Dynamic Heterogeneous Graph Attention Neural Architecture Search

Zeyang Zhang[1], Ziwei Zhang[1], Xin Wang[1], Yijian Qin[1], Zhou Qin[2], Wenwu Zhu[1]

[1]Tsinghua University, [2]Alibaba Group

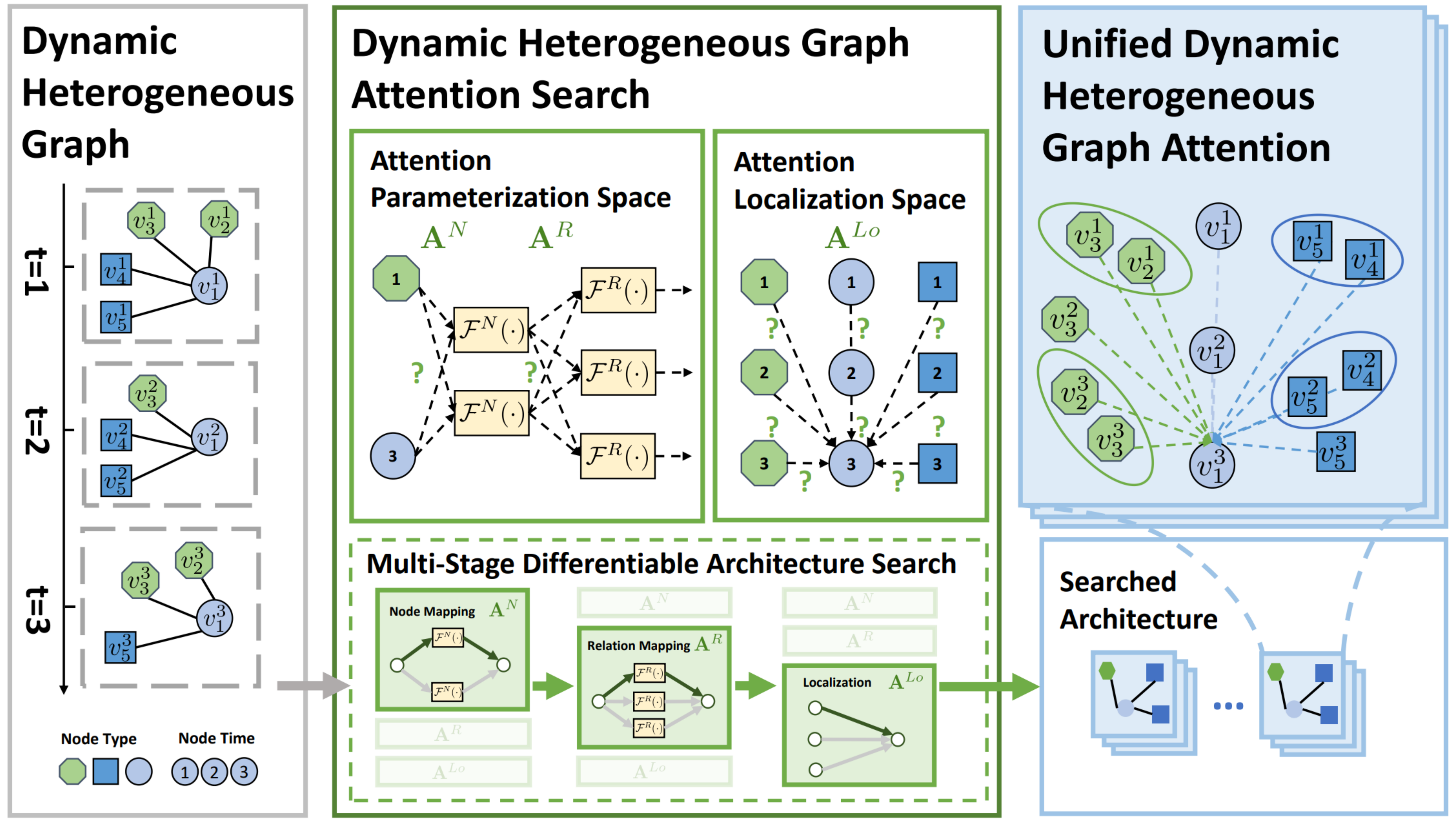
➢ Motivations

- **Dynamic heterogeneous graphs are ubiquitous in real-world**
  - Have applications including social networks, e-commerce networks, academic citation networks, etc.
  - Contain richer heterogeneous information represented as node and edge types, and dynamic information like evolving graph structures over time.
- **The existing dynamic heterogenous graph neural networks (DHGNNs) are limited due to**
  - Manual design require extensive human endeavors
  - Fixed architecture can not adapt to diverse scenarios
  - Tackle heterogeneous and dynamic information separately.
- **Our Goal : Automatically tailor an optimal DHGNN architecture and adapt to various dynamic heterogeneous graph scenarios with**
  - search space that jointly consider the complex spatial-temporal dependencies and heterogeneous interactions in graphs
  - search algorithm that efficiently search in the potentially large and complex search space for dynamic heterogeneous graphs

➢ Method

- We propose Dynamic Heterogeneous Graph Attention Neural Architecture Search (DHGAS) to automate DHGNN design with
  - **Unified dynamic heterogeneous graph attention** to jointly tackle spatio-temporal dependencies while capable of differentiating time/node/edge types
  - **Localization space** to determine where the attention should be applied and **parameterization space** to determine how the attention should be parameterized.
  - **Multi-stage differentiable search** algorithm to efficiently explore the space and stable the search process

➢ Model (DHGAS)

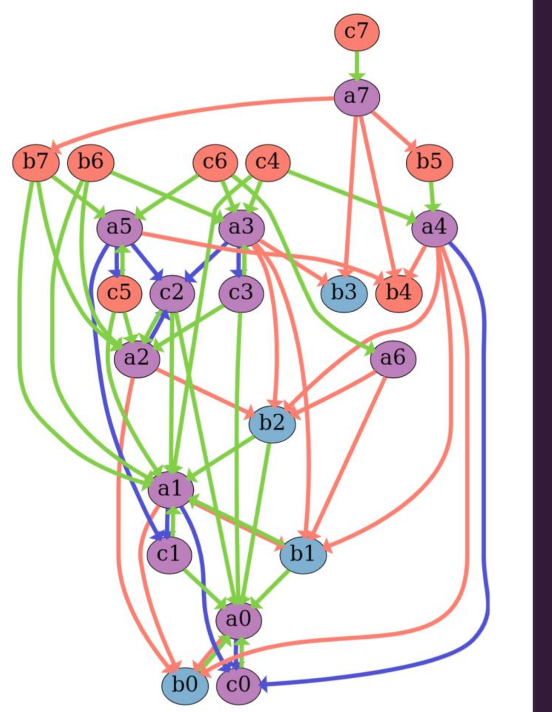


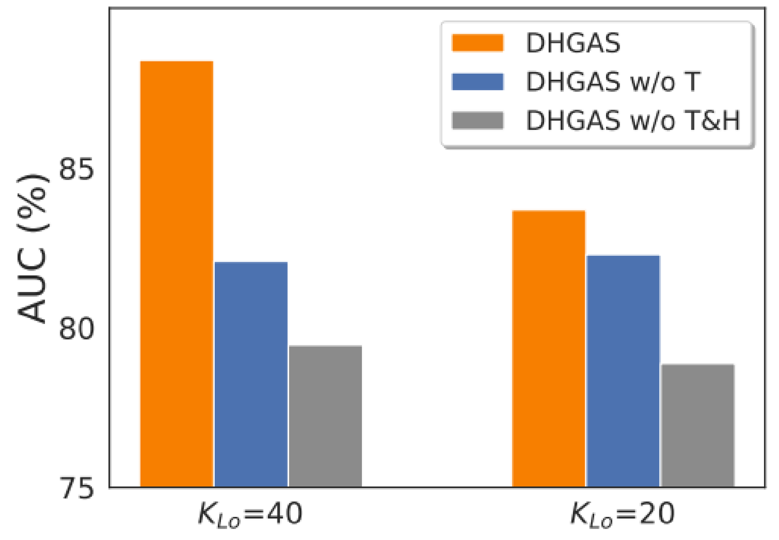
➢ Experiments

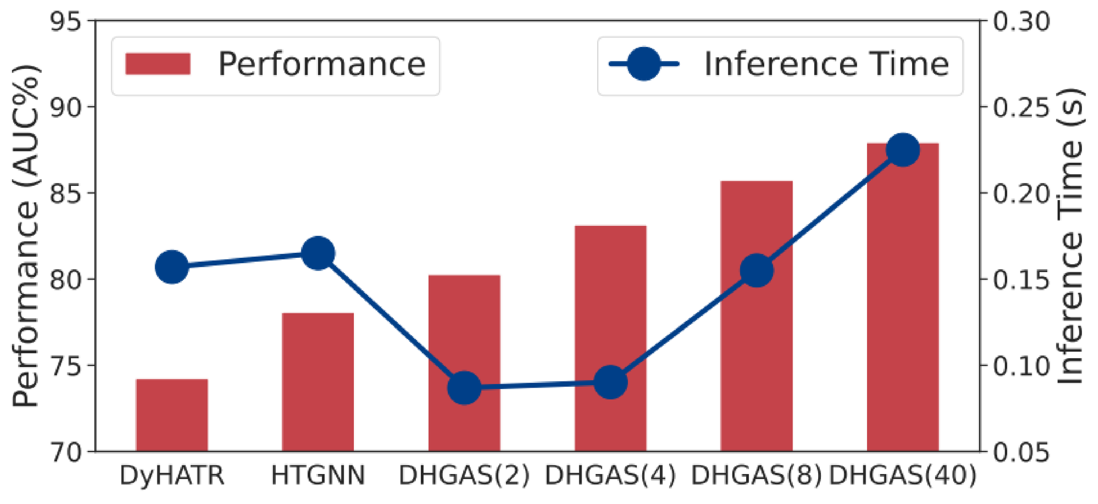
Real world datasets

DHGAS outperforms baselines by
1) jointly tackling dynamic and heterogeneous information
2) automatically tailoring optimal DHGNN for various scenarios

Task / Metric	Link Prediction (AUC%) ↑		Node Classification (F1%) ↑		Node Regression (MAE) ↓
Dataset	Aminer	Ecomm	Yelp	Drugs	COVID-19
GCN	73.84 ± 0.06	77.94 ± 0.22	37.02 ± 0.00	56.43 ± 0.21	846 ± 101
GAT	80.84 ± 0.96	78.49 ± 0.31	35.54 ± 0.00	57.06 ± 0.00	821 ± 91
RGCN	82.75 ± 0.12	82.27 ± 0.51	37.75 ± 0.00	57.97 ± 0.14	833 ± 95
HGT	78.43 ± 1.81	81.09 ± 0.52	34.62 ± 0.00	57.65 ± 0.01	805 ± 88
DyHATR	74.24 ± 2.09	71.69 ± 0.90	34.49 ± 0.16	55.51 ± 0.09	643 ± 36
HGT+	85.60 ± 0.12	76.68 ± 0.85	38.33 ± 0.00	59.09 ± 0.00	-
HTGNN	78.08 ± 0.80	76.78 ± 6.37	36.33 ± 0.07	56.24 ± 0.34	555 ± 34
GraphNAS	81.61 ± 0.98	79.37 ± 0.21	37.73 ± 0.00	57.13 ± 0.52	820 ± 43
DiffMG	85.04 ± 0.30	81.69 ± 0.06	38.65 ± 0.00	58.45 ± 0.15	629 ± 63
DHGAS	**88.13 ± 0.18**	**86.56 ± 0.58**	**41.99 ± 0.18**	**62.35 ± 0.03**	**536 ± 43**







Additional Results

DHGAS can exploit dynamic heterogenous information, permit efficiency tradeoff and automatically discover complex yet competitive DHGNN architectures for various datasets

Contact: Zeyang Zhang, Email: zy-zhang20@mails.tsinghua.edu.cn