Preserving Spatial-Temporal Relationship with Adaptive Node Sampling in Hierarchical Dynamic Graph Transformers

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MOTIVATIONS

- Dynamic Graph Transformers (DGTs) have demonstrated remarkable performance in various applications, such as social networks, traffic forecasting, and recommendation systems.
- Training DGTs for large graphs remains a challenge. Mini-batch training is usually used to alleviate this challenge but this approach often fails to capture complex dependencies or sacrifice performance.
- We propose the **A**daptive **N**ode **S**ampling in **H**ierarchical **D**ynamic **G**raph **T**ransformers (ASH-DGT) architecture that focuses on sampling the set of suitable nodes preserving spatial-temporal relationships in the dynamic graph for training DGTs.
- Unlike previous methods that use random sampling or structural sampling, our motivation is that the contribution of nodes to learning performance can be time-sensitive, while we still care about spatial correlation in the dynamic graph with consideration to the global and local structure of the graph.

METHOD

$$\text{Maximize} \quad R(\mathcal{T}) = \sum_{t\in\mathcal{T}, v\in\mathcal{V}} R_v^t$$

$$\text{Subject to} \quad \sum_{i\in\mathcal{N}(v)} p_i = 1, \qquad 0 < \gamma < 1$$

$$R_v^t = \frac{1}{N} \sum_{v\in\mathcal{S}(v)} A_v^t \cdot ||h_v^t||$$

Algorithm 1: Extent EXP3 Algorithm for node-wise sampling

Input : K: number of chosen nodes, η: number of neighbor nodes, γ: exploration rate
Output: : p: policy distribution
Initialize $w \leftarrow (1, 1, \dots, 1)$;
for *each iteration* **do**
  Compute $p = (p_1, p_2, \dots, p_\eta)$ with

$$p_i = (1-\gamma) \cdot \frac{w_i}{\sum_{i=1}^{\eta} w_i} + \frac{\gamma}{\eta}$$

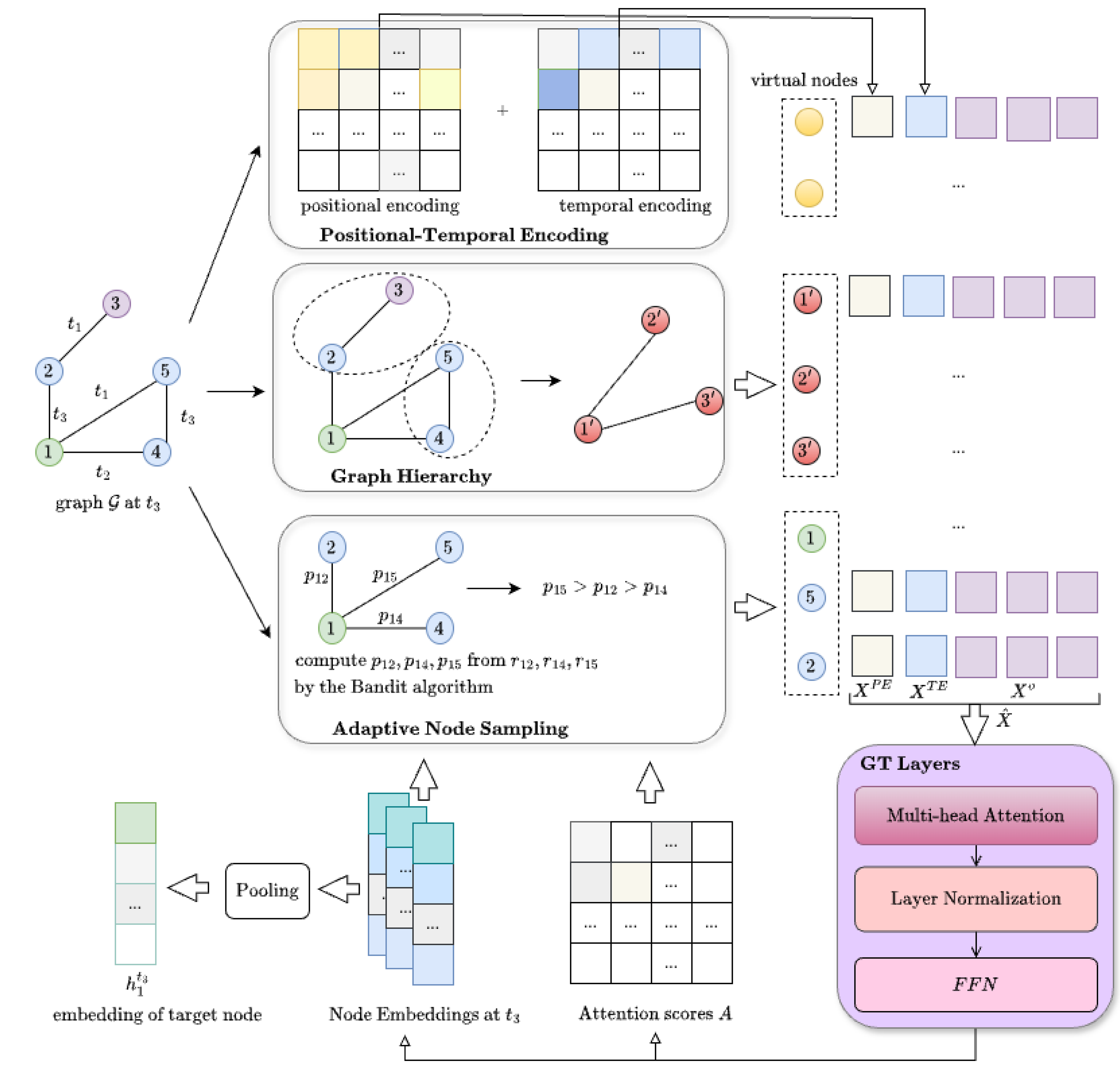
  Choose K nodes based on p; Compute reward r following eq.5,
  Update the weights using the EXP3 update:

$$w_i = w_i \cdot e^{-\eta \cdot \frac{r}{K \cdot p_i}}$$

end

Algorithm 2: Adaptive Sampling Iterative Process

Input : $G = (V, E, T)$: dynamic graph, H_0: initial node embeddings, t: maximum of time steps
Output: H^t: the updated node embedding
Initialize: $i \leftarrow 1$, $H \leftarrow H_0$;
while $i \leq numEpoch$ **do**
  for *each node* v *in* V **do**
    Train the policy p following the Algorithm 1; Sample neighbor nodes from p;
  end
  Training DGT;
  Updated node embeddings H^t for time step t; $i \leftarrow i + 1$
end



EXPERIMENTS & RESULTS

Dataset

Dataset	Wikipedia	Reddit	SocialEvo	ENRON	UCI	MOOC
# Nodes	9227	10984	74	184	1899	7145
# Edges	157474	672447	352180	2099520	59835	411749
# Edge feature dim	172	172	0	0	0	4
# Timespan	30 days	30 days	30 days	1316 days	193days	30 days

We split the data following the baseline TGN [1] with ratio of 70%/15%/15% for training, validation and test set. We compare our method with baselines on the node classification and link prediction tasks.

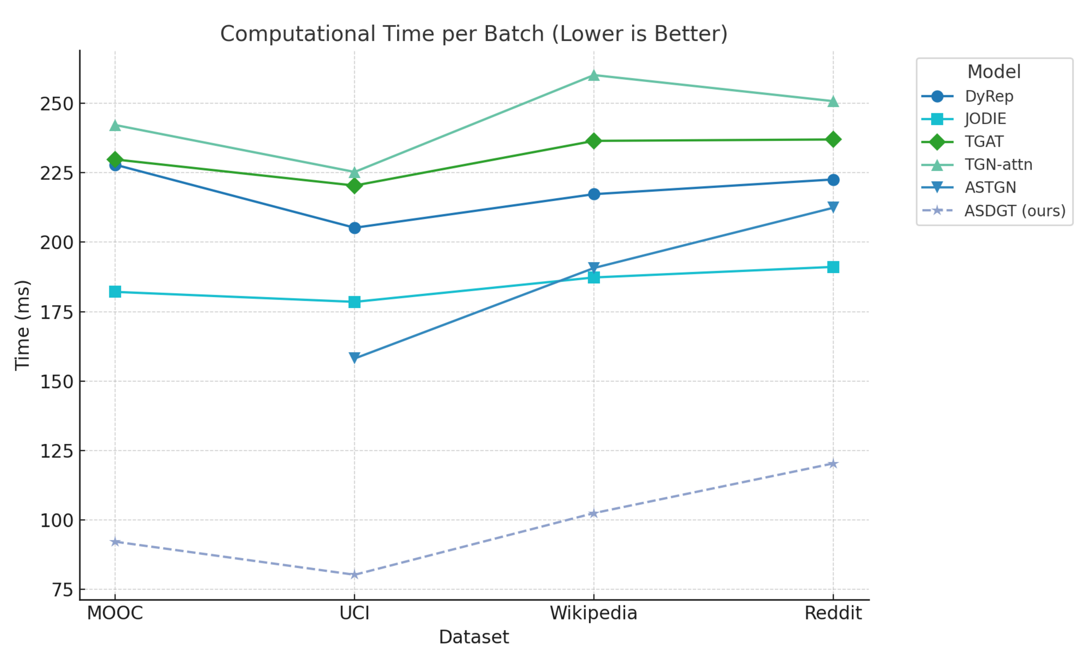
Node Classification Task

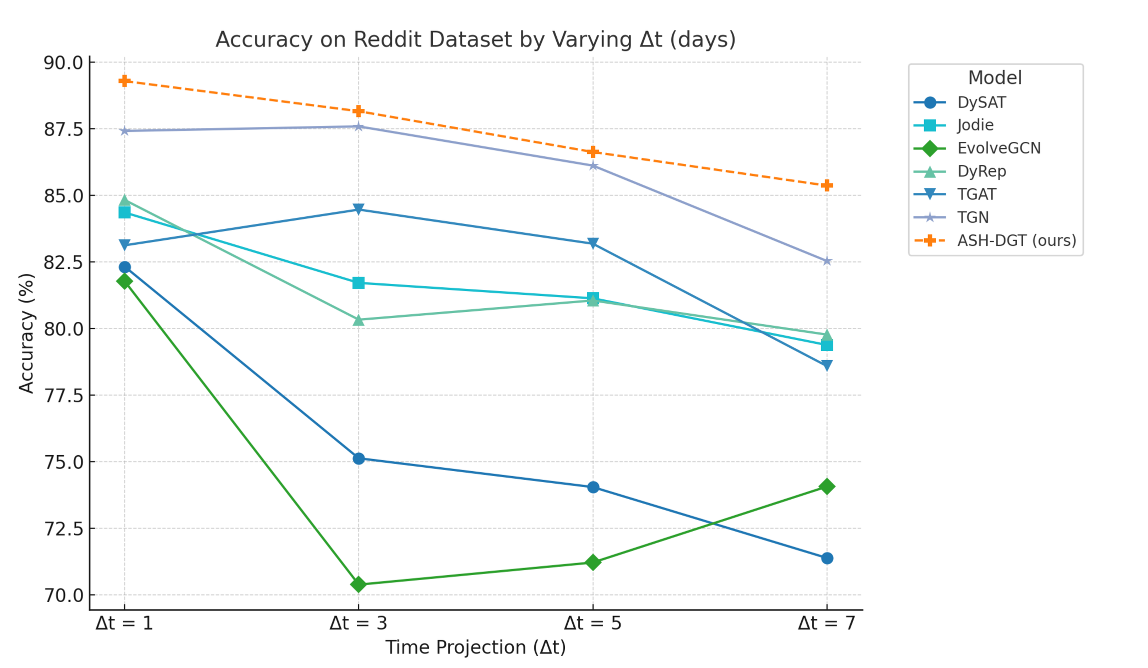
Model	MOOC	Wikipedia	Reddit
DySAT	72.11 ± 0.5	61.79 ± 0.3	74.82 ± 1.2
Jodie	73.39 ± 2.1	61.23 ± 2.5	84.35 ± 1.2
EvolveGCN	70.26 ± 0.5	63.41 ± 0.3	81.77 ± 1.2
TGAT	74.23 ± 1.2	65.43 ± 0.7	83.12 ± 0.7
DyRep	75.12 ± 0.7	62.79 ± 2.3	84.82 ± 2.2
TGN	77.47 ± 0.8	67.11 ± 0.9	87.41 ± 0.3
ASH-DGT (ours)	$\mathbf{79.08 \pm 0.5}$	$\mathbf{69.74 \pm 1.3}$	$\mathbf{89.12 \pm 0.3}$

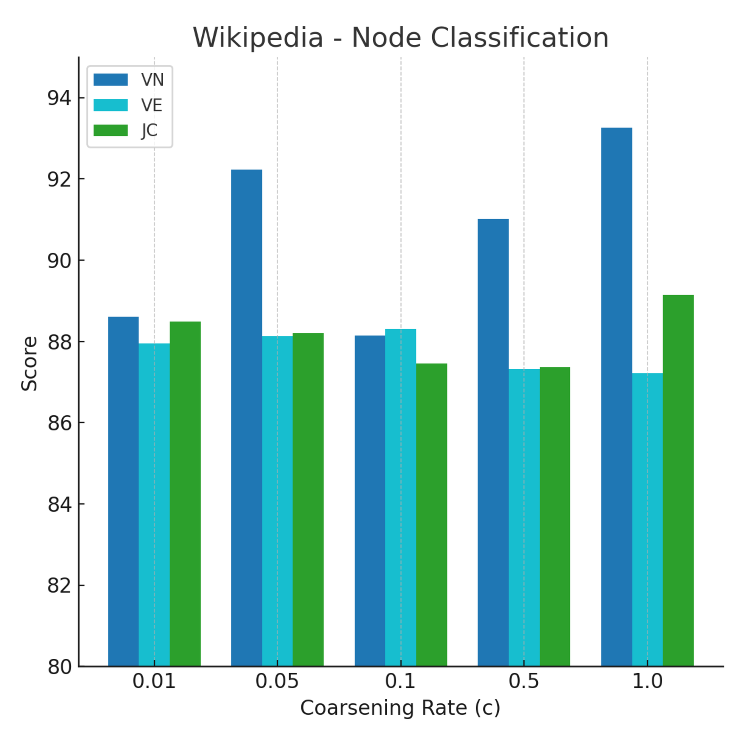
Link Prediction Task

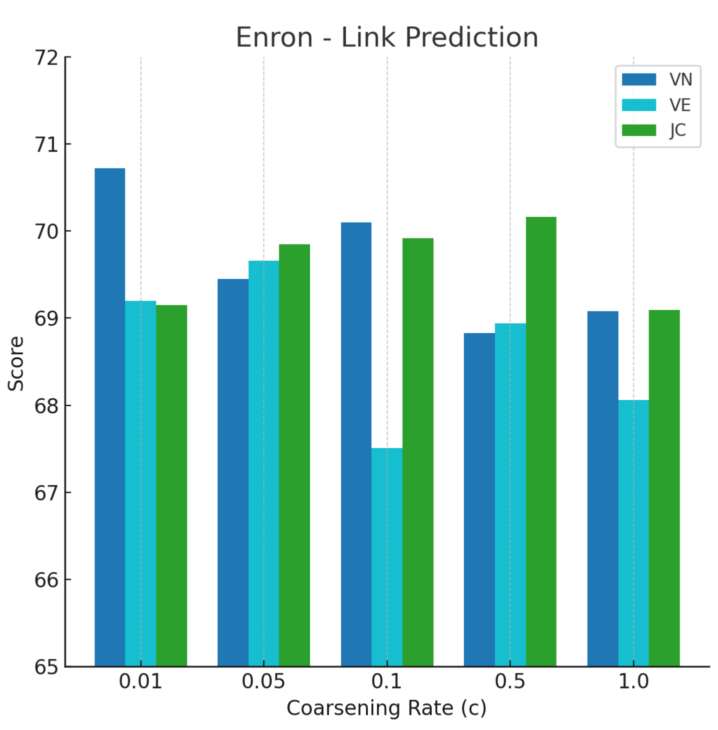
Dataset	Wikipedia		Reddit		MOOC	
Metric	AUC (%) ↑	AP (%) ↑	AUC (%) ↑	AP (%) ↑	AUC (%) ↑	AP (%) ↑
DyRep	77.40 ± 1.2	75.20 ± 1.1	67.36 ± 1.1	66.12 ± 1.0	90.49 ± 0.3	89.23 ± 0.4
JODIE	88.43 ± 0.7	87.95 ± 0.6	87.71 ± 0.4	87.43 ± 0.5	90.50 ± 0.1	90.20 ± 0.2
VGRNN	72.20 ± 0.6	71.00 ± 0.7	51.89 ± 0.2	50.56 ± 0.3	90.03 ± 0.4	89.00 ± 0.3
EvolveGCN	60.48 ± 0.5	58.74 ± 0.4	58.42 ± 0.4	57.33 ± 0.3	50.36 ± 0.8	49.76 ± 0.6
DynAERNN	71.00 ± 1.1	70.12 ± 1.0	83.37 ± 1.4	82.54 ± 1.3	89.34 ± 0.2	88.23 ± 0.3
TGAT	95.47 ± 0.1	94.89 ± 0.2	96.65 ± 0.1	95.98 ± 0.1	72.09 ± 0.3	70.95 ± 0.3
TGN-attn	95.72 ± 2.1	94.67 ± 1.9	96.12 ± 1.1	95.65 ± 1.0	81.64 ± 1.3	80.23 ± 1.1
ASTGN	96.92 ± 0.2	95.87 ± 0.3	98.97 ± 0.1	98.45 ± 0.1	92.75 ± 0.8	91.45 ± 0.7
ASH-DGT (ours)	$\mathbf{97.45 \pm 0.3}$	$\mathbf{96.50 \pm 0.2}$	$\mathbf{99.02 \pm 0.1}$	$\mathbf{98.76 \pm 0.1}$	$\mathbf{93.23 \pm 0.4}$	$\mathbf{92.10 \pm 0.3}$

Dataset	UCI		SocialEvo		Enron	
Metric	AP (%) ↑	AUC (%) ↑	AP (%) ↑	AUC (%) ↑	AP (%) ↑	AUC (%) ↑
DyRep	79.76 ± 0.1	81.02 ± 0.3	62.02 ± 1.7	64.35 ± 1.1	67.28 ± 1.3	68.55 ± 1.4
JODIE	78.02 ± 0.2	79.53 ± 0.5	60.01 ± 1.1	61.56 ± 1.2	63.10 ± 1.3	64.72 ± 1.0
EvolveGCN	76.63 ± 0.2	78.12 ± 0.4	56.90 ± 0.6	57.89 ± 0.5	57.37 ± 0.2	58.62 ± 0.3
TGAT	60.25 ± 0.2	61.32 ± 0.6	57.37 ± 0.6	58.91 ± 0.5	60.36 ± 0.7	61.67 ± 0.9
TGN-attn	64.21 ± 0.2	65.55 ± 0.4	58.11 ± 1.2	59.74 ± 0.8	62.47 ± 1.7	63.53 ± 1.3
ASTGN	81.52 ± 0.2	82.10 ± 0.3	62.41 ± 1.0	63.65 ± 1.2	69.12 ± 1.0	70.56 ± 0.9
ASH-DGT (ours)	$\mathbf{82.34 \pm 0.2}$	$\mathbf{83.21 \pm 0.2}$	$\mathbf{65.12 \pm 0.3}$	$\mathbf{66.45 \pm 0.4}$	$\mathbf{71.33 \pm 0.5}$	$\mathbf{72.67 \pm 0.4}$









CONCLUSION

We introduce an adaptive node sampling technique to preserve spatial-temporal relationships in hierarchical dynamic graph transformers. Through experiments, our approach demonstrates enhanced representation learning, leading to improved model performance and accuracy.

References:
[1] Emanuele Rossi et al, Temporal graph networks for for deep learning on dynamic graphs.

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