SEIGN: A Simple and Efficient Graph Neural Network for Large Dynamic Graphs





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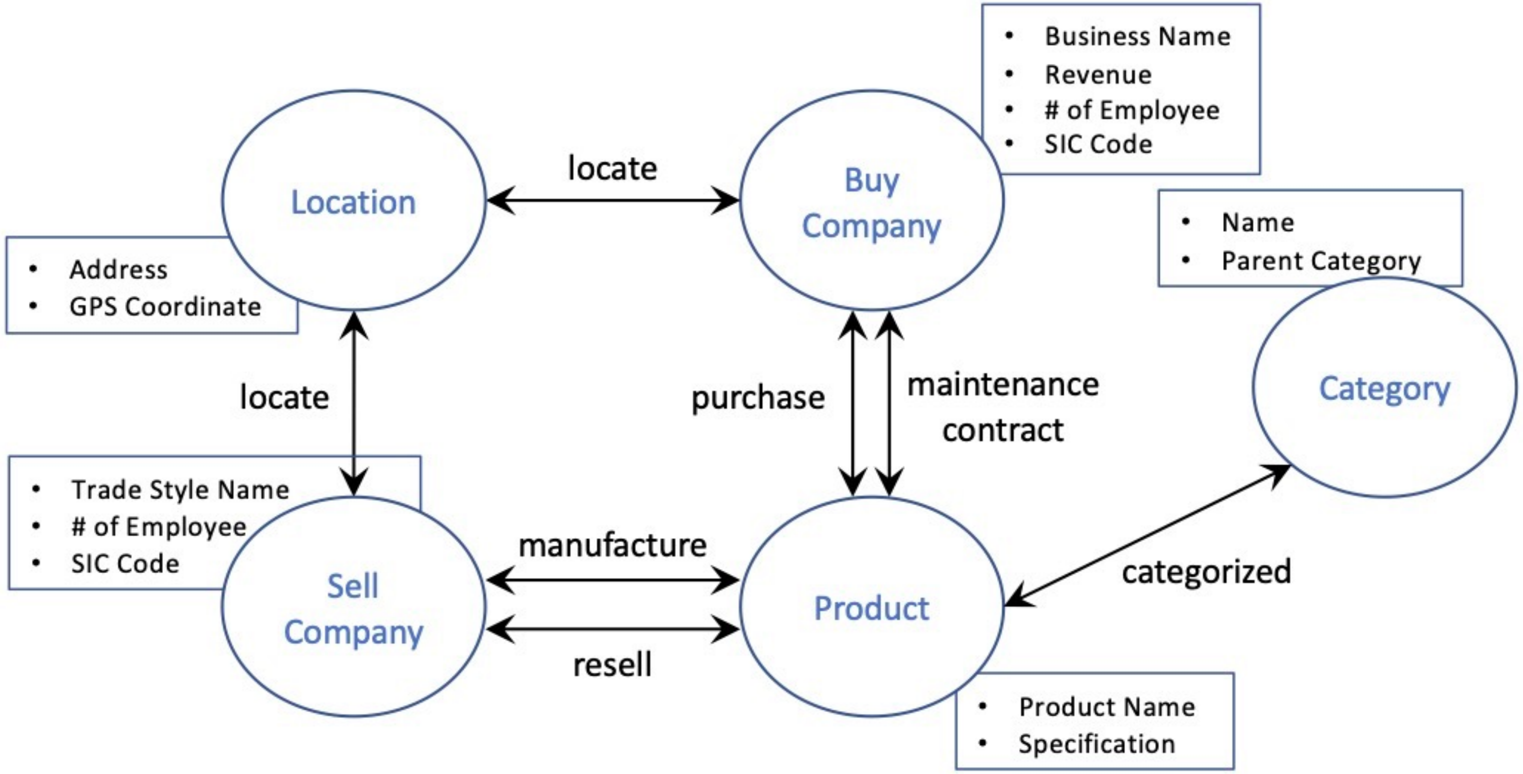
This work was completed when Xiao Qin, Chuan Lei and Giacomo Domeniconi were with IBM Research.

Outline

- ❑ Background
  - ❑ Discrete Time Dynamic Graphs (DTDGs)
  - ❑ Graph Neural Networks for DTDGs
  - ❑ Research Challenges
- ❑ Our Approach – SEIGN
  - ❑ Evolving Graph Model & Embedding
  - ❑ Inception Like Graph Neural Network
  - ❑ Parameter-free Message Passing
- ❑ Experimental Evaluation

Motivating Example – IT Procurement



Sheikh, Nasrullah, et al. Distributed Training of Knowledge Graph Embedding Models using Ray. EDBT 2022.

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Background – Discrete Time Dynamic Graphs (DTDGs)

- **Discrete-time Dynamic Graphs (DTDGs)**

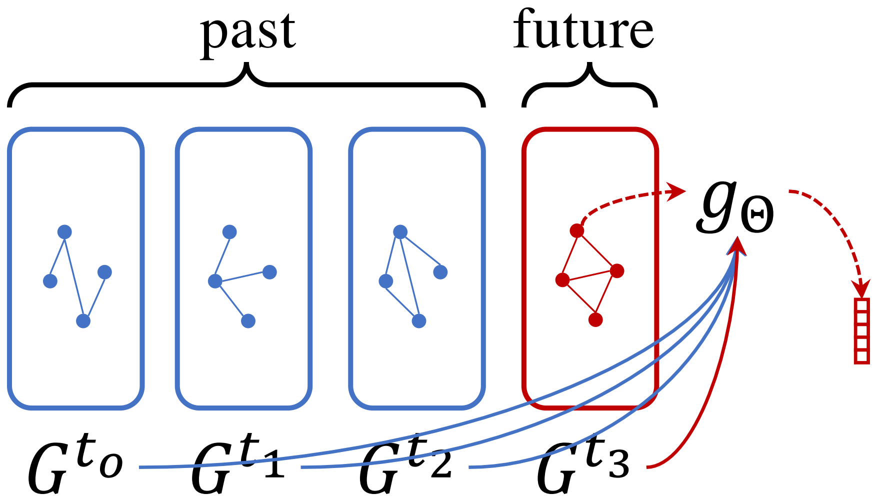
  $G^T = (G^{t0}, \ldots, G^{tn})$ # a sequence of static graphs (snapshots)

  $G^{ti} = \{V^{ti}, E^{ti}, X^{ti}\}$ # vertex, edge and feature sets

  $V^{ti} = \{v_1, \ldots, v_{|Vti|}\}$ # a set of nodes

  $E^{ti} = \{e_1, \ldots, e_{|Eti|}\}$ # a set of edges

  $X^{ti} = \{x_1, \ldots, x_{|Vti|}\}$ # a set of node features



- **Task**
  Learn the future node representation – predicting the future based on the past.

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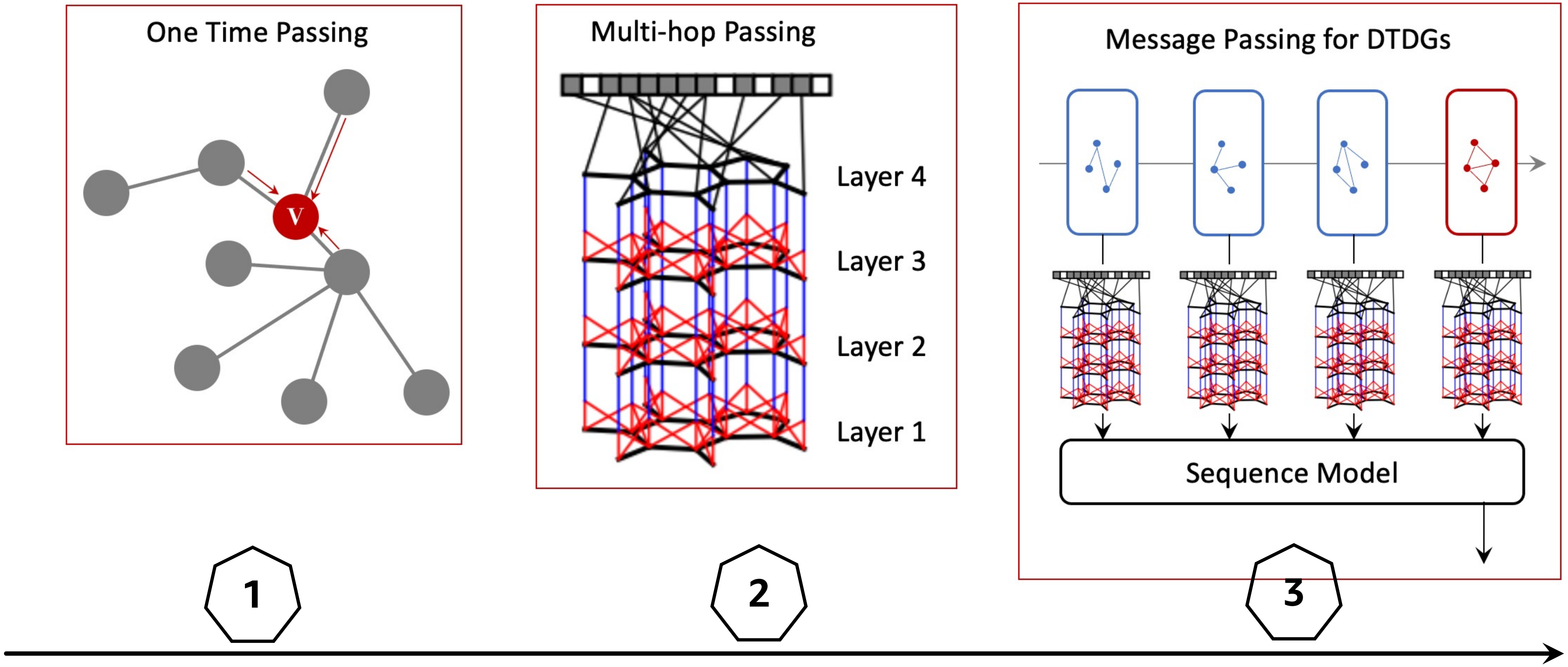
Background – Graph Neural Networks for DTDGs

Message passing-based methods



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Background – Research Challenges

Q1. How can the model be efficiently trained on large-scale DTDGs to exploit hardware accelerators with small memory footprint?

Q2. How can the model effectively capture the changing dynamics of the graphs?

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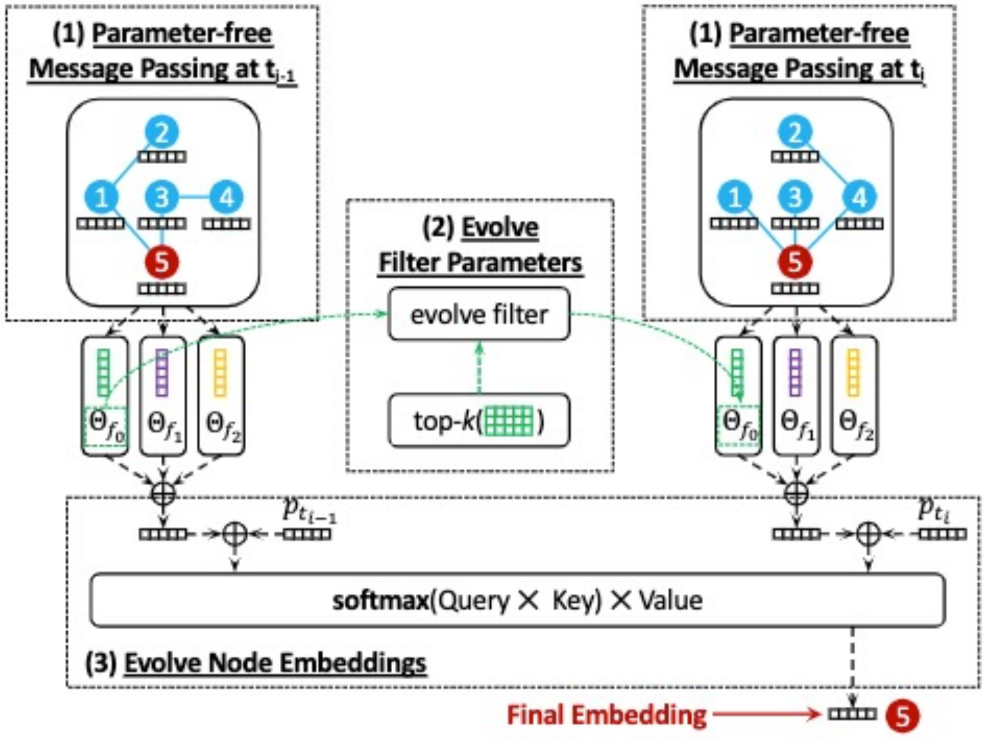
SEIGN Approach – A Quick Overview

Scalable **E**volving **I**nception **G**raph Neural **N**etwork (**SEIGN**)



An example of how v_5's (**red 5**) embedding is generated in 3 steps:

1. It participates in message passing (in every snapshot).

2. Its embedding for each snapshot is generated.

3. Its final embedding, taking all its embeddings from different snapshot into consideration, is generated for the downstream task.

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SEIGN Approach – Evolving Graph Model & Embedding

An answer to Q2 (effectiveness):

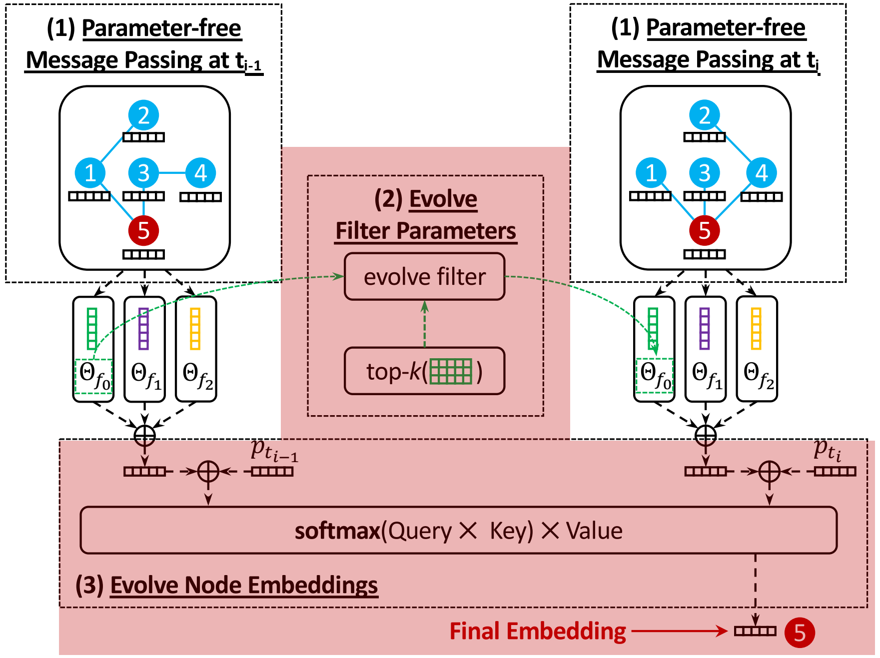
1. Evolve the node embedding

SEIGN uses self-attention mechanism to generate the final node embedding which summarize the embedding sequence.

2. Evolve the model parameters

SEIGN uses gated recurrent unit (GRU) to predict new model parameters based on the previous model parameters.

(We are going to talk about the model parameters next)



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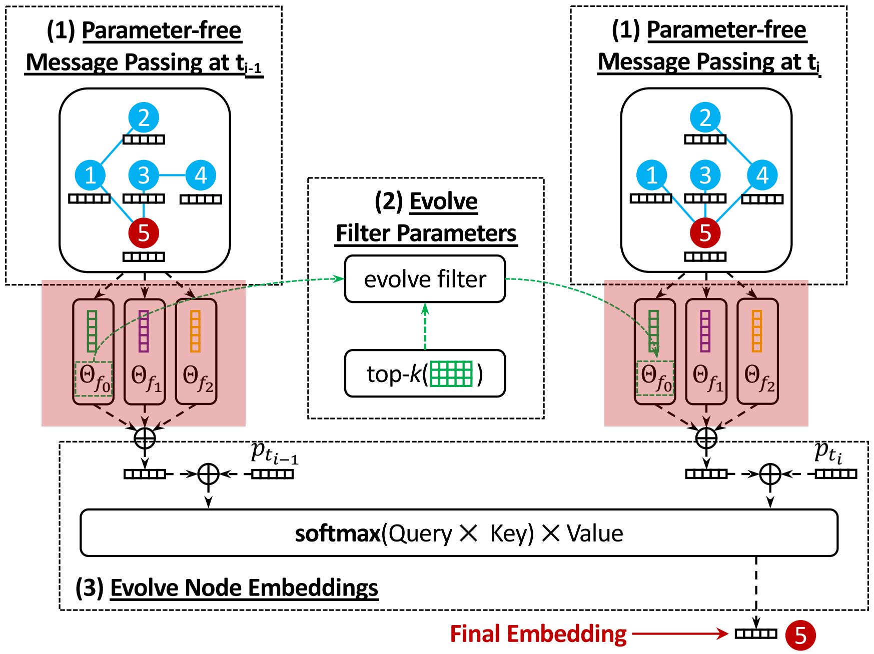
SEIGN Approach – Inception Like Graph Neural Network

Another answer to Q2 (effectiveness):

This design improves the model accuracy by combining 0 – k hop message passing results instead of using only the k-hop message passing result.



Parameters:

A set of learnable matrices that transform message passing results for each hop.

This sounds like a good idea for improving the accuracy.
But don't we make the model more complex just now?
What about the scalability?

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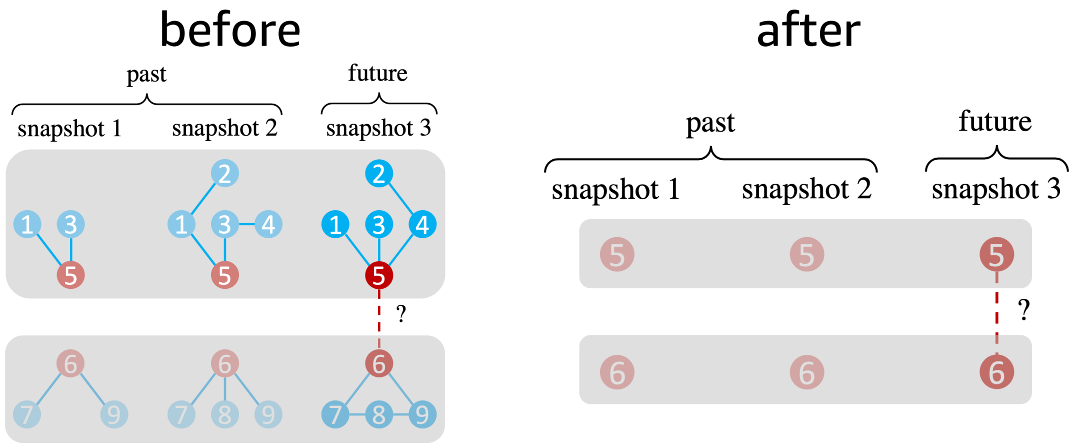
SEIGN Approach – Parameter-free Message Passing

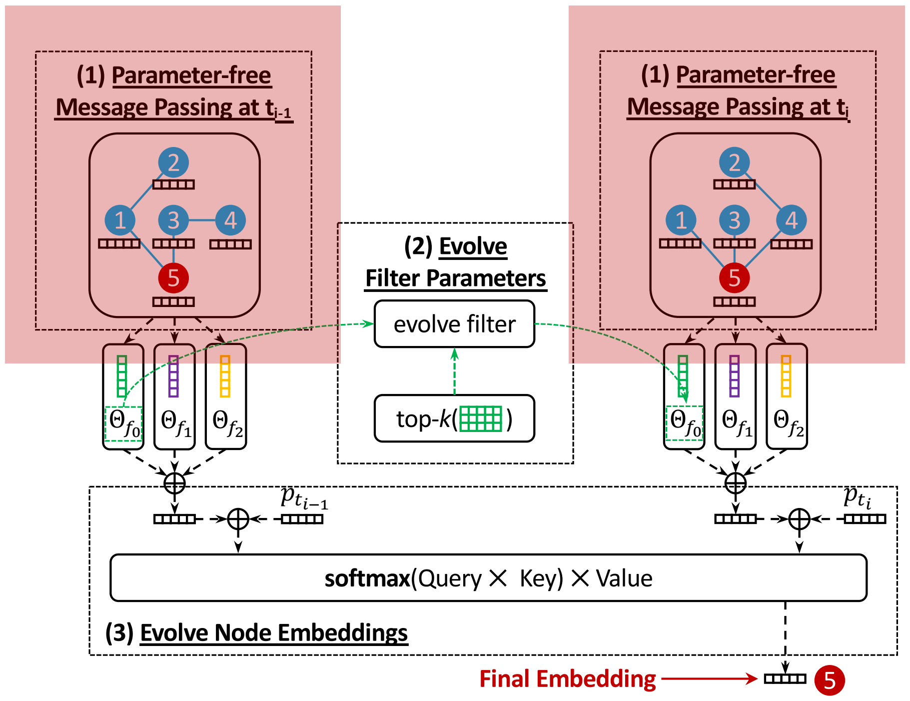
An answer to Q1 (efficiency):

X' = AX, where X is a linear diffusion operator

How does this help?

1. Fewer parameters 2. Less node dependencies





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Experimental Evaluation – Setup

Task: Link Prediction

$$\mathcal{L} = -\sum_{(v_i,v_j)\in\mathcal{E}^{t_k}} \log(\sigma(g_\Theta(v_i)\top g_\Theta(v_j))) - \sum_{(v_m,v_n)\notin\mathcal{E}^{t_k}} \log(\sigma(g_\Theta(v_m)\top g_\Theta(v_n))),$$

Datasets:

Dataset	UCI	Bitcoin	Company	ogbl-collab
# of nodes	1,899	5,881	24,108	235,868
# of edges	59,835	35,591	499,511	1,285,465
feature dim	128	128	768	128
# of snapshots	13	14	21	32
train/valid/test snapshots	10/2/2	9/2/2	17/2/2	28/2/2

Baselines:

- ❑ Shared GNN: GCN, GAT, SIGN
- ❑ GNN-to-sequence: DySAT
- ❑ Sequence-to-GNN: EvolveGCN

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Experimental Evaluation – Effectiveness

Baseline Comparison & Ablation Study

Methods	UCI			Bitcoin			Company			ogbl-collab		
	AUC↑	AP↑	F1↑(0.5)	AUC↑	AP↑	F1↑(0.5)	AUC↑	AP↑	F1↑(0.5)	AUC↑	AP↑	F1↑(0.5)
GCN	74.35±1.8	74.96±1.2	68.90±0.9	83.58±1.2	84.68±1.1	77.86±0.8	88.75±0.3	85.15±0.4	82.14±0.3	93.45±0.1	93.29±0.0	87.98±0.1
GAT	68.62±3.2	67.75±3.0	61.93±2.8	84.25±0.6	83.62±0.6	79.80±0.4	84.10±1.2	81.84±0.9	77.82±1.0	92.79±0.3	92.88±0.3	88.59±0.2
SIGN	74.98±0.3	69.92±0.4	74.54±0.2	87.03±0.1	85.70±0.1	**84.89**±0.2	92.72±0.1	89.11±0.1	86.22±0.2	97.07±0.0	96.10±0.1	82.80±0.1
GCRN	77.21±0.7	75.28±0.8	74.19±0.7	87.81±0.2	88.02±0.2	80.21±0.2	91.65±0.2	87.05±0.2	84.71±0.2	96.47±0.0	96.18±0.1	84.54±0.2
DySAT	77.46±0.6	76.54±0.6	73.06±0.7	88.82±0.1	88.19±0.2	82.01±0.2	92.45±0.0	88.07±0.1	86.10±0.0	95.18±0.2	95.05±0.3	87.34±0.1
EvolveGCN	76.09±1.0	75.65±0.9	71.07±0.9	85.53±0.4	84.82±0.5	79.23±0.3	89.22±0.1	86.40±0.2	79.84±0.1	96.06±0.2	95.61±0.2	**91.01**±0.3
EvolveDySAT	80.49±0.6	78.08±0.7	74.02±0.4	89.38±0.1	90.12±0.0	76.32±0.1	92.78±0.0	88.78±0.0	86.25±0.1	96.09±0.0	96.13±0.1	87.40±0.0
SEIGN-P	79.82±0.5	78.55±0.4	**75.44**±0.4	88.44±0.1	87.04±0.1	83.61±0.2	93.35±0.1	89.25±0.0	87.35±0.0	97.50±0.1	97.34±0.1	86.78±0.2
SEIGN-T	76.86±0.3	72.49±0.2	73.08±0.2	88.51±0.2	86.56±0.2	84.41±0.1	93.26±0.2	88.28±0.2	86.86±0.1	97.35±0.1	96.62±0.1	82.20±0.2
SEIGN	**80.83**±0.3	**81.36**±0.2	71.81±0.2	**90.12**±0.0	**91.13**±0.1	81.89±0.1	**94.34**±0.1	**90.09**±0.1	**88.39**±0.1	**98.33**±0.1	**98.49**±0.0	86.85±0.1

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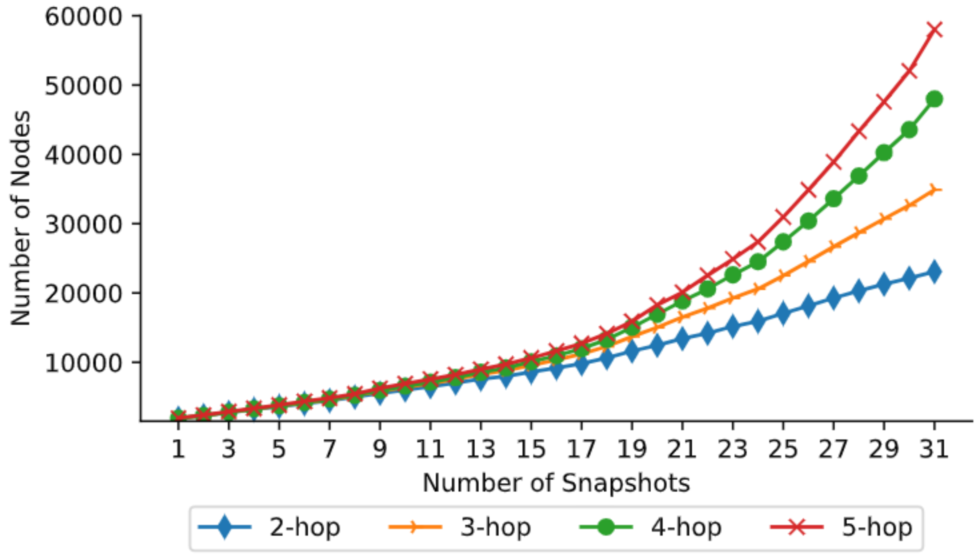
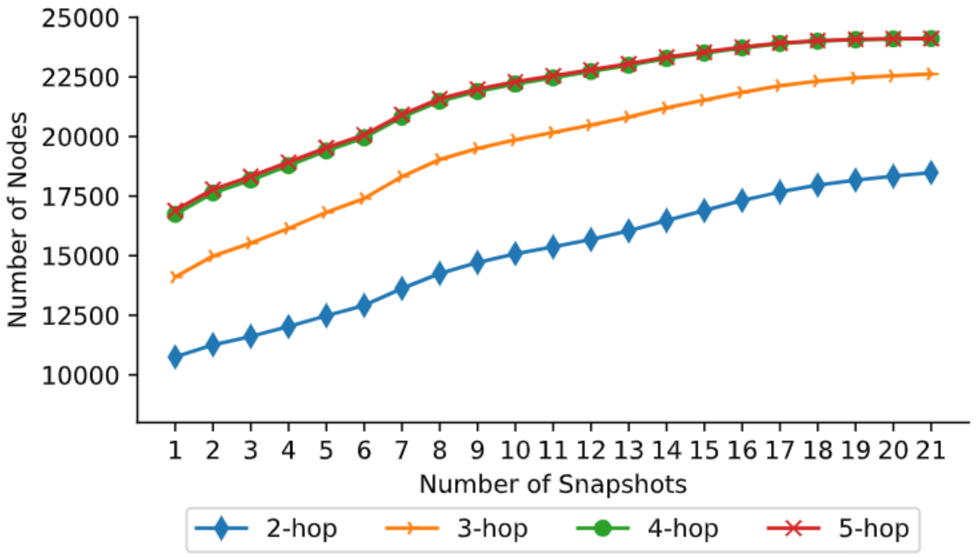
Experimental Evaluation – Explosion of Neighborhood

ogbl-collab



company



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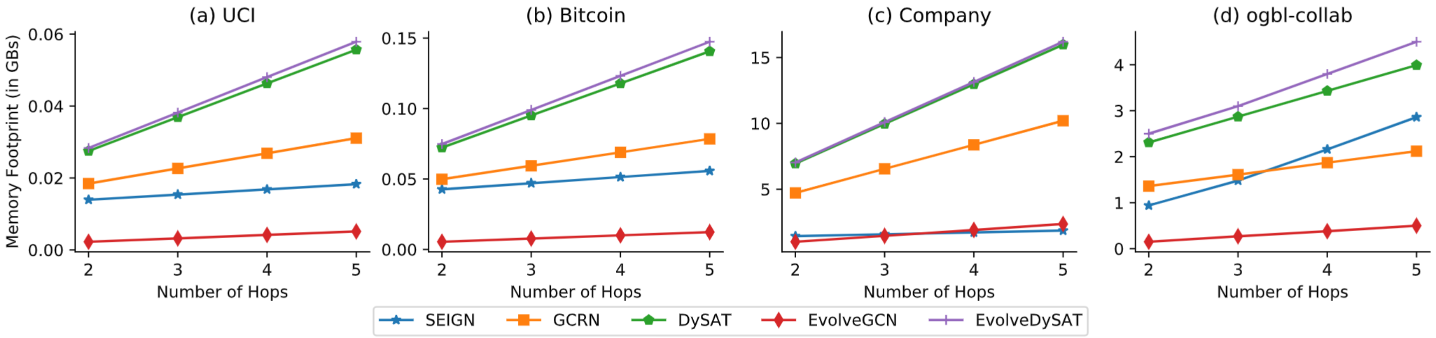
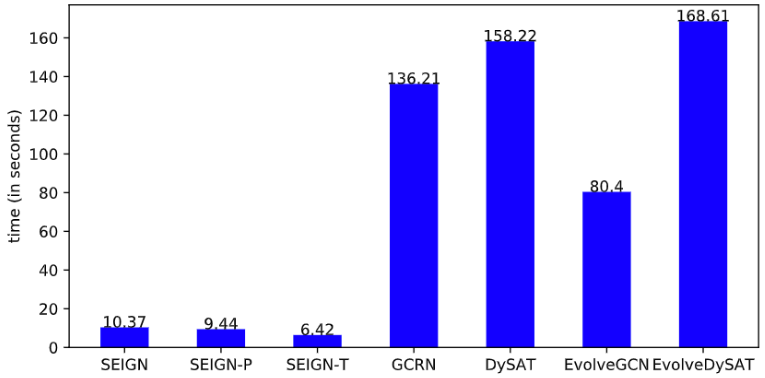
Experimental Evaluation – Explosion of Neighborhood

memory footprint (pytorch backward() call)

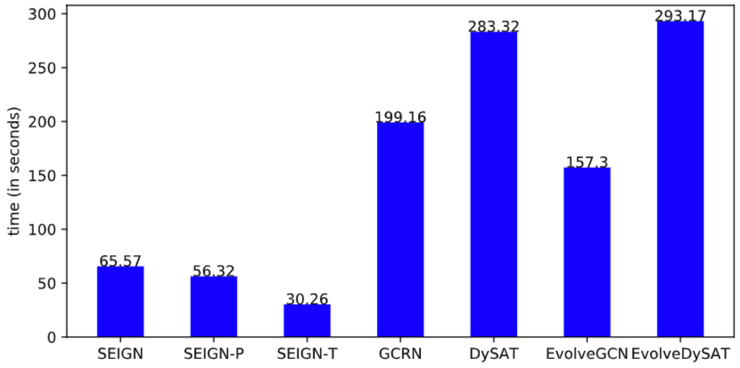


ogbl-collab



cpu time (training)

company



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Conclusion

- ❑ We introduce a simple and efficient representation learning method for DTDGs, called SEIGN.
- ❑ In our SEIGN neural network architecture, we propose to simultaneously evolve the graph model parameters and the representations from each graph snapshot to effectively capture the changing dynamics of the DTDGs.
- ❑ We further introduce an evolving graph inception architecture in SEIGN for DTDGs which enables efficient graph mini-batch construction and incurs a considerably lower training memory footprint.
- ❑ We evaluate the effectiveness of SEIGN in a position study and an ablation study. The position study compares our method against state-of-the-art approaches for an unsupervised training task on publicly available benchmarks as well as a real industrial dataset. We also demonstrate the efficiency of training SEIGN by providing various compute and memory profiles.

Thank you for listening! Do you have any question?





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