Improving Temporal Link Prediction via Temporal Walk Matrix Projection

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Background: Temporal Link Prediction

> Aims at predicting future links based on historical observations.



Future Graph

> Crucial for temporal graph learning and real-world applications.



- Relative Encodings
 - □ Indispensable module for effective temporal link prediction.
 - □ Additional node features (conditioned on the link to be predicted) to inject

the pairwise information that can not be capture by the message passing.



Timestamps:



Link В С A D [0,0] (D, F, t_3) [0,0][0,0] [0,0] [1,1][0,0] (D, A, t_3) [0,0][0,0][0,1][0,0][1.0] [0,0]

a) Message passing on the temporal graph can not capture the pairwise information.

b) Relative encoding $r_w^{(u,v,t)} = [g(u,w,t), g(v,w,t)],$ where $g(a, b, t) = \begin{cases} 1, & b \in \mathcal{N}_a(t) \\ 0, & \text{otherwise} \end{cases}$

Problems of Existing Relative Encodings

Concept. Existing relative encodings are derived from different heuristics.
The connections between different relative encodings are unclear.

2) **Method Design**. Most existing relative encodings are constructed based on structural connectivity, where the temporal information is ignored.

3) Computation. Constructing existing relative encodings always relies on time-consuming graph queries, making it the computational bottleneck.

A Unified View of Relative Encodings

Relative Encoding. Given an observed graph G_t and a link (u, v) to be predicted, the relative encoding for node *w* is the concatenation of two similarity features $r^{w|u}$ and $r^{w|v}$, which is $r^{w|(u,v)} = [r^{w|u}, r^{w|v}]$.

Unified View of the Similarity Feature. Existing similarity features $r^{w|u}$ can be unified into the function of temporal walk matrices. Formally, $r^{w|u} \in \mathbb{R}^k$ can be represented as

$$\boldsymbol{r}^{w|u} = g\left(\left[A_{u,w}^{(0)}(t), A_{u,w}^{(1)}(t), \cdots, A_{u,w}^{(k-1)}(t)\right]\right), \qquad A_{u,w}^{(i)}(t) = \sum_{W \in M_{u,w}^{i}} s(W),$$

A 4-step temporal walk from B to F

 $[(B,t), (C,t_A), (A,t_2), (D,t_2), (F,t_1)]$

Where $M_{u,w}^i$ is the set of i-step temporal walks from u to w and $s(\cdot)$ is a score function that maps a temporal walk to a scalar.

Timestamps: $t_1 < t_2 < t_3 < t_4 < t$ t_4 t_3 t_2 t_1 t_2 t_2 t_1 t_2 t_2 t_1 t_2 t_2 t_1

Temporal Graph G_t

A New Temporal Walk Matrix. We propose a new temporal walk matrix based on time decay effect, which simultaneously consider the temporal and structure information.

An Incremental Maintenance Algorithm. We propose an incremental algorithm to maintain the random projections of the proposed temporal walk matrices, which provably preserve the inner product between different rows of the matrices.

A Temporal Graph Network. We propose an effective and efficient temporal graph neural network, which construct relative encodings without time-consuming graph queries.

Experimental Results

SOTA performance on 13 benchmark datasets

Table 1: Transductive results for different baselines under the random negative sampling strategy. **blod** and <u>underline</u> highlight the best and second best result respectively.

Metric	Dataset	JODIE	DyRep	TGAT	TGN	CAWN	EdgeBank	TCL	GraphMixer	NAT	PINT	DyGForme	TPNet
	Wikipedia	96.50±0.14	94.86±0.00	96.94±0.05	98.45±0.06	98.76±0.03	90.37±0.00	96.47±0.10	97.25 ± 0.03	98.03±0.07	98.45 ± 0.04	99.03±0.02	99.32±0.03
	Reddit	$98.31{\scriptstyle \pm 0.14}$	$98.22_{\pm 0.04}$	$98.52{\scriptstyle\pm0.02}$	98.63 ± 0.00	$99.11{\scriptstyle \pm 0.01}$	94.86 ± 0.00	$97.53{\scriptstyle \pm 0.02}$	$97.31_{\pm 0.01}$	$99.13{\scriptstyle\pm0.10}$	$99.15{\scriptstyle \pm 0.02}$	99.22±0.01	99.27 ± 0.00
	MOOC	$80.23_{\pm 2.44}$	$81.97 \scriptstyle \pm 0.49$	85.84 ± 0.15	$89.15{\scriptstyle\pm1.00}$	$80.15{\scriptstyle \pm 0.25}$	$57.97{\scriptstyle \pm 0.00}$	82.38 ± 0.24	82.78±0.15	85.88±0.55	$88.08 \scriptstyle \pm 0.86$	$87.52_{\pm 0.40}$	96.39±0.00
	LastFM	70.85 ± 2.13	$71.92_{\pm 2.21}$	$73.42_{\pm 0.21}$	77.07±3.97	$86.99 \scriptstyle \pm 0.06$	79.29 ± 0.00	$67.27_{\pm 2.16}$	75.61±0.24	$88.02_{\pm 1.94}$	89.66 ± 1.41	93.00±0.12	94.50±0.08
	Enron	84.77±0.10	82.38±1.30	$71.12{\scriptstyle \pm 0.97}$	86.53 ± 1.11	$89.56 \scriptstyle \pm 0.00$	$83.53{\scriptstyle \pm 0.00}$	79.70±0.71	$82.25_{\pm 0.16}$	$90.60{\scriptstyle \pm 0.00}$	$92.20{\scriptstyle\pm0.15}$	92.47±0.12	92.90±0.17
	Social Evo.	89.89±0.55	88.87±0.30	93.16 ± 0.17	93.57 ± 0.17	84.96±0.00	74.95 ± 0.00	$93.13{\scriptstyle\pm0.10}$	93.37 ± 0.07	$88.92_{\pm 3.45}$	94.42 ± 0.03	94.73±0.01	94.73±0.02
AP	UCI	$89.43_{\pm 1.09}$	65.14±2.00	79.63 ± 0.70	92.34 ± 1.04	95.18 ± 0.06	$76.20{\scriptstyle \pm 0.00}$	89.57±1.60	93.25±0.07	$93.40{\scriptstyle \pm 0.26}$	96.45 ± 0.11	95.79±0.17	97.35±0.04
	Flights	95.60±1.73	95.29 ± 0.72	94.03±0.18	$97.95{\scriptstyle\pm0.14}$	98.51±0.01	89.35 ± 0.00	$91.23_{\pm 0.02}$	90.99±0.05	98.57 ± 0.12	98.80±0.02	98.91±0.01	98.93±0.02
	Can. Parl.	69.26 ± 0.31	66.54±2.76	70.73±0.72	70.88±2.34	69.82±2.34	64.55 ± 0.00	68.67 ± 2.67	77.04±0.46	79.72 ± 1.76	$68.36{\scriptstyle\pm1.43}$	97.36±0.4	90.28 ± 0.37
	US Legis.	75.05±1.12	75.34 ± 0.39	68.52±3.16	75.99±0.5#	70.58±0.48	58.39 ± 0.00	69.59 ± 0.48	70.74±1.02	78.71±0.87	74.85±0.97	71.11±0.50	80.58±0.28
	UN Trade	64.94 ± 0.31	63.21 ± 0.00	61.47±0.18	65.03±1.37	$65.39_{\pm 0.12}$	60.41 ± 0.00	62.21 ± 0.00	62.61 ± 0.27	$73.95{\scriptstyle\pm1.16}$	70.20 ± 0.58	66.46±1.20	87.24±0.05
	UN Vote	63.91 ± 0.81	62.81 ± 0.80	52.21 ± 0.08	65.72 ± 2.17	$52.84_{\pm 0.10}$	58.49 ± 0.00	51.90 ± 0.30	$52.11_{\pm 0.16}$	70.45±0.68	$66.25 \scriptstyle \pm 0.78$	55.55 ± 0.42	$75.12_{\pm 0.20}$
	Contact	$95.31{\scriptstyle\pm1.33}$	$95.98 \scriptstyle \pm 0.15$	$96.28 \scriptstyle \pm 0.09$	$96.89{\scriptstyle \pm 0.56}$	$90.26 \scriptstyle \pm 0.28$	$92.58 \scriptstyle \pm 0.00$	$92.44{\scriptstyle\pm0.13}$	$91.92{\scriptstyle\pm0.03}$	$97.39 \scriptstyle \pm 0.22$	$\underline{98.64}_{\pm 0.02}$	$98.29 \scriptstyle \pm 0.01$	$98.66_{\pm 0.01}$
	Avg. Rank	7.85	8.77	8.54	5.00	7.00	10.54	9.77	8.31	4.15	3.69	3.15	1.08
AUC	Wikipedia	96.33±0.07	94.37 ± 0.00	96.67±0.07	98.37±0.07	98.54±0.04	90.78 ± 0.00	95.84±0.18	96.92±0.03	$97.75{\scriptstyle\pm0.33}$	98.16±0.04	98.91±0.02	$99.30{\scriptstyle \pm 0.02}$
	Reddit	98.31 ± 0.05	98.17 ± 0.05	98.47 ± 0.03	98.60 ± 0.00	$99.01_{\pm 0.01}$	$95.37 \scriptstyle \pm 0.00$	97.42 ± 0.02	97.17 ± 0.02	$99.09{\scriptstyle \pm 0.10}$	99.09 ± 0.03	$99.15_{\pm 0.01}$	99.22 ± 0.00
	MOOC	$83.81_{\pm 2.00}$	85.03±0.58	87.11 ±0.10	91.21 ± 1.10	80.38±0.20	60.86 ± 0.00	$83.12{\scriptstyle \pm 0.18}$	84.01+0.17	87.42 ± 0.58	$90.55{\scriptstyle \pm 0.43}$	87.91±0.58	97.17 ± 0.08
	LastFM	$70.49{\scriptstyle\pm1.66}$	71.16±1.89	$71.59{\scriptstyle\pm0.18}$	78.47 ± 2.94	$85.92{\scriptstyle\pm0.10}$	$83.77{\scriptstyle\pm0.00}$	64.06 ± 1.10	73.53 ± 0.12	86.92 ± 2.72	89.28 ± 1.63	93.05±0.10	$94.39{\scriptstyle \pm 0.04}$
	Enron	87.96 ± 0.82	84.89±3.00	68.89±1.10	$88.32{\scriptstyle\pm0.09}$	$90.45_{\pm 0.14}$	87.05±0.00	75.74 ± 0.72	84.38 ± 0.21	91.68 ± 0.83	92.87 ± 0.04	93.33±0.13	93.98±0.26
	Social Evo.	$92.05{\scriptstyle \pm 0.46}$	90.76 ± 0.21	94.76 ± 0.16	$95.39{\scriptstyle \pm 0.17}$	87.34±0.08	81.60 ± 0.00	$94.84{\scriptstyle \pm 0.17}$	$95.23_{\pm 0.07}$	90.84±3.72	$96.16{\scriptstyle \pm 0.02}$	96.30±0.01	$96.43{\scriptstyle \pm 0.02}$
	UCI	90.44±0.49	68.77 ± 2.34	78.53 ± 0.74	92.03±1.13	93.87 ± 0.08	77.30 ± 0.00	87.82±1.36	91.81 ± 0.67	$92.31{\scriptstyle \pm 0.37}$	95.57±0.16	94.49 ± 0.26	96.79±0.05
	Flights	96.21±1.42	$95.95{\scriptstyle\pm0.62}$	94.13±0.17	98.22 ± 0.13	98.45 ± 0.01	$90.23{\scriptstyle \pm 0.00}$	$91.21{\scriptstyle\pm0.02}$	91.13 ± 0.01	$98.69{\scriptstyle\pm0.10}$	98.89±0.02	98.93 ± 0.01	99.00±0.02
	Can. Parl.	78.21 ± 0.23	$73.35{\scriptstyle\pm3.67}$	75.69 ± 0.78	76.99 ± 1.80	75.70±3.27	$64.14_{\pm 0.00}$	$72.46_{\pm 3.23}$	83.17 ± 0.53	$84.04{\scriptstyle\pm1.13}$	$77.96_{\pm 1.46}$	97.76±0.41	92.05 ± 0.34
	US Legis.	$82.85{\scriptstyle\pm1.07}$	82.28 ± 0.32	75.84±1.99	$83.34{\scriptstyle\pm0.43}$	77.16±0.39	62.57 ± 0.00	76.27±0.63	76.96±0.70	$85.36 \scriptstyle \pm 0.42$	82.10 ± 0.85	77.90±0.58	86.49±0.18
	UN Trade	69.62 ± 0.44	67.44±0.83	$64.01_{\pm 0.12}$	$69.10_{\pm 1.67}$	68.54 ± 0.18	$66.75 \scriptstyle \pm 0.00$	64.72±0.05	$65.52_{\pm 0.01}$	77.61±1.00	$74.87_{\pm 0.53}$	70.20±1.44	89.17 ± 0.46
	UN Vote	68.53±0.00	$67.18_{\pm 1.04}$	52.83 ± 1.12	$69.71_{\pm 2.00}$	53.09 ± 0.22	$62.97_{\pm 0.00}$	51.88 ± 0.30	52.46 ± 0.27	75.32 ± 0.68	70.69 ± 1.02	$57.12_{\pm 0.62}$	79.88±0.30
	Contact	$96.66 \scriptstyle \pm 0.89$	$96.48_{\pm 0.14}$	$96.95 \scriptstyle \pm 0.08$	$97.54 \scriptstyle \pm 0.35$	$89.99{\scriptstyle\pm0.34}$	$94.34{\scriptstyle\pm0.00}$	$94.15{\scriptstyle\pm0.09}$	$93.94{\scriptstyle\pm0.02}$	$97.79 \scriptstyle \pm 0.10$	$98.90{\scriptstyle \pm 0.02}$	$98.53 \scriptstyle \pm 0.01$	$98.91_{\pm0.01}$
	Avg. Rank	7.15	8.69	8.92	5.08	7.15	10.31	10.15	8.62	4.08	3.46	3.23	1.08

$33 \times \text{speedup compared to SOTA baseline}$





Code and tutorial

https://github.com/lxd99/TPNet

Thanks for listening !