

Complex Evolutional Pattern Learning for Temporal Knowledge Graph Reasoning

Zixuan Li^{1,2,3*}, Saiping Guan^{1,2}, Xiaolong Jin^{1,2}, Weihua Peng³, Yajuan Lyu³,
Yong Zhu³, Long Bai^{1,2}, Wei Li³, Jiafeng Guo^{1,2}, Xueqi Cheng^{1,2}

¹School of Computer Science and Technology, University of Chinese Academy of Sciences;

²CAS Key Laboratory of Network Data Science and Technology,

Institute of Computing Technology, Chinese Academy of Sciences; ³Baidu Inc.

{lizixuan, guansaiping, jinxiaolong}@ict.ac.cn

{pengweihua, lvayajuan, zhuyong}@baidu.com

Abstract

A Temporal Knowledge Graph (TKG) is a sequence of KGs corresponding to different timestamps. TKG reasoning aims to predict potential facts in the future given the historical KG sequences. One key of this task is to mine and understand evolutional patterns of facts from these sequences. The evolutional patterns are complex in two aspects, length-diversity and time-variability. Existing models for TKG reasoning focus on modeling fact sequences of a fixed length, which cannot discover complex evolutional patterns that vary in length. Furthermore, these models are all trained offline, which cannot well adapt to the changes of evolutional patterns from then on. Thus, we propose a new model, called Complex Evolutional Network (CEN), which uses a length-aware Convolutional Neural Network (CNN) to handle evolutional patterns of different lengths via an easy-to-difficult curriculum learning strategy. Besides, we propose to learn the model under the online setting so that it can adapt to the changes of evolutional patterns over time. Extensive experiments demonstrate that CEN obtains substantial performance improvement under both the traditional offline and the proposed online settings.

1 Introduction

Temporal Knowledge Graph (TKG) (Boschee et al., 2015; Gottschalk and Demidova, 2018, 2019; Zhao, 2020) has emerged as a very active research area over the last few years. Each fact in TKGs is a quadruple (*subject, relation, object, timestamp*). A TKG can be denoted as a sequence of KGs with timestamps, each of which contains all facts at the corresponding timestamp. TKG reasoning aims to answer queries about future facts, such as (*COVID-19, New medical case occur, ?, 2022-1-9*).

To predict future facts, one challenge is to dive deep into the related historical facts, which reflect

the preferences of the related entities and affect their future behaviors to a certain degree. Such facts, usually temporally adjacent, may carry informative sequential patterns, called evolutional patterns in this paper. For example, [(*COVID-19, Infect, A, 2021-12-21*), (*A, Discuss with, B, 2021-12-25*)], (*B, Go to, Shop, 2021-12-28*)] is an informative evolutional pattern for the above query implied in historical KGs. There are two kinds of models to model evolutional patterns, namely, query-specific and entire graph based models. The first kind of models (Jin et al., 2020; Li et al., 2021a; Sun et al., 2021; Han et al., 2020a, 2021; Zhu et al., 2021) extract useful structures (i.e., paths or subgraphs) for each individual query from the historical KG sequence and further predict the future facts by mining evolutional patterns from these structures. This kind of models may inevitably neglect some useful evolutional patterns. Therefore, the entire graph based models (Deng et al., 2020; Li et al., 2021a) take a sequence of entire KGs as the input and encode evolutional patterns among them, which exhibit superiority to the query-specific models.

However, they all ignore the length-diversity and time-variability of evolutional patterns. **Length-diversity**: The lengths of evolutional patterns are diverse. For example, [(*COVID-19, Infect, A, 2021-12-21*), (*A, Discuss with, B, 2021-12-25*)], (*B, Go to, Shop, 2021-12-28*)] is a useful evolutional pattern of length 3 to predict the query (*COVID-19, New medical case occur, ?, 2022-1-9*) and [(*COVID-19, Infect, A, 2021-12-21*), (*A, Go to, Shop, 2021-12-30*)] is also a useful evolutional pattern of length 2 for this query. Previous models extract evolutional patterns of a fixed length, which cannot handle evolutional patterns of diverse lengths. **Time-variability**: Evolutional patterns change over time. For example, (*COVID-19, Infect, A, 2019-12-9*) and (*COVID-19, Infect, A, 2022-1-9*) may lead to different results due to the wide usage of the COVID-19 vaccines. Previous models learn from

^{*}This work was done while the first author was doing internship at Baidu Inc.

the historical training data, which fail in modeling the time-variability of evolutionary patterns after that.

Upon the above observations, we propose Complex Evolutional Network (CEN) to deal with the above two challenges. For length-diversity, CEN learns evolutionary patterns from historical KG sequences of different lengths via an Relational Graph Neural Network (RGCN) based KG sequence encoder and a length-aware Convolutional Neural Network (CNN) based evolutionary representation decoder. Besides, the model is trained via an easy-to-difficult curriculum learning strategy incrementally according to the length of KG sequences. For time-variability, we learn CEN under an online setting and combine CEN with a temporal regularization unit to alleviate the catastrophic forgetting problem (McCloskey and Cohen, 1989).

In general, this paper makes the following contributions:

- We address, for the first time, the problems of length-diversity and time-variability of evolutionary patterns for TKG reasoning.
- For length-diversity, we propose a length-aware CNN to learn evolutionary patterns with different lengths in a curriculum learning manner. For time-variability, we propose to learn the model under an online setting to adapt to the changes of evolutionary patterns.
- Experiments demonstrate that the proposed CEN model achieves better performance on TKG reasoning under both the traditional offline and the proposed online settings.

2 Related Work

The TKG reasoning task primarily has two settings, interpolation and extrapolation. This paper focus on the extrapolation setting. In what follows, we will introduce related work on both settings:

TKG Reasoning under the interpolation setting. This setting aims to complete the missing facts at past timestamps (Jiang et al., 2016; Leblay and Chekol, 2018; Dasgupta et al., 2018; Garcia-Duran et al., 2018; Goel et al., 2020; Wu et al., 2020). For example, TTransE (Leblay and Chekol, 2018) extends TransE (Bordes et al., 2013) by adding the temporal constraints; HyTE (Dasgupta et al., 2018) projects the entities and relations to time-aware hyperplanes to generate representations

for different timestamps. Above all, they cannot obtain the representations of the unseen timestamps and are not suitable for the extrapolation setting.

TKG Reasoning under the extrapolation setting This setting aims to predict facts at future timestamps, which can be categorized into two groups: query-specific and entire graph based models. Query-specific models focus on modeling the query-specific history. For example, RE-NET (Jin et al., 2020) captures the evolutionary patterns implied in the subgraph sequences of a fixed length specific to the query. CyGNet (Zhu et al., 2021) captures repetitive patterns by modeling repetitive facts. xERTE (Han et al., 2020a) learns to find the query-related subgraphs of a fixed hop number. CluSTeR (Li et al., 2021a) and TITer (Sun et al., 2021) both adopt reinforcement learning to discover evolutionary patterns in query-related paths of a fixed length. Unlike the query-specific models, entire graph based models encode the latest historical KG sequence of a fixed-length. RE-GCN (Li et al., 2021b) captures the evolutionary patterns into the representations of all the entities by modeling KG sequence of a fixed-length at latest a few timestamps. Glean (Deng et al., 2020) introduces event descriptions to enrich the information of the entities.

3 Problem Formulation

A TKG $G = \{G_1, G_2, \dots, G_t, \dots\}$, where $G_t = (\mathcal{V}, \mathcal{R}, \mathcal{E}_t)$, is a directed multi-relational graph. \mathcal{V} is the set of entities, \mathcal{R} is the set of relations, and \mathcal{E}_t is the set of facts at timestamp t . The TKG reasoning task aims to answer queries like $(s, r, ?, t_q)$ or $(?, r, o, t_q)$ with the historical KG sequence $\{G_1, G_2, \dots, G_{t_q-1}\}$ given, where $s, o \in \mathcal{V}$, $r \in \mathcal{R}$ and t_q are the subject/object entity, the relation and the query timestamp, respectively. Following Jin et al. (2020), KGs from timestamps 1 to T_1 , T_1 to T_2 , T_2 to T_3 ($T_1 < T_2 < T_3$) are used as the training, validation and test sets, respectively. Under the traditional offline setting, models are trained only using the training set ($t_q \leq T_1$), while under the online setting, the model will be updated by KGs before t_q ($T_1 < t_q \leq T_3$) continually. Without loss of generality, we describe our model as predicting the missing object entity.

4 Methodology

We propose CEN to deal with the length-diversity and time-variability challenges of evolutionary pat-

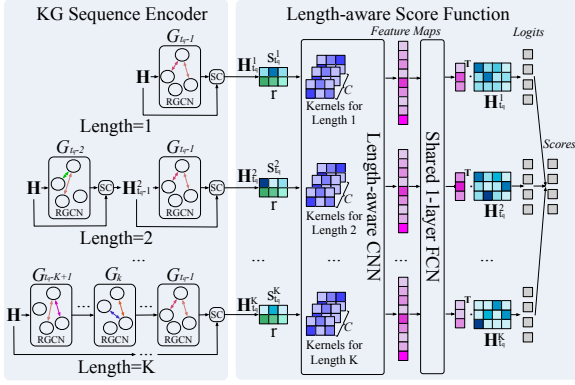


Figure 1: An diagram of the basic CEN model.

tern learning for TKG reasoning. Specifically, CEN consists of a basic model as well as a curriculum learning strategy for the former challenge and an online learning strategy for the latter challenge.

4.1 Basic CEN Model

As shown in Figure 1, the basic model of CEN contains a KG sequence encoder and an evolutionary representation decoder. The KG sequence encoder encodes the latest historical KG sequences of different lengths to corresponding evolutionary representations of entities. Then, the evolutionary representation decoder calculates the scores of all entities for the query based on these representations.

KG Sequence Encoder. Its inputs include the latest historical KG sequences of lengths from 1 to K , initial representations of entities $\mathbf{H} \in \mathbb{R}^{|\mathcal{V}| \times d}$ and relation representations $\mathbf{R} \in \mathbb{R}^{|\mathcal{R}| \times d}$, where d is the dimension of the representations. Take the KG sequence of length $k = 2$ for example, for each KG in the input sequence $\{G_{t_q-2}, G_{t_q-1}\}$, it iteratively calculates the evolutionary representations of entities \mathbf{H}_t^2 at the corresponding timestamps $t \in \{t_q - 1, t_q\}$ as follows:

$$\hat{\mathbf{H}}_t^2 = RGCN(\mathbf{H}_{t-1}^2, \mathbf{R}, G_{t-1}), \quad (1)$$

$$\mathbf{H}_t^2 = SC(\hat{\mathbf{H}}_t^2, \mathbf{H}_{t-1}^2), \quad (2)$$

where $RGCN(\cdot)$ and SC denote the shared RGCN layer and the skip connection unit proposed in RE-GCN (Li et al., 2021b). For the initial timestamp $t_q - 1$, $\mathbf{H}_{t_q-2}^2$ is set to \mathbf{H} . \mathbf{R} is shared across timestamps, which is different from RE-GCN. By reusing the encoder for KG sequences of different lengths, we obtain K entity evolution representations at the query timestamp: $\{\mathbf{H}_{t_q}^1, \dots, \mathbf{H}_{t_q}^k, \dots, \mathbf{H}_{t_q}^K\}$.

Evolutional Representation Decoder. Multiple evolutionary representations contain evolutionary pat-

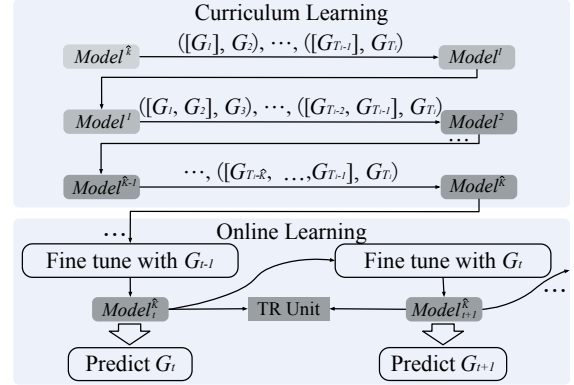


Figure 2: The learning procedure of the proposed model.

terns of multiple lengths. To distinguish the influences of the length-diverse evolutionary patterns, we design a length-aware CNN, which uses K separate channels to model the above K evolutionary representations. Specifically, for a query $(s, r, ?, t_q)$, the representations of s ($\mathbf{s}_{t_q}^1, \dots, \mathbf{s}_{t_q}^k, \dots, \mathbf{s}_{t_q}^K$) and r (\mathbf{r}) are looked up from multiple representations of entities $\{\mathbf{H}_{t_q}^1, \dots, \mathbf{H}_{t_q}^k, \dots, \mathbf{H}_{t_q}^K\}$ and the shared relation representations \mathbf{R} . For historical KG sequence of length k , k^{th} channel with C different kernels of size $2 \times M$ is used to decode the concatenation of $\mathbf{s}_{t_q}^k$ and \mathbf{r} . Specifically, the feature maps are calculated as below,

$$\mathbf{m}_c^k(s, r, t_q) = Conv_{2D}(\mathbf{w}_c^k, [\mathbf{s}_{t_q}^k; \mathbf{r}]), \quad (3)$$

where $Conv_{2D}$ denotes the 2D convolution operation, \mathbf{w}_c^k ($0 \leq c < C$) are the trainable parameters in c^{th} kernel of k^{th} channel and $\mathbf{m}_c^k(s, r, t_q) \in \mathbb{R}^{1 \times d}$. After that, it concatenates the output vectors from C kernels yielding a vector: $\mathbf{m}^k(s, r, t_q) \in \mathbb{R}^{C \times d}$. For K channels, it outputs a list of vectors: $[\mathbf{m}^1(s, r, t_q), \dots, \mathbf{m}^k(s, r, t_q), \dots, \mathbf{m}^K(s, r, t_q)]$. Then, each vector is fed into a shared 1-layer Fully Connected Network (FCN) with $\mathbf{W}_3 \in \mathbb{R}^{C \times d}$ as its parameters and the final score of a candidate entity o is the sum of the logits from multiple evolutionary representations: $\sum_{k=1}^K \mathbf{m}^k(s, r, t_q) \mathbf{W}_3 \mathbf{o}^k$, where \mathbf{o}^k is the evolutionary representation of length k for o . Then we seen it as a multi-class learning problem and use the cross-entropy as its objective function.

4.2 Curriculum Learning for Length-diversity

Longer historical KG sequences contain more historical facts and longer evolutionary patterns, which is more challenging to learn. Similar to human learning procedures, the models can benefit from an easy-to-difficult curriculum. Besides, how to

Datasets	ICEWS14	ICEWS18	WIKI
$\#\mathcal{E}$	6,869	23,033	12,554
$\#\mathcal{R}$	230	256	24
$\#Train$	74,845	373,018	539,286
$\#Valid$	8,514	45,995	67,538
$\#Test$	7,371	49,545	63,110
T_3	1 day	1 day	1 year

Table 1: Statistics of the datasets. $\#Train$, $\#Valid$, $\#Test$ are the numbers of facts in the training, validation and test sets.

choose the maximum length of evolutionary patterns is vital to CEN. Thus, we design the curriculum learning strategy to learn the length-diverse evolutionary patterns from short to long and adaptively select the optimal maximum length \hat{K} . As shown at the top of Figure 2, we start from the minimum length \hat{k} ($\hat{k} = 1$ for example) and gradually move on to longer history in the training set. The model stops the curriculum and gets the optimal \hat{K} when the MRR metric decreases or the length is up to maximum length K . Note that, curriculum learning is conducted under the traditional offline setting and $Model^{\hat{K}}$ is used as the pre-trained model for online learning.

4.3 Online Learning for Time-variability

To handle the time-variability of evolutionary patterns, one simple and direct method is to update the model according to the newly occurred facts. Thus, as shown in the bottom of Figure 2, for timestamp $t + 1$ ($T_1 < t + 1 < T_3$), $Model_t^{\hat{K}}$ is fine-tuned to get $Model_{t+1}^{\hat{K}}$ by predicting the facts in the KG at the last timestamp G_t with historical KG sequences as inputs. Furthermore, to balance the knowledge of new evolutionary patterns and the existing ones, we use a Temporal Regularization unit (TR unit) (Daruna et al., 2021; Wu et al., 2021). We apply an $L2$ regularization constraint between two temporally adjacent models to smooth the drastic change of the parameters.

4.4 Analysis on Computational Complexity

We analyze the computational complexity of CEN. We view the computational complexities of the RGCN unit and ConvTransE as constants. Then, the time complexity of the RGCN at a timestamp t is $O(|\mathcal{E}|)$, where $|\mathcal{E}|$ is the maximum number of facts at timestamps in history. As we unroll m ($m = \hat{K} - \hat{k}$) sequences, the time complexity of the KG sequence encoder is finally $O(m^2|\mathcal{E}|)$. Thus, the time complexity of CEN is $O(m^2|\mathcal{E}| + m)$.

5 Experiments

Experimental Setup. We adopt three widely-used datasets, ICEWS14 (Li et al., 2021b), ICEWS18 (Jin et al., 2020), and WIKI (Leblay and Chekol, 2018) to evaluate CEN. Dataset statistics are demonstrated in Table 1. Due to the space limitation, the CEN model is only compared with the latest models of TKG reasoning: CyGNet (Zhu et al., 2021), RE-NET (Jin et al., 2020), xERTE (Han et al., 2020a), TG-Tucker (Han et al., 2021), TG-DistMult (Han et al., 2021), TiTer (Sun et al., 2021) and RE-GCN (Li et al., 2021b). In the experiments, we adopt MRR (Mean Reciprocal Rank) and Hits@{1,3,10} as the metrics for TKG reasoning. We averaged the metrics over five runs. Note that, following Han et al. (2020b), we adopt an improved filtered setting where the timestamps of facts are considered, called time-aware filtered setting. Take a typical query $(s, r, ?, t_1)$ with answer o_1 in the test set for example, and assume there is another two facts (s, r, o_2, t_2) and (s, r, o_3, t_1) . Under this time-aware filtered setting, only o_3 will be considered as a correct answer and thus removed from the ranking list of candidate answers.

Implementation Details. In the experiments, the optimal minimum lengths of evolutionary patterns \hat{k} for ICEWS14, ICEWS18, WIKI are 3, 3, 2, respectively. The maximum length K for all datasets is set to 10. For all datasets, the kernel width M is set to 3, and C is set to 50. For each fact (s, r, o, t) in the test set, we evaluate CEN on two queries $(s, r, ?, t)$ and $(?, r, o, t)$. The dimension d of relation representations and entity representations is set to 200 on all datasets. Adam (Kingma and Ba, 2014) is adopted for parameter learning with the learning rate of 0.001 on all datasets. The number of RGCN layers is set to 2 and the dropout rate for each layer to 0.2. For the online setting, we set the max epochs of the fine-tuning at each timestamp to 30. For predicting G_t , G_{t-2} is used as the validation set. We fine tune the pre-trained CEN from $T_1 + 1$ to T_3 and report the results at the test timestamps (T_2 to T_3) in Table 3. The experiments are carried out on Tesla V100. Codes are available at <https://github.com/Lee-zix/CEN>.

5.1 Experimental Results

Results under the Offline Setting. The results under the traditional offline setting are presented in Table 2. CEN consistently outperforms the

Model	ICEWS14				ICEWS18				WIKI			
	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10
CyGNet	35.05	25.73	39.01	53.55	24.93	15.90	28.28	42.61	33.89	29.06	36.10	41.86
RE-NET	36.93	26.83	39.51	54.78	28.81	19.05	32.44	47.51	49.66	46.88	51.19	53.48
xERTE	40.02	32.06	44.63	56.17	29.31	21.03	33.51	46.48	71.14	68.05	76.11	79.01
TG-Tucker	-	-	-	-	28.68	19.35	32.17	47.04	50.43	48.52	51.47	53.58
TG-DistMult	-	-	-	-	26.75	17.92	30.08	44.09	51.15	49.66	52.16	53.35
TITer	40.97	32.28	45.45	57.10	29.98	22.05	33.46	44.83	75.50	72.96	77.49	79.02
RE-GCN	40.39	30.66	44.96	59.21	30.58	21.01	34.34	48.75	77.55	73.75	80.38	83.68
CEN	42.20	32.08	47.46	61.31	31.50	21.70	35.44	50.59	78.93	75.05	81.90	84.90

Table 2: Experimental results on TKG reasoning (in percentage) under the offline setting.

Model	ICEWS14				ICEWS18				WIKI			
	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10
CEN(-TR)	39.28	30.05	43.58	57.01	31.11	21.41	35.09	50.27	81.92	77.93	85.23	87.63
CEN	43.34	33.18	48.49	62.58	32.66	22.55	36.81	52.50	79.67	75.63	83.00	85.58

Table 3: Experimental results on TKG reasoning (in percentage) under the online setting.

metrics	MRR	H@1	H@3	H@10
CEN	42.20	32.08	47.46	61.31
CEN(-CL)	41.50	31.53	46.50	60.81
CEN(-LA)	41.52	31.49	46.74	60.65

Table 4: Ablation Study of CEN on ICEWS14.

baselines on MRR, Hits@3, and Hits@10 on all datasets, which justifies the effectiveness of modeling the evolutionary patterns of different lengths. On ICEWS datasets, CEN underperforms TITer on Hits@1 because TITer retrieves the answer through explicit paths, which usually gets high Hits@1. Whereas, CEN recalls more answer entities by aggregating the information from multiple evolutionary patterns, which may be the reason for its high performance on Hits@3 and Hits@10.

Results under the Online Setting. Under the online setting, the model is updated via historical facts at the testset. Thus, it cannot be directly compared with the baselines designed for the offline setting. As shown in Table 3, on ICEWS datasets CEN outperforms CEN(-TR) (CEN without TR unit), which implies the effectiveness of TR unit to balance the knowledge of new evolutionary patterns and the existing ones. On WIKI, CEN(-TR) gets better performance. It is because that the time interval between two adjacent timestamps in WIKI (one year) is much larger than ICEWS datasets (one day) and contains more time-variable evolutionary patterns. TR unit limits the model to adapt to new knowledge and is not suitable for this dataset.

Ablation Study. To investigate the contributions of curriculum learning strategy and the length-aware CNN, we conduct ablation studies for CEN

on the test set of ICEWS14 under the traditional offline setting, which are shown in Table 4. CEN(-CL) denotes CEN without the curriculum learning strategy. The underperformance of CEN(-CL) demonstrates the effectiveness of the curriculum learning strategy. CEN(-LA) denotes the model replacing the length-aware CNN with a traditional CNN. The underperformance of CEN(-LA) implies the effectiveness of the length-aware CNN.

6 Conclusions

In this paper, we proposed Complex Evolutional Network (CEN) for TKG reasoning, which deals with two challenges in modeling the complex evolutionary patterns: length-diversity and time-variability. For length-diversity, CEN adopts a length-aware CNN to learn evolutionary patterns of different lengths and is trained under a curriculum learning strategy. For time-variability, we explored a new online setting, where the model is expected to be updated to new evolutionary patterns emerging over time. Experimental results demonstrate the superiority of the proposed model under both the offline and the online settings.

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