcal{T}\}\) be a tKG and let \(c^i_x\) be the core information at step \(i\), then the periphery \(p^i_x \subset G\) consists of the following tuples:

\[
p^i_x = \{(u_p, r_p, v_p, t_p) \in G \setminus c^i_x | \exists (u_c, r_c, v_c, t_c) \in c^i_x : (u_p = u_c \lor u_p = v_c) \land |t_q - t_p| < \Delta tknn\},
\]

where \(\Delta tknn\) is the \(k\)-nearest neighbor distance w.r.t. the query time \(t_q\).

We define the state \(s^i_x\) of each topology starting from \(x \in \{u_q, v_q\}\) at iteration \(i\) by joining the core (Eq. 5) and periphery (Eq. 1) information:

\[
s^i_x := c^i_x \cup p^i_x \tag{2}
\]

Finally, the overall state is defined as the union of both topologies. We define:

\[
S^i = \bigcup_{x \in \{u_q, v_q\}} s^i_x \tag{3}
\]

The intuition is that the proposed agent follows links not solely starting at one particular entity, which would result in single inference paths. Instead, the state space describes a set of quadruples comprising the local query entities’ information.

3.2.2 Action Space \(A\)

Generally, the set of feasible actions is defined as the set of relation types \(\mathcal{R}\) within the tKG, i.e., \(\mathcal{A} := \mathcal{R}\).

At iteration \(i\), it comprises all relation types included in the union of the periphery information of the topologies starting from \(u_q\) and \(v_q\):

\[
A^i := \{p_p | (u_p, r_p, v_p, t_p) \in \bigcup_{x \in \{u_q, v_q\}} p^i_x \} \tag{4}
\]

Example 1 Fig. 1 shows three steps with \(tknn = 2\) of the agent’s exploration. For a concise representation, we show the steps only for one query entity \(x \in \{u_q, v_q\}\). Starting from \(x\), the agent gathers incident relations (cond. i) fulfilling the temporal proximity (cond. ii)). Red crosses indicate relations being incident to one of the entities within the topology but can be pruned as they are not temporal nearest neighbors. For a query \(q = (u_q, ?, v_q, t_q)\), the agent chooses amongst \(|N_{tknn}(q)| = 2\) relations at step 1. The lighter (darker) areas highlight the periphery (core) information. Initially, the core information is the empty set. The agent’s actions are illustrated by green edges. Therefore, the agent iteratively learns more about an entity’s neighborhood.

3.2.3 Transition

The transition function \(tr : S \times A \rightarrow S\) is defined as \(tr(S^i, a^i) = (c^{i+1}_{u_q}, p^{i+1}_{u_q}, c^{i+1}_{v_q}, p^{i+1}_{v_q})\), where \(S^i\) denotes the state in the \(i\)-th iteration and \(a^i \in A^i\) denotes the action. In the following, the update procedures for the core and periphery information are unfolded in more detail:
Core. Initially, \( c_x^0 \) is empty. The information stored in \( c_x^i \) is extended iteratively with quadruples taken from \( p_x \) where the relation type matches the agent’s chosen action \( a^i \) in the \( i \)-th iteration. We define:
\[
c_x^i := \{ c_x^{i-1} \cup y^i \}, \quad c_x^0 := \emptyset, \quad \text{where } y^i = \{ q | \forall q = (u_p, r_p, v_p, t_p) \in p_x : r_p = a^i \}. \tag{5}
\]
Intuitively, \( y^i \) denotes the subset of quadruples for which the relation type matches the agent’s selected action \( a^i \). To conclude, \( c_x^i \) comprises for each iteration the history of all traversed facts.

Periphery. Subsequent to the update procedure of the core’s information according to Eq. 5, the update of the periphery is initiated. Intuitively, it is updated by quadruples being reachable by the updated core’s information such that Eq. 1 holds again.

3.2.4 Reward \( R \)
The agent receives a terminal reward of 1 if the query entities’ core information overlap in at least one entity, and 0 otherwise. All intermediate states receive a reward of 0. We define the reward as:
\[
\text{reward}^i = \mathbb{1}\{ \text{ent}(c_x^{i+1}) \cap \text{ent}(c_y^{i+1}) \}, \tag{6}
\]
where \( \text{ent}(\cdot) \) extracts the subject and head entities of quadruples.

An episode in this MDP ends after receiving a reward or performing a maximum of \( I \) steps. Each query \( (u_q, ?, v_q, t_q) \) might result in a different sequence of action or relation types which can be directly interpreted as reasoning sequence upon the \( tKG \). Furthermore, we can apply these reasoning sequences to any query tuple and receive a binary result if the path connects subject and object. Thus, using \( m \) reasoning sequences can be used to generate an \( m \)-dimensional binary feature vector which can be used in the downstream path of predicate prediction. For prediction, we use a linear layer with a successive softmax function for classification.

3.3 Model architecture
3.3.1 Calculating Fingerprints
On traversing the \( tKG \) starting from \( x \in \{ u_q, v_q \} \), the agent iteratively gathers information about their respective neighborhood. As discussed in Sec. 3.2, the current state \( s_x^i \) of \( x \) at iteration \( i \) is defined by a topology’s core information \( c_x^i \) and its periphery \( p_x^i \). The computation of the fingerprint translates the herein stored information about the relations and their respective timestamp into a \( d_f \)-dimensional vector. First of all, we apply an embedding layer \( \psi : r \rightarrow \mathbb{R}^{d_f} \) to represent the relations in \( s_x^i \), and correspondingly, an embedding layer \( \xi : t \rightarrow \mathbb{R}^{d_t} \) for the temporal information. Concatenating both embeddings, we receive the following matrix representation of \( s_x^i \):
\[
\mathbb{X}_{s_x^i} = \|0_{(u,r,v,t) \in s_x^i} (\psi(r) \parallel_1 \xi(t)) \|_l, \tag{7}
\]
where \( \parallel_l \) denotes the concatenation in the \( l \)-th dimension. Thus, \( \mathbb{X}_{s_x^i} \) has the shape \( |s_x^i| \times (d_r + d_t) \). Next, \( \mathbb{X}_{s_x^i} \) is fed into an MLP which generates a \( |s_x^i| \times d_f \)-dimensional vector. Finally, a max-pooling operation on the \( 0 \)-th dimension yields a \( d_f \)-dimensional fingerprint. We describe this non-linear transformation by \( \Phi : s_x \rightarrow \Phi(s_x) \in \mathbb{R}^{d_f} \). Finally, the overall low-dimensional state representation is defined as the concatenation of the query’s
subject and object representation:

\[ \tilde{s}^i := \Phi(s^i_{uq})||\Phi(s^i_{vq}) \]  

(8)

**Example 2** The calculation of a fingerprint is illustrated in Fig. (right). The core’s information of the topology (green) is concatenated with the relations’ information given in the periphery (red). The input to the MLP is provided by the concatenation of the relation embeddings with their respective temporal embeddings. Applying a maxpooling operation, the network yields the fingerprint \( \Phi_x \) of the observed topology.

### 3.3.2 Q-network

The RL frameworks in (Xiong et al., 2017; Das et al., 2018; Lin et al., 2018; Shen et al., 2018) have to handle large action spaces leading to problems whenever we lack training labels for multiple actions. Each of the earlier works proposes workarounds either by defining a more sophisticated reward function (Xiong et al., 2017; Lin et al., 2018) or by combining the learning procedure with MCTS (Shen et al., 2018) to tackle the sparse reward setting. Our model uses DQN with action masking for relations having been identified in the periphery as described in Sec. 3.2.1.

Having computed the fingerprints for both topologies, we concatenate them \( \Phi_{uq} || \Phi_{vq} \) (cf. sec 3.2.1) and get a \( (2 \cdot df) \)-dimensional input vector for the Q-net. Thereafter, we compute the Q-values for all relation types. An MLP is used as function approximator \( \hat{q}_\theta = \hat{q}_\theta(s, a; \theta) \).

We utilize the information stored in \( p_{xq} \) to mask out all unreachable semantic links. We define a binary mask \( \Omega^i \in \{0, 1\}^{|R|} \) that retains only the information of traversable predicates in the agent’s current state. Formally, it is defined as:

\[ \Omega^i(r) = \begin{cases} 1 & \text{if } r \in \text{rel}(p_{uq} \cup p_{vq}) \\ 0 & \text{otherwise.} \end{cases} \]

(9)

where \( \text{rel}(\cdot) \) extracts the relation types of quadruples. The network’s outputs for all predicates is defined by \( f(s^i, \theta) = [\hat{q}(s^i, a_0), \hat{q}(s^i, a_1), \ldots, \hat{q}(s^i, a_n)] \), where the output \( f(s^i, \theta) \) describes the q-values of state \( s^i \) under all possible actions in the \( i \)-th iteration. We apply the Hadamard product for masking:

\[ f_{\Omega^i}(s^i, \theta) = [\hat{q}(s^i, a_0), \hat{q}(s^i, a_1), \ldots, \hat{q}(s^i, a_n)] \odot \Omega^i, \]

(10)
yielding only relevant Q-values the agent has to take into consideration. The architecture is illustrated in Fig. 2 where exemplarily two relation types are masked out in the final output.

### 3.3.3 Deep Q-Learning - Learning Procedure

In deep Q-learning, we apply a function approximator \( \hat{q}_\theta = \hat{q}_\theta(s, a; \theta) \), where \( \theta \) are the model’s parameters. The objective function being optimized is straightforward defined as:

\[ L(\theta) = \mathbb{E} \left[ (r(s^i, a^i) + \gamma \max_a \hat{q}_\theta(s^{i+1}, a) - \hat{q}_\theta(s^i, a^i))^2 \right] \]

for an effective learning procedure, using a Replay Memory is of discernible utility (Mnih et al., 2013). Hence, we store the transitions \((s^i, a^i, \text{reward}^i, s^{i+1})\) in \( D \), and a training batch is generated by sampling from the replay memory, \((s^i, a^i, \text{reward}^i, s^{i+1}) \sim D\).

### 4 Evaluation

#### 4.1 Experimental Settings

**Datasets.** The Integrated Crisis Early Warning System (ICEWS) dataset (García-Durán et al., 2018) encodes political events with timestamps.  

The repository is organized in dumps storing information about events that occurred from 1995 to 2015: \textit{ICEWS14} contains events of 2014; and \textit{ICEWS05-15} contains events from 2005 to 2015.

For an effective learning procedure, using a Replay Memory is of discernible utility (Mnih et al., 2013). Hence, we store the transitions \((s^i, a^i, \text{reward}^i, s^{i+1})\) in \( D \), and a training batch is generated by sampling from the replay memory, \((s^i, a^i, \text{reward}^i, s^{i+1}) \sim D\).

The \textit{YAGO15K} dataset (García-Durán et al., 2018) is a modification of FB15k (Leblay and Chekol, 2018) including either the temporal information \(<\text{occursSince}>\) or \(<\text{occursUntil}>\) for only

![Figure 2: Q-Net with action masking](image-url)

Table 1: Dataset statistics

|        | ICEWS14 | ICEWS05-15 | YAGO15K |
|--------|---------|------------|---------|
| # Entities | 7,128   | 10,094     | 15,403  |
| # Relations | 230     | 251        | 32      |
| # Temporal Info. | 365     | 4017       | 188     |
| [train]     | 72,826  | 368,962    | 110,441 |
| [validation] | 8,817   | 45,858     | 13,792  |
| [test]      | 8,789   | 46,056     | 13,813  |

1 Additional information can be found at http://www.icews.com/
some facts. To capture these scatteredly given temporal information, we modify the shape of the input matrix $\mathbf{X}_{s_t}$ to a $|s| \times (d_r + 2d_l)$ matrix, i.e., we obtain one $d_l$-dimensional vector for $\langle \text{occursSince} \rangle$, and one for $\langle \text{occursUntil} \rangle$.

The statistics of the datasets are summarized in Table 1.

Adaptions of Competitors.

**TNTComplex.** In (Lacroix et al., 2020), the authors set up an objective function being suitable for entity prediction queries, i.e., $(u_q, r_q, ?, t_q)$. For predicate prediction, we modify the loss function along the relational tube of the 4-order tensor. Following their notation, for each train tuple $(i, j, k, l)$, we define their loss function as:

$$\tilde{l}(\tilde{X}):(i, j, k, l) = -\tilde{X}_{i,j,k,l} + \log \left( \sum_{j'} \exp(\tilde{X}_{i,j',k,l}) \right)$$

**DE-TransE/-DistMult/-SimpleE.** In (Goel et al., 2020), the authors present a diachronic embedding building on-top of existing embedding methods for static KGs. Due to the associative property of the scoring functions, the objective functions stay the same for the predicate prediction task. However, for evaluation, instead of corrupting the subject/objects entities, we falsify the relations and compute the ranking metrics accordingly. As the temporal information is only sparsely annotated in YAGO15k, the missing information refers to the same (null) embedding vector such that the diachronic embeddings can be at least applied for the existing temporal information.

**Evaluation protocol.** We evaluate all methods in the setting of predicate prediction, i.e., for queries $(u_q, ?, v_q, t_q)$. In the test set, we rank the ground-truth relation type $r$ against all other candidates. The candidate set is filtered, i.e., the set for $(u, ?, v, t)$ exclude any $r'$ where $(u, r', v, t)$ appears in the train/val/test set.

**Implementation Details.** Our model is implemented in PyTorch, and trained on a single GPU. The MLP for calculating the fingerprint uses two hidden layers, each with 16 neurons. The output (fingerprint) is a $d_f = 16$ dimensional vector. We use an embedding size of $d_r = d_l = 10$ for the relations and temporal information. The agent’s episode length is restricted to 5, resulting in a maximal path length of 10. The MLP of the DQN consists of 2 layers with 16 neurons in the first hidden layer and 32 in the second. As weight decay for the fingerprint network and DQN, we use a value of 0.0001 and a decay factor of $\gamma = 0.99$. For restricting the exploration w.r.t the temporal information, we use $tknn$ in the range $[5, 10, 15, 20, 30]$. The buffer of the replay memory is set to 1,000. We use RMSprop as optimizer with a learning rate of 0.0001 and a batch size of 64. We apply an epsilon greedy strategy with an exponential decay, where $\epsilon_{start} = 1.0$, $\epsilon_{end} = 0.05$ and $\epsilon_{decay} = 0.00001$. Code availability: <git-link-on-publication>.

### 4.2 Predicate Prediction

We use the standard evaluation metrics used in the literature, i.e., mean reciprocal rank (MRR) and Hits@$k$, where $k \in \{1, 10\}$. The MRR is the average of the inverse of the mean rank assigned to the true fact over all candidates, whereas Hits@$k$ is a measurement for the percentage a true fact is ranked within the top-$k$ candidate facts. As explained in Sec. 3.2.4, for our reasoning, we use topologies found by the agent as binary features. For each predicate, we sort the the topologies according to the number of times they connected query entities successfully. We pick the top-$m \in \{15, 25, 50\}$ most observed topologies for each relation. Taking more topologies into account yields more distinctive feature vectors, e.g., for ICEWS05-15 the best results were obtained by using $m = 50$ topologies. In Table 2, we summarize the results of the predicate prediction task on the ICEWS14, ICEWS05-15, and YAGO15K dataset. Our approach reaches results which are in line with state-of-the-art results on ICEWS14, and is the best on ICEWS05-15 where we can include more temporal information. On YAGO15K, where time intervals are scatteredly encoded by the relation types $\langle \text{occursSince} \rangle$ and $\langle \text{occursUntil} \rangle$, our method beats the modified TNTComplex and DE-xxx approaches for solving predicate prediction w.r.t the MRR score and Hits@1. The evolution unit of RE-GCN expects as input the temporal information which is not ensured to be given on the YAGO15k dataset, hence, the results are omitted.

### 4.3 Effectiveness

#### 4.3.1 Influence of Parameter $tkNN$

**On Predicate Prediction.** Table 3 shows the results on ICEWS14 with varying $tknn \in \{5, 15, 25, 50\}$. Naturally, the running time for each episode and consequently, for each epoch increases with taking more information into account. We also observe that there is a sweet spot for $tknn$, where results are best. Hence,
Table 2: Predicate prediction results. Best/Second best results are highlighted in bold/underlined.

| Model                              | ICEWS14 | ICEWS05-15 | YAGO15K |
|------------------------------------|---------|------------|---------|
|                                    | MRR     | Hits@10    | Hits@1  | MRR     | Hits@10    | Hits@1  | MRR     | Hits@10    | Hits@1  |
| TNTComplex (Lacroix et al., 2020) | 0.2691  | 0.5266     | 0.1701  | 0.2398  | 0.4775     | 0.1327  | 0.5852  | 0.9699     | 0.3168  |
| DE-SimplE (Goel et al., 2020)     | 0.5074  | 0.7573     | 0.3882  | 0.4289  | 0.6551     | 0.3162  | 0.2749  | 0.4228     | 0.1852  |
| DE-TransE (Goel et al., 2020)     | 0.2068  | 0.3119     | 0.1364  | 0.1928  | 0.3486     | 0.1074  | 0.3906  | 0.4827     | 0.3120  |
| DE-DistMult (Goel et al., 2020)   | 0.4613  | 0.7370     | 0.3261  | 0.3197  | 0.5243     | 0.2129  | 0.2459  | 0.4298     | 0.1457  |
| RE-GCN (Li et al., 2021c)         |         |            |         |         |            |         |         |            |         |
| APPTeK                             | 0.4889  | 0.7749     | 0.3421  | 0.4844  | 0.8246     | 0.3222  | 0.6041  | 0.9547     | 0.3537  |

Table 3: Predicate Prediction on ICEWS14 with varying tkNN, \( m = 25 \), and the respective running times.

| tkNN | MRR@10 | MRR@1 | time[ms]/episode | time[s]/epoch |
|------|--------|-------|-----------------|---------------|
| 5    | 0.4297 | 0.7563| 0.2849          | 23            | 1598          |
| 15   | 0.4593 | 0.7549| 0.3183          | 33            | 2245          |
| 25   | 0.4716 | 0.7591| 0.3269          | 41            | 2975          |
| 50   | 0.4469 | 0.7425| 0.3079          | 66            | 4473          |

while increasing \( tkNN \), the agent is able to gather more information about the neighborhood of the query entities. However, capping the number of quadruples at some point prevents the influence of temporally unconnected events.

**Figure 3:** Avg. number of possible actions w.r.t. the current step for \( tkNN \in \{5, 10, 20\} \) on ICEWS14 (left) and ICEWS05-15 (right).

On Action Space. Fig. 3 (left) illustrates the influence of \( tkNN \) on the action space for ICEWS14. It displays the average number of possible relations for \( tkNN \in \{5, 10, 20\} \) in each step. While increasing the value for \( tkNN \), we increase the agent’s view on the temporal dimension. Naturally, there is a higher chance for various relation types to be in the candidate set. In Fig. 3 (right) the effect is illustrated on the larger dataset ICEWS05-15. Due to the more dense nature of the dataset, applying a filtering step on the temporal dimension is of utmost importance to keep the action space as low as possible, but large enough such that the agent can connect topologies of \( u_q \) and \( v_q \).

### 4.3.2 Reward history

In Fig. 4, the agent’s reward history for \( tkNN \in \{5, 10, 20\} \) is shown for ICEWS14 (Fig. 4a) and ICEWS05-15 (Fig. 4b). The colored lines show the reward history with a moving average window of 500, and the red line with a size of 1,000. On ICEWS05-15 we reach slightly better rewards for the same values of \( tkNN \). This is due to the sparseness of ICEWS14. There are less connections being incident to entities as we only take a time span of 1 year into account. Increasing the value for \( tkNN \), we consider more relations at each step resulting in more overlapping parts for both topologies. On the other hand, processing a larger amount of relations increases the running time.

**Figure 4:** Reward for \( tkNN \in \{5, 10, 20\} \)

**Figure 5:** Success rate of relation types.
4.3.3 Success Rate for Individual Links

Fig. 5a/5b illustrates the success rate of 5 individual links in ICEWS14/ICEWS05-15. Generally, taking a larger time span into account helps for finding descriptive topologies. Moreover, some relations have a high correlation connecting the same entities. In such cases, the agent finds instantly a direct path that interconnects both query entities, given that the relations are also temporal nearest neighbors. From a semantical point of view, e.g., ‘Make statement’ or ‘Consult’ are predicates used for a verbal exchange, which do correlate and interconnect the same entities within a time frame. For densely connected graph structures, the exploration of topologies will result faster in an overlap in at least one entity such that the success rate reaches a maximum in early stages.

4.4 Qualitative Analysis of Topologies

In Fig. 6, we present exemplary topologies. The query relation between two entities (orange) is shown on top of each column; two relevant topologies are shown below. For predicting, e.g., ‘Protest violently, Riot’, one way to find a path to the object is by expanding the subject’s topology by ‘Use unconventional violence’ fulfilling the temporal constraint w.r.t the query. As the agent expands according to a relation type and not by single quadruples, we might get additional connections to other entities (lavender). For ‘Reduce or break diplomatic relations’, the agent found a connection by expanding both query entities by ‘Make Statement’. As the latter is a predominant and very generic relation type, it occurs more often in the dataset. For relational reasoning, these kind of relation types yield indistinguishable features exacerbating the prediction when used as a single feature.

In the last example, we see topologies being used to infer ‘Reject’. Both topologies use generic relation types ‘Accuse’ and ‘Criticize or Denounce’ which might not be decisive features on their own, but using them together as binary path features yields a more conclusive feature vector. Hence, taking more topologies into account facilitates predicate prediction.

5 Conclusion

We propose an RL approach for predicate prediction on temporal Knowledge Graphs (tKG) suitable for human interpretation. Given a query (subject, ?, object, time), we train an RL agent that gathers information from both query entities, simultaneously. The most representative topologies connecting two entities can then be used in downstream tasks like predicting the relation type holding between them. Our architecture computes vector representations (fingerprints), of the topologies starting from each of the query entities. Afterwards both fingerprints are concatenated and used to calculate Q-values for relation types (actions) being incident to the observed topologies. To capture the temporal aspect when choosing a relation type, we limit the possible action by temporal proximity to the query. Our evaluation shows i) the reasoning topologies can be used as features to infer the predicate between two entities; ii) our model allows for modeling time intervals; iii) the influence of the temporal proximity to the action space; and iv), we additionally gain a more in-depth insight into the reasons for a prediction by analyzing the inferred topologies.
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