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Exploring Temporal Knowledge Graphs with Compositional Interactions and Diachronic Mechanisms

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Abstract.
Temporal Knowledge Graphs (TKGs) organize dynamic real-world facts, adding a time dimension to the multi-relational graph structure of Knowledge Graphs (KGs). We leverage the expressive power of graph convolutional networks (GCNs) for modeling TKGs, recognizing similarities with handling graph-structured data and utilizing complex geometry. Our approach emphasizes compositional interactions between relations and entities, integrating a diachronic mechanism to enhance representation with both graph structure and temporal dynamics. Experimental results on benchmark datasets, employing various composition operators, showcase the effectiveness of our model in link prediction tasks.

1 Introduction

Knowledge Graphs (KGs) are effective representations of real-world entities and relationships, but they struggle to accommodate dynamic changes in reality. Static KGs fail to accurately depict facts or events that evolve over time, as illustrated by the changing U.S. presidents in the triplet *(?, president of, US)*. Temporal Knowledge Graphs (TKGs) address this limitation by incorporating a time dimension, enabling them to capture evolving facts and events more effectively. Despite their enhanced capabilities, TKGs often remain incomplete due to their dynamic nature, underscoring the importance of Temporal Knowledge Graphs Completion (TKGC) for uncovering new insights.

Previous studies like ComplEx-GNN [1] and ComplexGCN [2] have shown the potential improvement of using complex numbers in Knowledge Graph Embedding (KGE) to model entities and relations. These works modified graph convolutional networks (GCNs) to handle complex values, focusing on entities but neglecting relation information. Our research extends this by employing Graph Neural Networks (GNNs) to model relation-aware interactions using various operators, showcasing the power of complex geometry. Additionally, we incorporate temporal features into entity and relation embeddings using Diachronic Embedding (DE), aiming to enhance link prediction accuracy in Temporal KGE

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(TKGE). This approach enriches understanding of temporal dynamics and improves embedding quality for more effective link prediction.

Our main contributions to this work are as follows:

- We propose a novel CE-CGCN model designed for learning complex representations of multi-relational TKGs with time-dependency using GCNs, filling a gap in existing models.
- We build a variaty of complex-valued composition operators to illustrate the expressiveness of complex space in relation-aware TKGE, highlighting the versatility and potential of complex geometry in modeling intricate relationships.
- The model is validated through experimentation on two benchmark datasets showing its effectiveness for link prediction.

2 Related work

Link prediction on TKGs is crucial for predicting missing links where facts change over time. Several methods have explored complex geometry in KGE models for enhancing link prediction tasks in TKGs. For example, ComplEx-GNN [1] and ComplexGCN [2] showed that leveraging complex numbers improves the representation of entities and relations, but they neglected relational information, limiting their ability to model dynamic relationships effectively. Models like RotatE [3] used complex numbers for rotational transformation but struggled with more complex patterns.

Recent TKGC research focuses on incorporating temporal features into embeddings. DE [4] approaches highlighted the importance of time-dependent dynamics. Similarly, TComplEx [5] extended the ComplEx model [6] to temporal settings, but often lacked integrated mechanisms for complex interactions. LorenTzE [7] expand the temporal dependency into the high-dimensional Lorentz, but neglected the graph structure information; HGAT [8] use RGCN to enrich the entity representation with relation-aware and hierarchical-aware mechanism; HyTE [9] used hyperplane-based, improving performance but facing challenges in intricate interactions within complex geometry.

Overall, TKGC research emphasizes dynamic and relation-aware models that capture the evolving nature of knowledge graphs. The strengths and weaknesses of previous models highlight the potential for innovative use of complex geometry, DE, and efficient performance on benchmarks. Our paper aligns with this goal, proposing an improved model that enhances representation learning and dynamic interaction modeling.

3 Methodology

Preliminary and Notation: We denote TKGs as $\mathcal{G}(\mathcal{E}, \mathcal{R}, \mathcal{F}, \mathcal{T})$ where $\mathcal{E}$ is the set of entities, $\mathcal{R}$ is the set of relations, $\mathcal{T}$ is the set of all timestamps, and $\mathcal{F}$ is

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the set of positive quadruplets. For complex numbers, let $z = a + bi \in \mathbb{C}$ where $\mathrm{Re}(z) = a,\ \mathrm{Im}(z) = b$ represent for the real and imaginary part correspondingly.

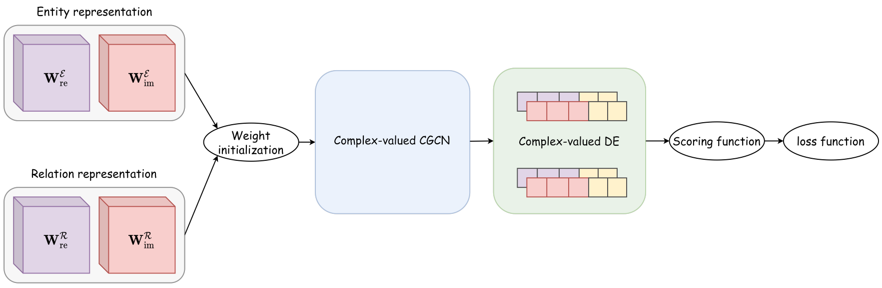

Fig. 1: The overall architecture of CE-CGCN includes 6 main components corresponding with 6 main stages for link prediction progress.

Fig. 1 illustrates the overall architecture of CE-CGCN. Initially, we embed the entities $\mathcal{E}$ and relations $\mathcal{R}$ into complex geometry as $\mathbf{W}_{\mathrm{re}}$ and $\mathbf{W}_{\mathrm{im}}$. After Xavier's initialization [10], we conduct relation-aware representation learning using Complex-valued CGCN. Next, we introduce a new Complex-valued DE to enrich the representation with temporal features. Finally, we utilize the ComplEx scoring function to evaluate the plausibility of forming quadruplets.

3.1 Complex-valued CGCN

Based on the foundation model of CompGCN [11] on the real space, we utilize three separate relation-type matrices $\mathbf{W}_{\lambda(r)}$ to model three types of relations $\lambda(r)$, including the base (source) relation $\mathcal{R}_{src}$, its reverse $\mathcal{R}_{inv}$, and self-loop $\mathcal{R}_{\top}$, and formulate two composition operations on the complex geometry, which take the entity and relation-type specific complex vectors as input:

Subtraction:

$$\varphi(\mathbf{h}_s, \mathbf{h}_r) = \mathbf{h}_s - \mathbf{h}_r = \mathrm{Re}(\mathbf{h}_s) - \mathrm{Re}(\mathbf{h}_r) + i(\mathrm{Im}(\mathbf{h}_s) - \mathrm{Im}(\mathbf{h}_r)) \tag{1}$$

Multiplication:

$$\begin{aligned}\varphi(\mathbf{h}_s, \mathbf{h}_r) = \mathbf{h}_s * \mathbf{h}_r &= \mathrm{Re}(\mathbf{h}_s)\mathrm{Re}(\mathbf{h}_r) - \mathrm{Im}(\mathbf{h}_s)\mathrm{Im}(\mathbf{h}_r) \\ &+ i(\mathrm{Re}(\mathbf{h}_s)\mathrm{Im}(\mathbf{h}_r) + \mathrm{Im}(\mathbf{h}_s)\mathrm{Re}(\mathbf{h}_r))\end{aligned} \tag{2}$$

In the update phase at Eq. 3, neighbor information is aggregated based on complex multiplication of $\mathbf{W}_{\lambda(r)}$ and $\varphi(\cdot)$. Then, we perform relation-type awareness by ensuring that each dot-product embedding equally contributes to the entity embedding. After applying the activation function σ, we obtain the final entity embedding $\mathbf{h}^l_o$ at the l-th layer. The equations below demonstrate the progression for both the real and imaginary components:

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$$\mathbf{h}_o^{l+1} \overset{\text{(c)}}{=} \sigma\left(\sum_{(s,r)\in\mathcal{N}(o)} \mathbf{W}_{\lambda(r)}\varphi(\mathbf{h}_s^l, \mathbf{h}_r^l)\right) \tag{3}$$

$$\mathbf{h}_r^{l+1} \overset{\text{(d)}}{=} \mathbf{W}_{\text{rel}}\mathbf{h}_r^l \tag{4}$$

where $\mathcal{N}(o)$ is the set of outgoing edges from node o. Meanwhile, (d) arises from the relation updating phase, with $\mathbf{W}_{\text{rel}}$ being the relation embedding matrix.

3.2 Complex-valued DE

We introduce the Complex-valued DE, an entity and relation-specific DE method based on DE [4], which allows parameter-sharing and control over the γ fraction of static and temporal features over time. Let $\mathbf{z}^t[i] \in \mathbf{z}^t$ denote the vector embedding $\mathbf{z}^t$ of the i-th component in the temporal embedding for both entities and relations, and $\mathbf{a}_o$, $\mathbf{w}_o$, and $\mathbf{b}_o$ represent relation-entity specific vectors. The activation function σ uses sine for the imaginary component and cosine for the real component. Finally, we concatenate the static and temporal representations to obtain the temporal dependency embedding:

$$\mathbf{z}_o^t[i] = \sum_{\mathbf{t}_i\in\mathbf{t}} \mathbf{a}_o[i]\sigma\left(\mathbf{w}_o[i]\mathbf{t}_i + \mathbf{b}_o[i]\right) \tag{5}$$

$$\mathbf{h}_o = \left[\mathbf{h}_o^l \mid\mid \mathbf{z}_o^t\right] \tag{6}$$

3.3 Complex scoring function

We utilize the ComplEx [6] scoring function, which exploits intricate interactions in complex geometry. Then, minimize the loss using the Cross Entropy Loss.

$$\begin{aligned}\phi(s,r,o) &= \text{Re}(\mathbf{h}_r)\text{Re}(\mathbf{h}_s)\text{Re}(\mathbf{h}_o) + \text{Re}(\mathbf{h}_r)\text{Im}(\mathbf{h}_s)\text{Im}(\mathbf{h}_o) \\ &+ \text{Im}(\mathbf{h}_r)\text{Re}(\mathbf{h}_s)\text{Im}(\mathbf{h}_o) - \text{Re}(\mathbf{h}_r)\text{Im}(\mathbf{h}_s)\text{Re}(\mathbf{h}_o)\end{aligned} \tag{7}$$

4 Experiment

4.1 Setup

Dataset and Metrics: We employ two standard benchmark datasets for the link prediction task: ICEWS14 [12] and ICWES05-15 [12], which provided statistics on Table 1. Furthermore, we evaluate the performance using Mean Reciprocal Rank (MRR) and Hits@K (1, 3, 10).
Baselines and Implementation: We compare our work with some static models: RotatE and ComplEx. For temporal baselines, we compare CE-CGCN with DE models and other models mentioned in section 2. We used PyTorch version 1.13.1. The hyperparameters include learning rate, embedding size, GCN size and γ is used to control the static and temporal contribution correspondingly.

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Dataset	$\lvert\mathcal{E}\rvert$	$\lvert\mathcal{R}\rvert$	$\lvert\mathcal{T}\rvert$	$\lvert\mathcal{F}\rvert$	$\lvert\mathcal{F}_{\text{train}}\rvert$	$\lvert\mathcal{F}_{\text{valid}}\rvert$	$\lvert\mathcal{F}_{\text{test}}\rvert$
ICEWS14	6869	230	365	96730	72826	8941	8963
ICEWS05-15	10094	251	4017	461329	368962	46275	46092

Table 1: Dataset statistics

Model	ICEWS14				ICWES05-15			
	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10
ComplEx	.470	.350	.530	.700	.490	.370	.550	.720
RotatE	.418	.291	.478	.690	.304	0.164	.355	.595
TTransE	.227	.072	.301	.582	.243	.086	.315	.609
TA-DisMult	.477	.363	-	.686	.474	.346	-	**.728**
HyTE	.297	.108	.416	.655	.316	.116	.445	.681
LorenTzE	.320	.102	.470	.704	.354	.168	.471	.708
HGAT	.389	.297	.424	.564	-	-	-	-
DE-TransE	.326	.124	.467	.686	.314	.108	.453	.685
DE-DistMult	.501	.392	.569	.708	.484	.366	.546	.718
CE-CGCN	**.529**	**.423**	**.596**	**.723**	**.492**	**0.373**	**.553**	.726

Table 2: Link Prediction results on the ICEWS14 and ICEWS05-15 datasets

4.2 Results

In Table 2, our model achieves the best performance in all metrics (except H@10) on both datasets. On ICEWS14, the CE-CGCN model outperforms the static models, which demonstrates the importance of temporal dependency embeddings produced by the Complex-valued DE. Additionally, compared to DE-TransE and DE-DisMult models, our approach achieves nearly 29.9% and 3.1% higher Hits@1, and 2.6% higher Hits@10 on average, which confirm the ability to enrich representations by integrating complex-valued embeddings and composition operators in GCNs. Regarding ICWES05-15, our model surpasses LorenTzE and DE models, achieving approximately 10.5% higher performance on average compared to these three aforementioned models. By leveraging the intricate interactions within complex geometry using GCNs, CE-CGCN demonstrates efficiency compared to high-dimensional space approach like Lorentz.

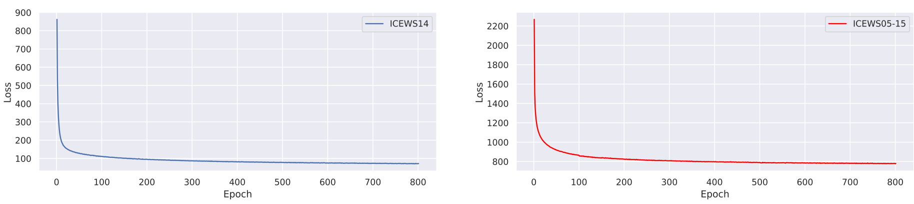

Fig. 2: The training loss curves for the ICEWS14 and ICEWS05-15 datasets

As shown in Fig. 2, the loss curve for ICEWS05-15 consistently remained lower than that of ICEWS14. Training convergence occurs rapidly within the

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first 200 epochs but requires at least 400 epochs on both benchmark datasets.

5 Conclusion

In this paper, we have presented CE-CGCN, which leverages the latent interactions between relations and entities through various composition operations in complex geometry. The experimental results have demonstrated the effectiveness of integrating complex-valued representations with temporal dynamics for TKGC. In the future, we investigate into the time evolution tendencies during the GCNs updating phase.

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