Time-aware Random Walk Diffusion to Improve Dynamic Graph Learning

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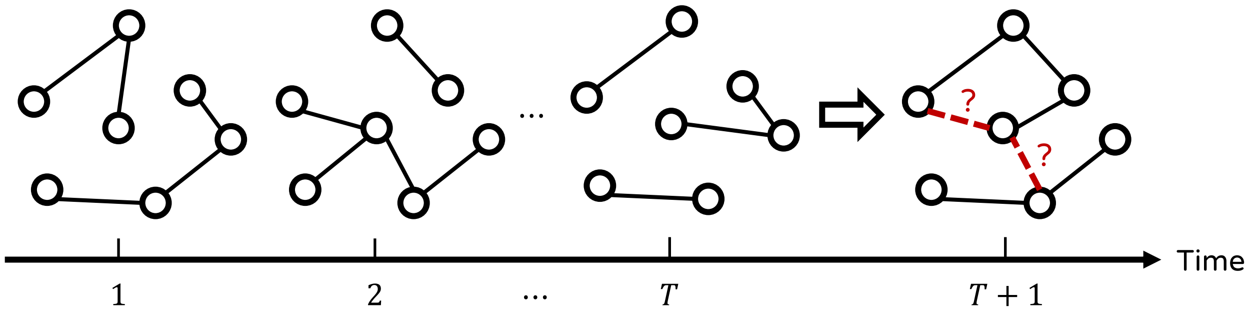
Outline

- ❑ Introduction
- ❑ Motivation
- ❑ Proposed Method
- ❑ Experiments
- ❑ Conclusion

Research Question

❑ Real-world graphs change over time!

- Learning dynamic graphs is important in **link prediction**, **traffic forecasting**, **temporal knowledge completion**, etc.
- As a sequence of graph snapshots (discrete-time dynamic graph)



Link prediction on a dynamic graph

❑ Data Augmentation is essential for ML models

- How can we augment a dynamic graph to improve dynamic graph learning?

Problem Definition

❑ Dynamic graph learning aims to learn

$$\mathbf{H}_t = \mathcal{F}_\Theta(\boldsymbol{A}_t, \mathbf{F}_t, \mathbf{H}_{t-1})$$

- $\mathcal{F}_\Theta$ is a dynamic GNN model with parameter Θ
- $\boldsymbol{A}_t$ is an adjacency matrix of a dynamic graph $\mathcal{G}$ at time t
- $\mathbf{F}_t$ and $\mathbf{H}_t$ are node features and hidden embeddings, resp.

❑ Dynamic graph augmentation

- **Input**: a sequence $\{\boldsymbol{A}_1, \cdots, \boldsymbol{A}_T\}$ of adjacency matrices in $\mathcal{G}$
- **Output**: a new sequence $\{\boldsymbol{\mathcal{X}}_1, \cdots, \boldsymbol{\mathcal{X}}_T\}$ of augmented adjacency matrices
  - **We want the new adjacency matrices to improve the performance of a model $\mathcal{F}_\Theta(\cdot)$**

Previous Approaches

- Most existing methods mainly transform spatial structure of a single static graph
  - Drop-based methods
    - e.g., randomly drop a few of edges or nodes at each epoch
  - Diffusion-based methods
    - e.g., add new edges weighted by graph diffusion

- However, those aren't suitable for dynamic graphs
  - Naively applying a static method to each graph snapshot could not capture temporal dynamics!

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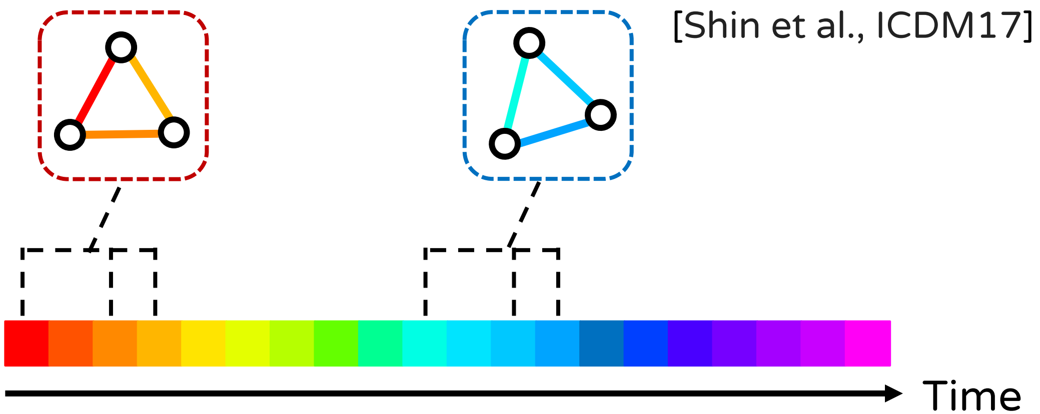
Motivation (1)

❑ Dynamic graph augmentation

- Consider **temporal dynamics** as well as **spatial structure**
- Inspired from temporal and spatial localities

❑ Temporal locality

- Objects (e.g., triangle) tend to be **more affected by more recent edges than older ones** in real dynamic graphs
  - e.g., triangles with edges close in time than with edges far in time

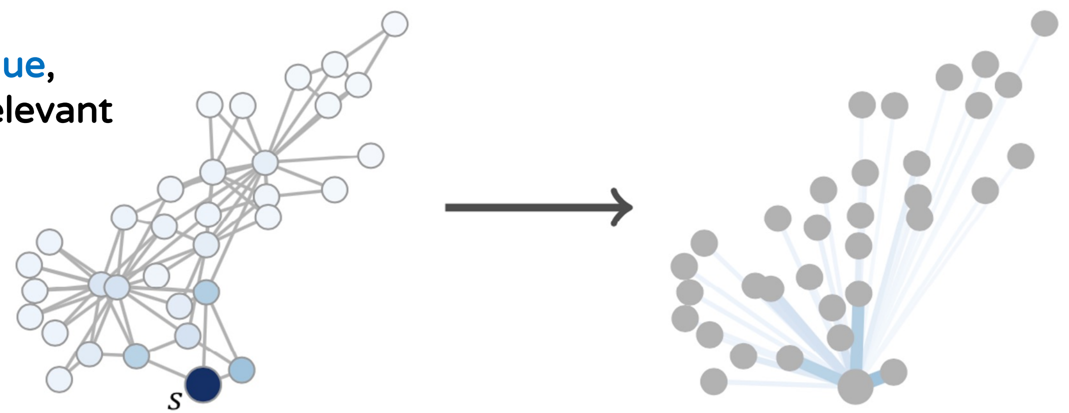


Motivation (2)

❑ Spatial locality

- Objects (e.g., node) tend to be **more affected by nearby nodes than distant ones**
- Graph diffusion using RWR enhances **spatial locality**
  - **Random Walk with Restart (RWR)** uses a random surfer who does random walk or restart from seed node s
  - $\Rightarrow$ Node-to-node proximity (diffusion) scores **spatially localized** to s

More blue,
More relevant



Diffusion scores w.r.t. seed node s Diffusion scores $\Rightarrow$ edge weights

[Klicpera et al., NeurIPS19]

Research Challenges

- ❑ **Previous work ignores temporal locality**
  - But, newly augmented edges need to be more affected by more recent edges
- ❑ **Graph diffusion enhances spatial locality**
  - But, it leads to a fully dense adjacency matrix that can degrade computational efficiency

Challenges:
- **Q1.** How can we augment spatio-temporal locality?
- **Q2.** How can we avoid to generate dense matrices while preserving enhanced data?

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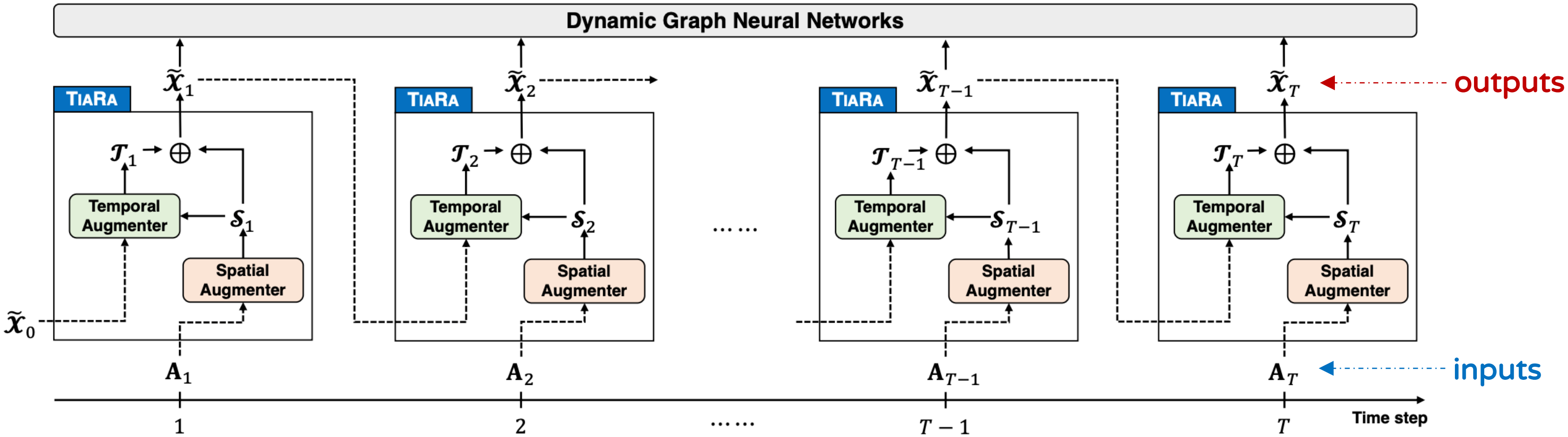
Proposed Method

❑ TiaRa (Time-aware Random Walk Diffusion)

- **Aims to enhance spatio-temporal locality!**



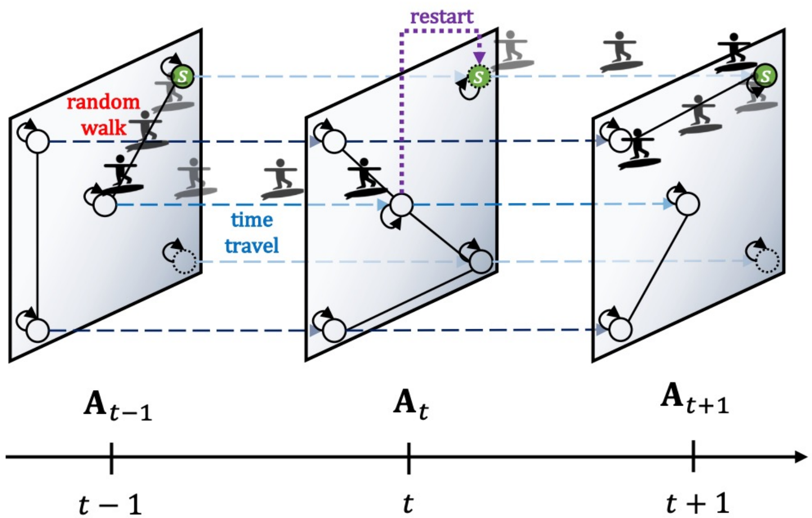
❑ Our approaches

- 1) Make a random surfer time-aware (TRWR)
- 2) Derive spatio-temporally diffusion matrices from TRWR
- 3) Sparsify the diffusion matrices for efficiency

Time-aware RWR (TRWR)

❑ Virtually connect nodes toward the future

- Then, the surfer also can travel along the time axis
  - Not backward since future (test) data should be prevented
- Leads to diffusion scores spatio-temporally localized
  - Now, we can insert new edges based on the diffusion scores!



Classical RWR [Tong et al., ICDM06]

$$\underbrace{\mathbf{x}_s}_{\text{Diffusion scores w.r.t. } s} = \underbrace{(1-\alpha)\tilde{\boldsymbol{\mathcal{A}}}^\top \mathbf{x}_s}_{\text{Random walk}} + \underbrace{\alpha \mathbf{i}_s}_{\text{Restart}}$$

⇩

Time-aware RWR

$$\underbrace{\mathbf{x}_{t,s}}_{\text{Diffusion scores w.r.t. } s \text{ at time } t} = \underbrace{(1-\alpha-\beta)\boldsymbol{\mathcal{A}}_t^\top \mathbf{x}_{t,s}}_{\text{Random walk}} + \underbrace{\alpha \mathbf{i}_s}_{\text{Restart}} + \underbrace{\beta \mathbf{x}_{t-1,s}}_{\text{Time travel}}$$

Diffusion Matrix of TRWR

Details

- Diffusion matrix $\mathcal{X}_t$ of TRWR is represented as:

$$\boldsymbol{\mathcal{X}}_t = (1-\gamma)\underbrace{(\boldsymbol{\mathcal{L}}_t^{\text{rwr}}\boldsymbol{I}_n)}_{\substack{\text{Spatial augmenter} \\ \boldsymbol{\mathcal{S}}_t}} + \gamma\underbrace{(\boldsymbol{\mathcal{L}}_t^{\text{rwr}}\boldsymbol{\mathcal{X}}_{t-1})}_{\substack{\text{Temporal augmenter} \\ \boldsymbol{\mathcal{T}}_t}}$$

- Notations
  - $\boldsymbol{\mathcal{X}}_t = \{\boldsymbol{x}_{t,s}\}$ contains diffusion scores of TRWR w.r.t. all nodes s
  - $\gamma = \beta/(\alpha+\beta)$ is a ratio of temporal locality
  - $\boldsymbol{\mathcal{L}}_t^{\text{rwr}}$ is a diffusion matrix of RWR at only time t

- In other words, $\boldsymbol{\mathcal{X}}_t$ is a linear combination of $\boldsymbol{\mathcal{S}}_t$ and $\boldsymbol{\mathcal{T}}_t$

Diffusion Matrix of TRWR

Details

❑ Theorem for dynamic graph augmentation

$$\mathcal{X}_t \propto \overbrace{\underbrace{\gamma^0 \mathcal{L}_t^{\text{rwr}} + \gamma^1 \mathcal{L}_{t \leftsquigarrow t-1}^{\text{rwr}} + \cdots + \gamma^{t-2} \mathcal{L}_{t \leftsquigarrow 2}^{\text{rwr}} + \frac{\gamma^{t-1}}{1-\gamma} \boxed{\mathcal{L}_{t \leftsquigarrow 1}^{\text{rwr}}}}_{\Longleftarrow \text{Emphasized} \qquad\qquad \text{Decayed} \Longrightarrow}}^{\text{Augmentation of spatial and temporal localities}} \qquad 0 < \gamma < 1$$

$$\boxed{\mathcal{L}_t^{\text{rwr}} \times \mathcal{L}_{t-1}^{\text{rwr}} \times \cdots \times \mathcal{L}_1^{\text{rwr}}}$$

- Can capture temporal locality as well as spatial locality
  - $\mathcal{L}_t^{\text{rwr}}$ indicates a matrix in which a spatial locality is enhanced
  - $\mathcal{X}_t$ is more affected by more recent data than older ones where a temporal locality is enhanced
    - Old information is decaying over time by γ (temporal decay ratio)
  - See the detailed proof in the paper!

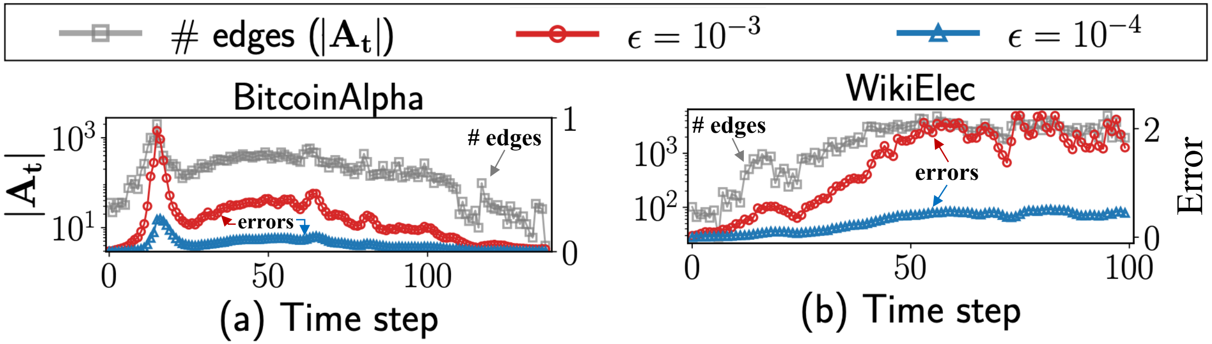
Sparsification and Its Effects

❑ Set elements of $\mathcal{X}_t$ less than ϵ to zero

- As scores are localized, very tiny entries are unlikely to affect the performance [Klicpera et al., NeurIPS19]

❑ Analytical results

- # of non-zeros of $\mathcal{X}_t$ becomes $O(n/\epsilon)$
  - Where n is # of nodes, and it's much smaller than $O(n^2)$
- Its approximation errors don't explode over time
  - Less affected by previous errors; rather, it is ∝ # of edges



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Experimental Setup

❑ Baseline augmentation methods

- DropEdge, GDC, and Merge

❑ Dynamic GNN models

- GCN, GCRN and EvolveGCN (EGCN)

❑ Datasets

	# nodes	# edges	# time steps	# labels
Datasets	n	m	T	L
BitcoinAlpha	3,783	31,748	138	2
WikiElec	7,125	212,854	100	2
RedditBody	35,776	484,460	88	2
Brain	5,000	1,955,488	12	10
DBLP-3	4,257	23,540	10	3
DBLP-5	6,606	42,815	10	5
Reddit	8,291	264,050	10	4

Temporal Link Prediction

❑ Aims to predict if an edge appears in the future

- Augment the adjacency matrix at each time
- Train a GNN with data from time 1 to $t-1$
- Predict test edges time t

▲ improvement
▼ degradation

	AUC	BitcoinAlpha			WikiElec			RedditBody		
		GCN	GCRN	EGCN	GCN	GCRN	EGCN	GCN	GCRN	EGCN
	NONE	57.3±1.6	80.3±6.0	58.8±1.1	59.9±0.9	72.1±2.4	66.9±3.7	77.6±0.4	88.9±0.3	77.6±0.2
Augmentation baseline	DROPEDGE	▼56.3±1.0	▼73.9±2.2	▼57.4±0.9	▼50.1±1.0	▼56.0±9.3	▼47.9±6.4	▼73.0±0.4	▼77.0±1.7	▼71.9±0.7
	GDC	▲57.5±1.6	▼77.3±6.5	▼57.4±1.2	▲62.8±0.8	▼67.9±1.0	▼63.1±0.7	▼74.6±0.0	▼86.4±0.3	▼73.8±0.3
	MERGE	▲66.8±2.6	▲93.1±0.4	▲61.0±9.2	▲60.6±1.7	▼68.4±3.2	▼60.7±1.3	▼69.7±0.7	▲89.8±0.5	▲80.3±0.5
	TIARA	▲**76.0±1.3**	▲**94.6±0.8**	▲**77.2±1.4**	▲**69.0±1.2**	▲**73.4±2.2**	▲**69.1±0.3**	▲**80.8±0.6**	▲**90.2±0.4**	▲**82.0±0.1**

TiaRa consistently improves the performance of dynamic GNNs, and outperforms other augmentation methods

Node Classification

❑ Aims to classify a label of a node

- A graph and features change over time
- Train a GNN with training nodes from time 1 and t
- Classify test nodes at time t

▲ improvement
▼ degradation

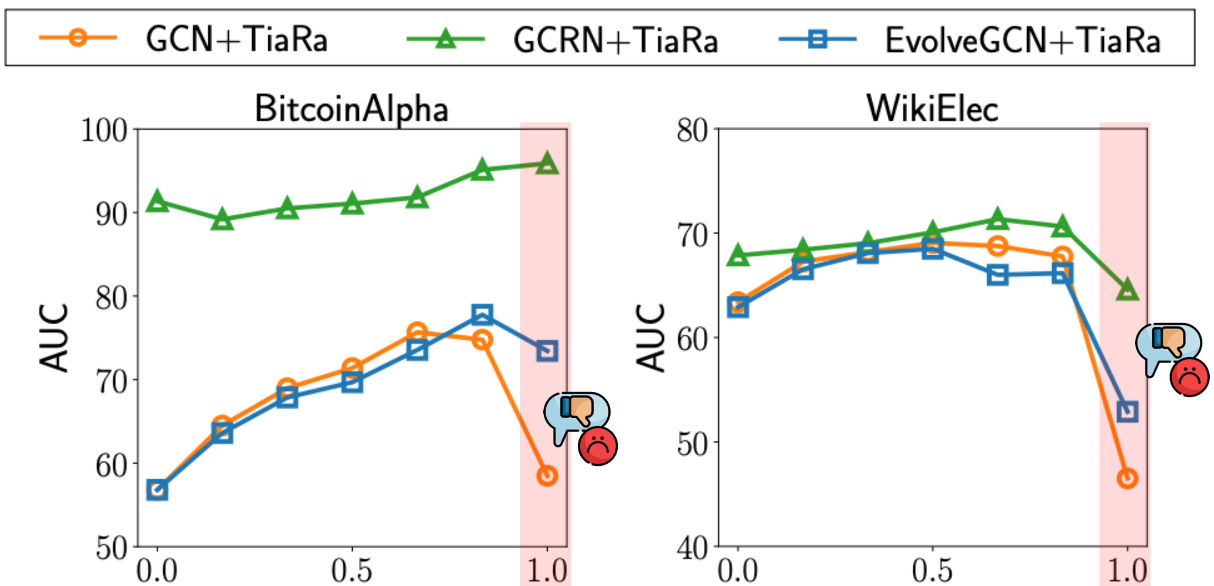
Augmention baseline	Macro F1	Brain			Reddit			DBLP-3			DBLP-5		
		GCN	GCRN	EGCN	GCN	GCRN	EGCN	GCN	GCRN	EGCN	GCN	GCRN	EGCN
	None	44.7±0.8	66.8±1.0	43.4±0.7	18.2±2.9	40.4±1.6	18.6±2.3	53.4±2.6	83.1±0.6	51.3±2.7	69.6±0.9	75.4±0.7	68.5±0.6
	DropEdge	▼35.2±1.7	▲67.8±0.6	▼39.7±1.8	▲**19.4±0.8**	▼40.3±1.4	▼18.0±2.7	▲55.8±1.9	▲84.3±0.6	▲52.4±1.7	▲70.5±0.5	▲75.6±0.7	▼68.0±0.7
	GDC	▲63.2±1.2	▲88.0±1.5	▲67.3±1.3	▼17.5±2.3	▲41.0±1.6	▼18.5±2.8	▲53.4±2.1	▲84.7±0.5	▲52.8±2.2	▲70.0±0.7	▲75.5±1.2	▲69.1±1.0
	Merge	▼34.4±3.4	▼63.2±1.6	▲53.0±0.9	▲19.3±3.0	▼39.6±0.8	▲20.4±3.0	▲54.9±3.1	▼83.0±1.4	▲53.3±1.2	▲70.8±0.4	▼74.5±0.8	▲69.7±1.6
	TiaRa	▲**68.7±1.2**	▲**91.3±1.0**	▲**72.0±0.6**	▲18.4±3.0	▲**41.5±1.5**	▲**21.9±1.6**	▲**57.5±2.2**	▲**84.9±1.6**	▲**56.4±1.8**	▲**71.1±0.6**	▲**77.9±0.4**	▲**70.1±1.0**

TiaRa also works on the node classification task!

Effect of Hyperparameters (1)

❑ Effect of temporal decay ratio γ

- Mostly, AUC decreases drastically when $\gamma \rightarrow 1$
- Using the information of all time steps is a poor choice
- Important to properly mix spatial & temporal information

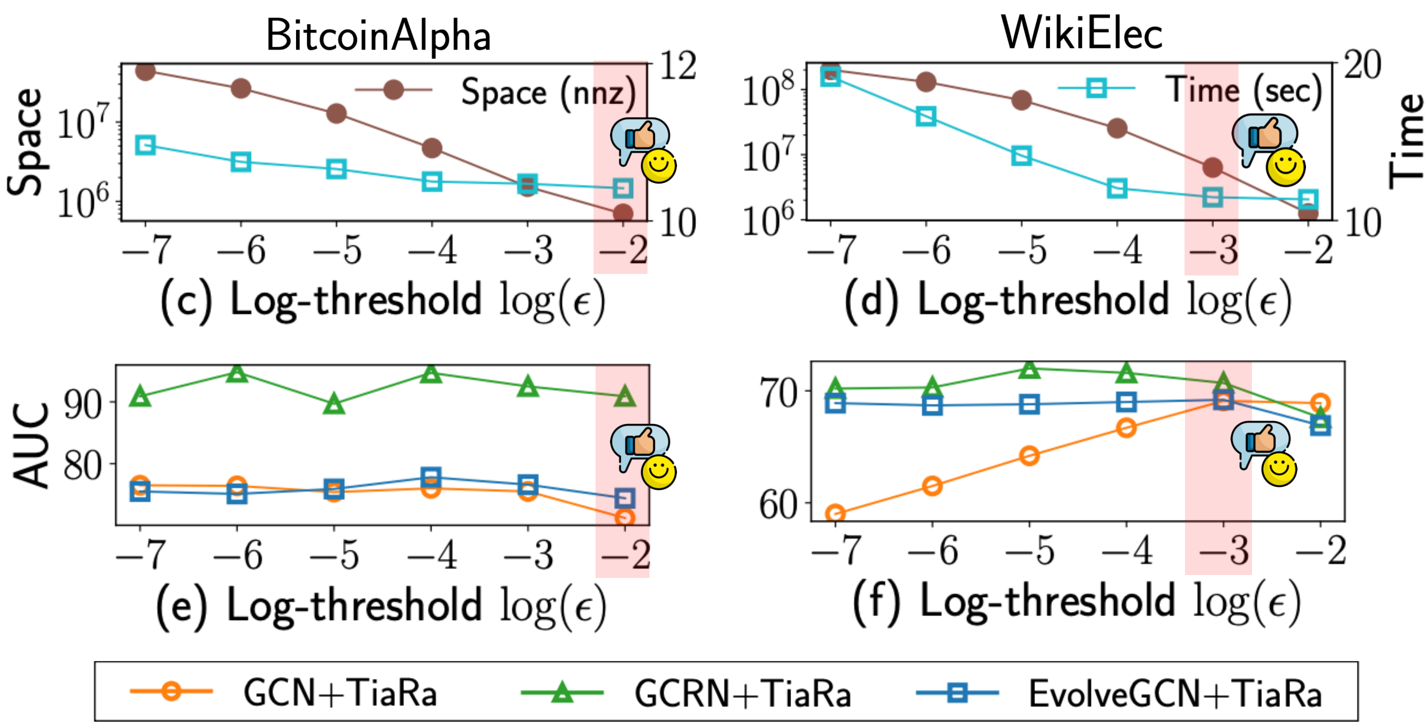


(a) Temporal decay ratio γ (b) Temporal decay ratio γ

Effect of Hyperparameters (2)

❑ Effect of filtering threshold ϵ

- Large ϵ improves efficiency while keeping accuracy



Sparsification makes TiaRa efficient and paractically usable!

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Conclusion

❑ TiaRa (Time-aware Random Walk Diffusion)

- 1) Make a random surfer time-aware (TRWR)
- 2) Derive spatio-temporally diffusions from TRWR
- 3) Sparsify the diffusion matrices for efficiency

❑ Aids dynamic GNNs in providing better accuracy

- Temporal locality as well as spatial locality are caputred
- Sparsification makes TiaRa efficient & paractically usable
- TiaRa improves the performance of dynamic GNNs

Thank You

Jong-whi Lee

Code: https://github.com/dev-jwel/TiaRa

Appendix

Computation of TiaRa

❑ Computing the augmented adjacency matrix $\mathcal{X}_t$

- Use Power iteration
  - Avoid matrix inversion
  - Repeatedly multiply the adjacency matrix
  - Guarantee convergence to the final answer

Algorithm 1: TIARA at time t

Require: adjacency matrix $\mathbf{A}_t$, previous time-aware diffusion matrix $\tilde{\boldsymbol{\mathcal{X}}}_{t-1}$, restart probability α, time travel probability β, number K of iterations, filtering threshold ϵ

Ensure: time-aware diffusion matrix $\tilde{\boldsymbol{\mathcal{X}}}_t^\top$

$\tilde{\boldsymbol{\mathcal{A}}}_t \leftarrow \mathbf{D}_t^{-1}\mathbf{A}_t$ where $\mathbf{D}_t = \mathrm{diag}(\mathbf{A}_t\mathbf{1})$

$\boldsymbol{\mathcal{L}}_t^{\mathrm{rwr}} \leftarrow$ POWER-ITERATION$(\tilde{\boldsymbol{\mathcal{A}}}_t, \alpha, \beta, K)$

$\boldsymbol{\mathcal{S}}_t \leftarrow \boldsymbol{\mathcal{L}}_t^{\mathrm{rwr}}$ ▷ **Spatial augmenter**

$\boldsymbol{\mathcal{T}}_t \leftarrow \boldsymbol{\mathcal{S}}_t\tilde{\boldsymbol{\mathcal{X}}}_{t-1}$ ▷ **Temporal augmenter**

$\boldsymbol{\mathcal{X}}_t \leftarrow (1-\gamma)\boldsymbol{\mathcal{S}}_t + \gamma\boldsymbol{\mathcal{T}}_t$ where $\gamma = \beta/(\alpha+\beta)$

$\tilde{\boldsymbol{\mathcal{X}}}_t \leftarrow$ filter entries of $\boldsymbol{\mathcal{X}}_t$ if their weights are $< \epsilon$

normalize $\tilde{\boldsymbol{\mathcal{X}}}_t$ column-wise

return $\tilde{\boldsymbol{\mathcal{X}}}_t^\top$

function POWER-ITERATION$(\tilde{\boldsymbol{\mathcal{A}}}_t, \alpha, \beta, K)$

  set $c \leftarrow 1-\alpha-\beta$ and $\mathbf{M}_t^{(0)} \leftarrow \boldsymbol{\mathcal{I}}_n$

  for $k \leftarrow 1$ to K **do**

    $\mathbf{M}_t^{(k)} \leftarrow \boldsymbol{\mathcal{I}}_n + c\tilde{\boldsymbol{\mathcal{A}}}_t^\top\mathbf{M}_t^{(k-1)}$

  $\boldsymbol{\mathcal{L}}_t^{\mathrm{rwr}} \leftarrow (1-c)\mathbf{M}_t^{(K)}$ where $\mathbf{M}_t^{(K)} \approxeq \mathbf{L}_t^{-1}$

  normalize $\boldsymbol{\mathcal{L}}_t^{\mathrm{rwr}}$ column-wise and **return** $\boldsymbol{\mathcal{L}}_t^{\mathrm{rwr}}$

end function

Computational Complexity

❑ Time complexity of TiaRa

- $O(n_t n/\epsilon + n_t^2 K)$ time at each time step
  - n_t: # of activated nodes (forming edges at time t)
  - n: # of total nodes
  - ϵ: filtering threshold (typically, 10^{-2} or 10^{-3})
  - K: # of power iteration

Datasets	n	$\lfloor \bar{n}_t \rfloor$
BitcoinAlpha	3,783	105
WikiElec	7,125	354
RedditBody	35,776	2,465
Brain	5,000	5,000
DBLP-3	4,257	782
DBLP-5	6,606	1,212
Reddit	8,291	2,071

- Takes $O(n)$ time in real-world dynamic graphs
  - $n_t \ll n$, and ϵ^{-1} and K are constant
- Takes $O(n^2)$ time in dense graphs ($n_t = n$)

❑ Space complexity of TiaRa

- Takes $O(n/\epsilon)$ space for augmentation at each time step

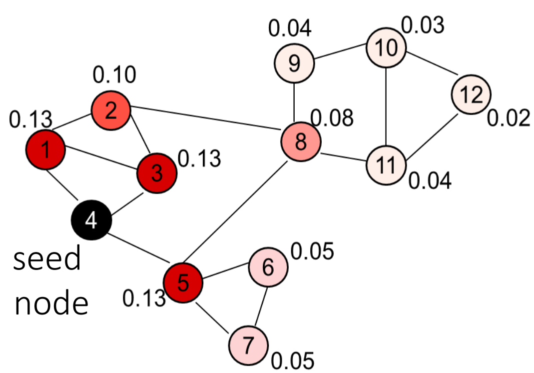
RWR Diffusion Matix $\mathcal{L}_t^{\mathrm{rwr}}$

❑ The term is derived from the equation of TRWR

$$\mathbf{x}_{t,s} = (1-\alpha-\beta)\boldsymbol{\mathcal{A}}_t^{\top}\mathbf{x}_{t,s} + \alpha\mathbf{i}_s + \beta\mathbf{x}_{t-1,s}$$

$$\Rightarrow \left(\boldsymbol{I}_n - (1-\alpha-\beta)\boldsymbol{\mathcal{A}}_t^{\top}\right)\mathbf{x}_{t,s} = \alpha\mathbf{i}_s + \beta\mathbf{x}_{t-1,s}$$

- Suppose $\mathbf{L}_t = \boldsymbol{I}_n - (1-\alpha-\beta)\boldsymbol{\mathcal{A}}_t^{\top}$
- Then, $\mathcal{L}_t^{\mathrm{rwr}} = (\alpha+\beta)\mathbf{L}_t^{-1}$
    - RWR scores of all pairs of nodes with restart probability $\alpha+\beta$



	Node 4
Node 1	0.13
Node 2	0.10
Node 3	0.13
Node 4	0.22
Node 5	0.13
Node 6	0.05
Node 7	0.05
Node 8	0.08
Node 9	0.04
Node 10	0.03
Node 11	0.04
Node 12	0.02

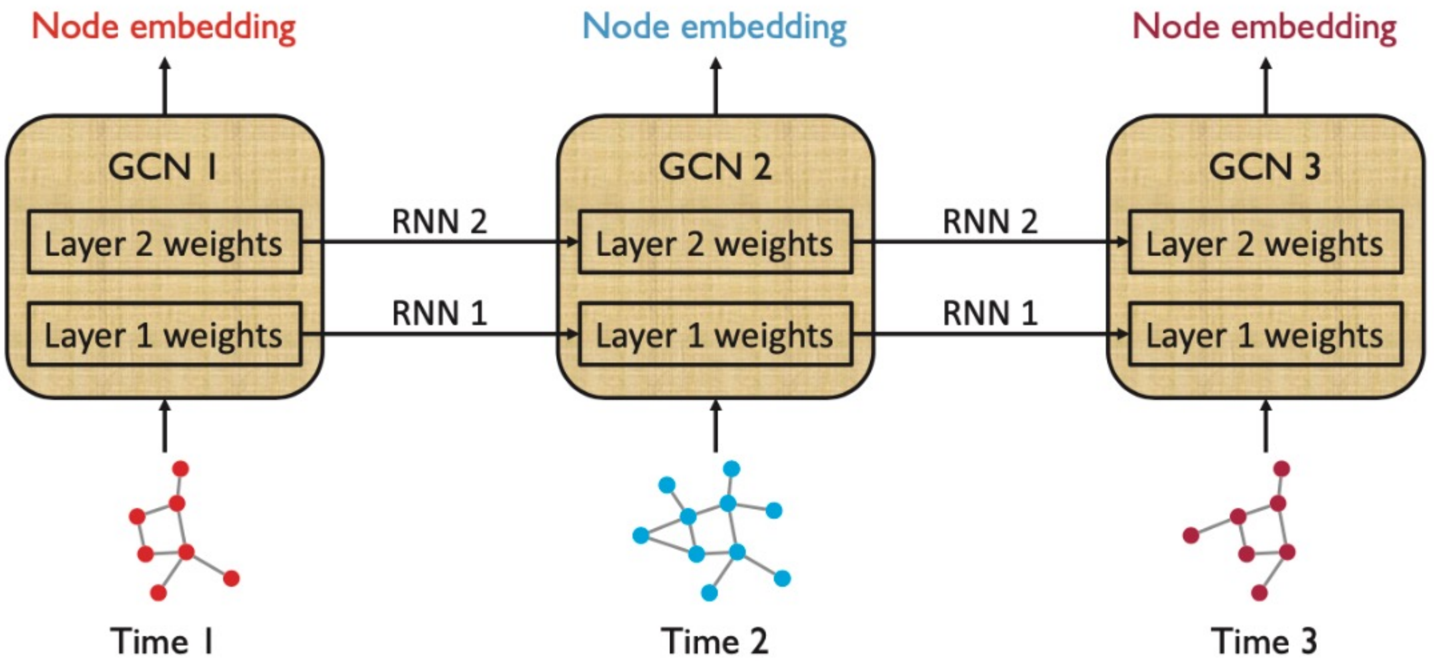
[Tong et al., ICDM06]

Input: an adjacency matrix **Output**: RWR scores w.r.t. seed

Dynamic Graph Learning

❑ Dynamic Graph Neural Networks

- Combined with GCNs and RNNs (e.g., GCRN, EvolveGCN)
- Formally expressed as a learnable function $\mathcal{F}_\Theta(\cdot)$



Overview of EvolveGCN

[Pareja et al., AAAI20]