Advances in Multigraph Neural Networks

Graphs&Data@TUDelft

13-02-2025

H. Çağrı Bilgi

Supervised by Assoc. Prof. Kubilay Atasu

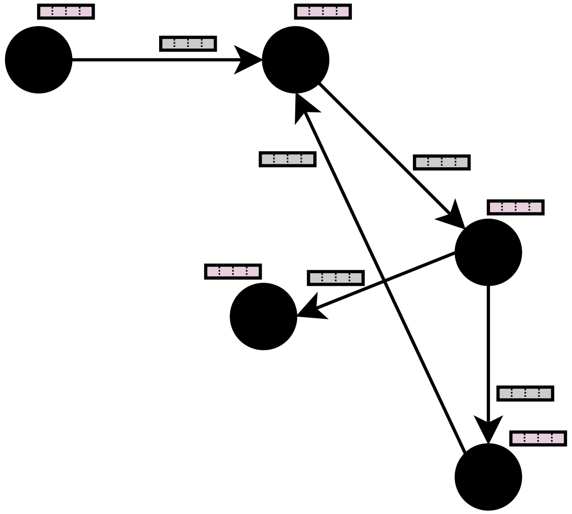
TU Delft

Outline

- Introduction
  - Motivation for Multigraph Neural Networks
- Related Work
  - Limitations of Existing Solutions for Multigraphs.
- MEGA-GNN: Our Proposed Solution
  - Motivation
  - Multigraph Message Passing with Multi-edge Aggregations
  - Why does a Two-stage Aggregation Make Sense?
  - Bi-directional Message Passing
  - Properties
- Experiments & Results
- Conclusion

Introduction

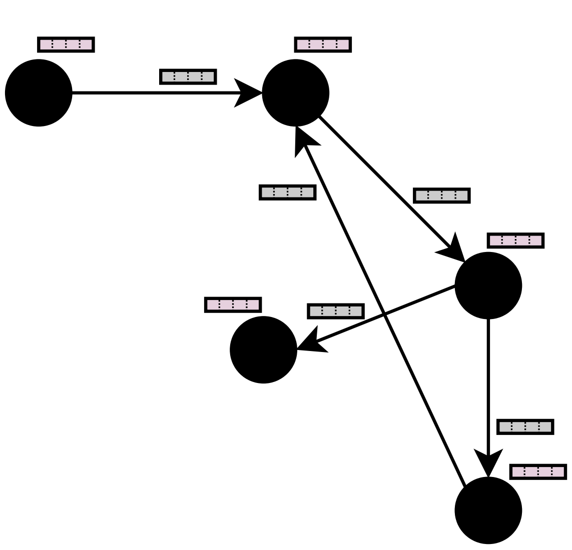
Motivation for Multigraph Neural Networks



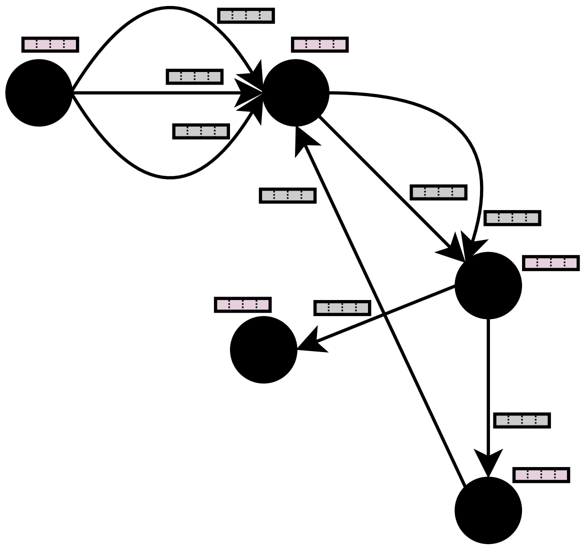
Simple graph with node and edge attributes

Introduction

Motivation for Multigraph Neural Networks



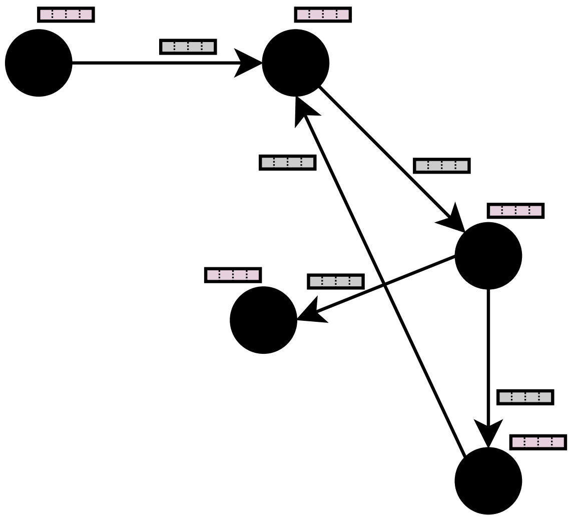
Simple graph with node
and edge attributes



Multigraph with node
and edge attributes

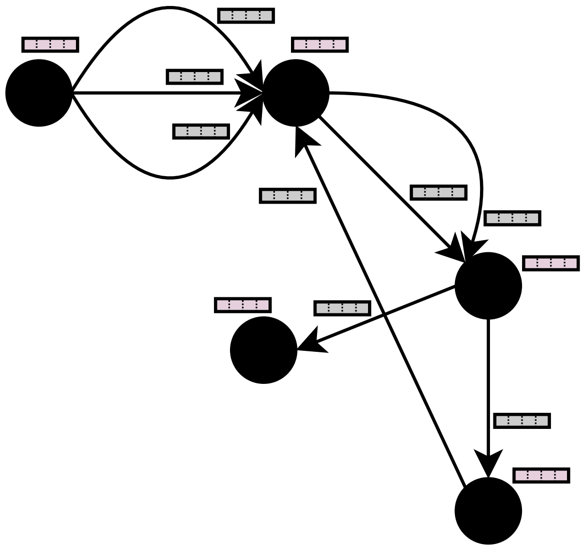
Introduction

Motivation for Multigraph Neural Networks



Simple graph with node and edge attributes

(Battaglia et al. 2018 [3])



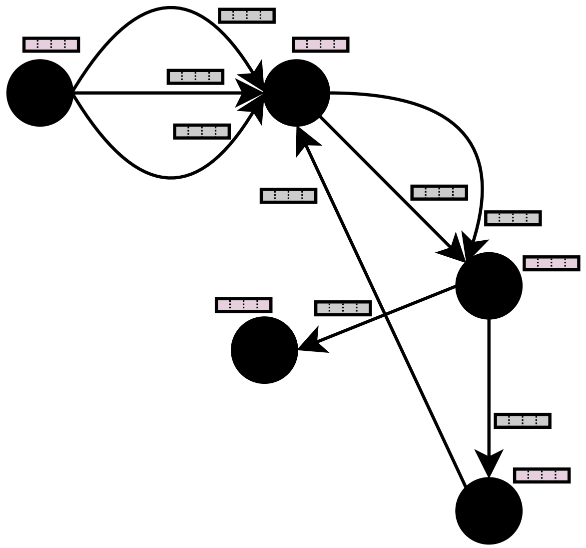
Multigraph with node and edge attributes

ADAMM (Sotiropoulos et al. [1])
Multi-GNN (Egressy et al. [2])

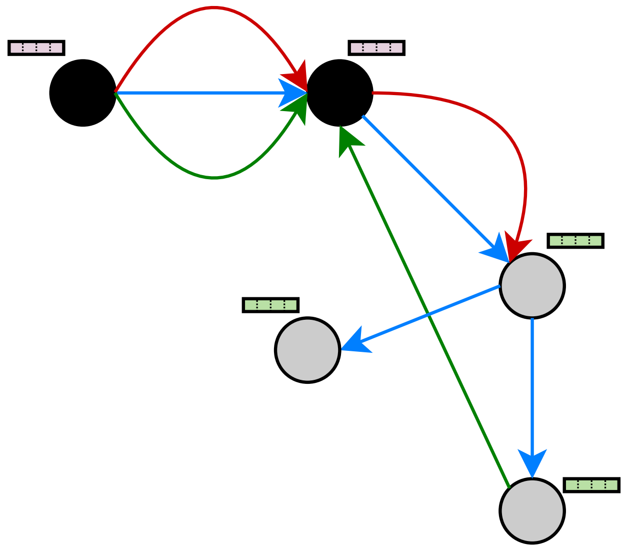
[1] Sotiropoulos K, Zhao L, Liang PJ, Akoglu L. ADAMM: Anomaly Detection of Attributed Multi-graphs with Metadata: A Unified Neural Network Approach. 2023 IEEE International Conference on Big Data.
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 AAAI.
[3] Battaglia, Peter W., et al. Relational inductive biases, deep learning, and graph networks. arXiv preprint 2018.

Introduction

Motivation for Multigraph Neural Networks



Multigraph with node and edge attributes

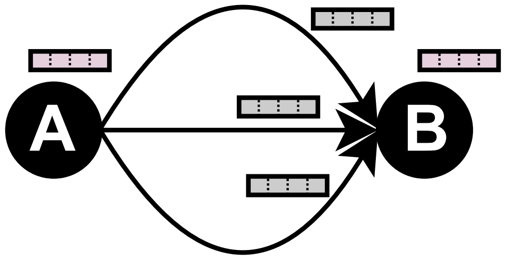


Multi-relational graph with different edge types

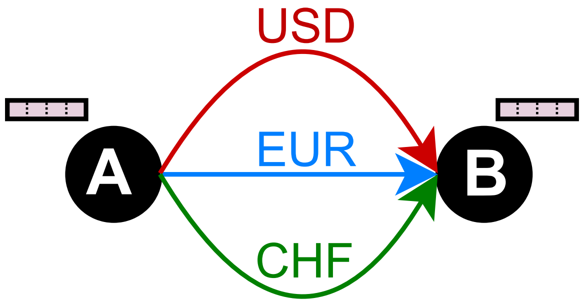
Introduction

The difference between Multigraphs and Multi-relational graphs

Trans. ID	Timestamp	Source bank ID	Source Account	Target bank ID	Target Account	Amount	Currency	Payment type
0	5/3/19 12:45	1	A	2	B	1400	USD	Cheque
1	5/15/19 7:34	1	A	2	B	710	EUR	ACH
2	5/18/19 16:55	1	A	2	B	950	CHF	Credit card
3	6/1/19 10:06	2	C	3	D	1200	CHF	Wire



Multigraph with node and edge attributes



Multi-relational graph with different edge types

ADAMM (Sotiropoulos et al. [1])
Multi-GNN (Egressy et al. [2])

R-GCN (Schlichtkrull et al. [4])
CompGCN (Vashishth et al. [5])

[4] Schlichtkrull, Michael, et al. Modeling relational data with graph convolutional networks. 2018 ESWC.
[5] Vashishth, Shikhar, et al. "Composition-based multi-relational graph convolutional networks." 2020 ICLR.

Related Work

Limitations of Existing Solutions for Multigraphs

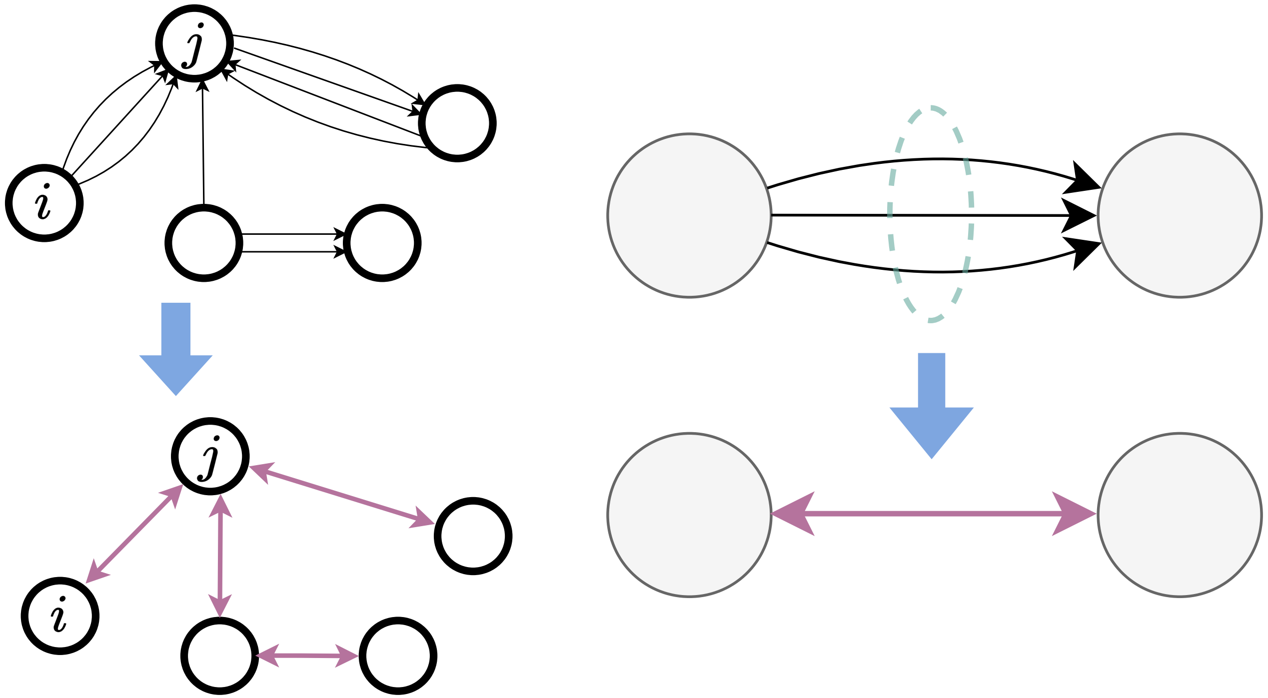
1. ADAMM (Sotiropoulos et. al. [1]) Transforms multigraph into a simple graph.

[1] Sotiropoulos K, Zhao L, Liang PJ, Akoglu L. ADAMM: Anomaly Detection of Attributed Multi-graphs with Metadata: A Unified Neural Network Approach. 2023 IEEE International Conference on Big Data.

Related Work

Limitations of Existing Solutions for Multigraphs

1. ADAMM (Sotiropoulos et. al. [1]) Transforms multigraph into a simple graph.



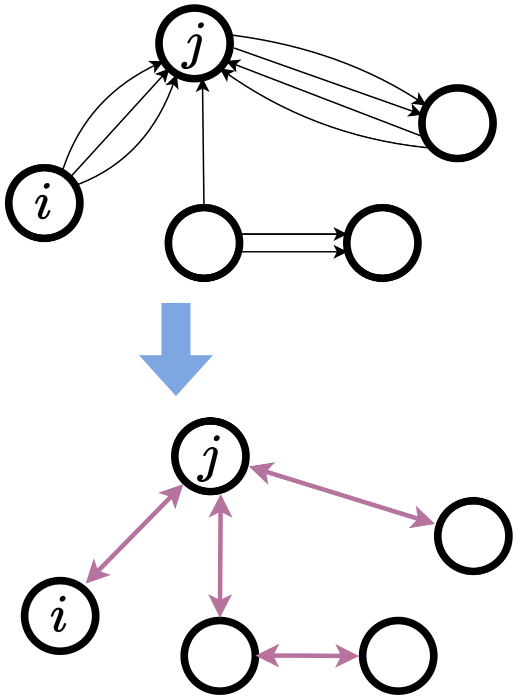
[1] Sotiropoulos K, Zhao L, Liang PJ, Akoglu L. ADAMM: Anomaly Detection of Attributed Multi-graphs with Metadata: A Unified Neural Network Approach. 2023 IEEE International Conference on Big Data.

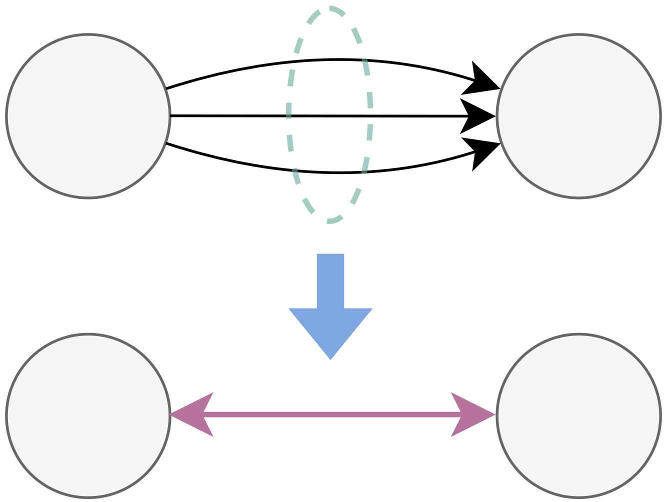
Related Work

Limitations of Existing Solutions for Multigraphs

1. ADAMM (Sotiropoulos et. al. [1]) Transforms multigraph into a simple graph

- Loses the original topology of the multigraph.
- Cannot produce embeddings for individual edges. Hence, not effective on edge classification.





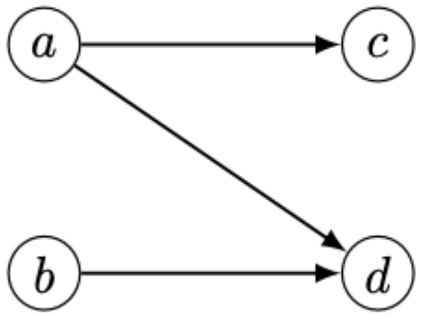
[1] Sotiropoulos K, Zhao L, Liang PJ, Akoglu L. ADAMM: Anomaly Detection of Attributed Multi-graphs with Metadata: A Unified Neural Network Approach. 2023 IEEE International Conference on Big Data.

Related Work

Limitations of Existing Solutions for Multigraphs

2. Multi-GNN (Egressy et al. [2]) Introduce three multigraph adaptations on the base GNN model.

Reverse MP



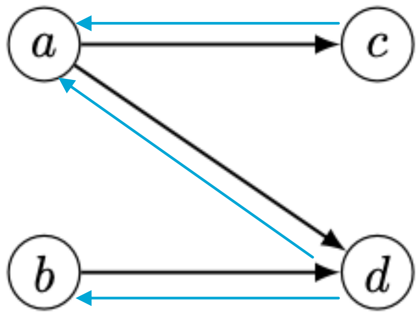
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Related Work

Limitations of Existing Solutions for Multigraphs

2. Multi-GNN (Egressy et al. [2]) Introduce three multigraph adaptations on the base GNN model.

Reverse MP



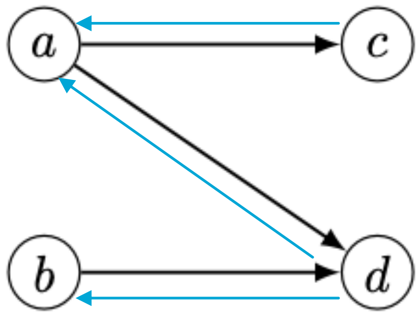
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Related Work

Limitations of Existing Solutions for Multigraphs

2. Multi-GNN (Egressy et al. [2]) Introduce three multigraph adaptations on the base GNN model.

Reverse MP



Messages from **incoming** and **outgoing** neighbors are aggregated separately

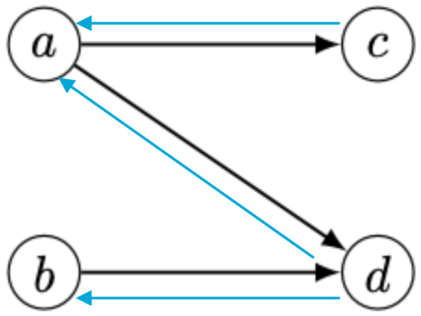
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Related Work

Limitations of Existing Solutions for Multigraphs

2. Multi-GNN (Egressy et al. [2]) Introduce three multigraph adaptations on the base GNN model.

Reverse MP



Messages from **incoming** and **outgoing** neighbors are aggregated <u>separately</u>

Increases expressivity as this allows for the computation of out-degree.

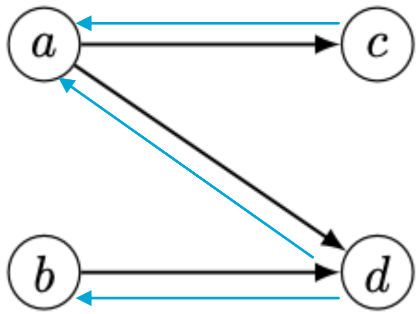
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Related Work

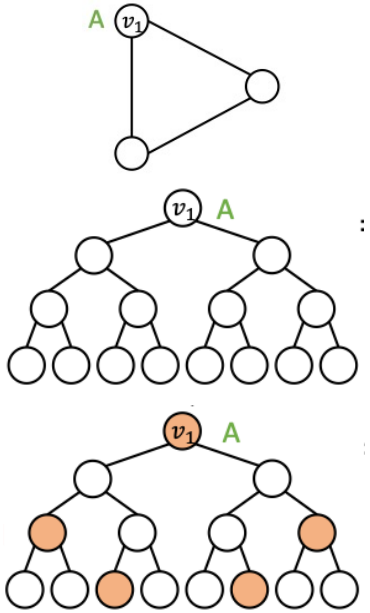
Limitations of Existing Solutions for Multigraphs

2. Multi-GNN (Egressy et al. [2]) Introduce three multigraph adaptations on the base GNN model.

Reverse MP



EgoIDs



The **center node** is marked with a distinct feature to recognize when a sequence of messages cycles back around it.

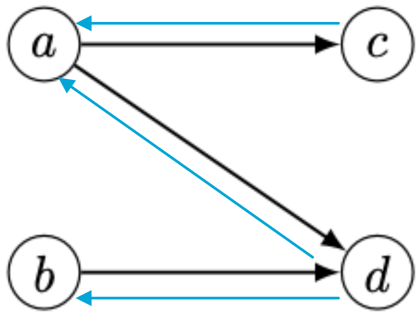
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Related Work

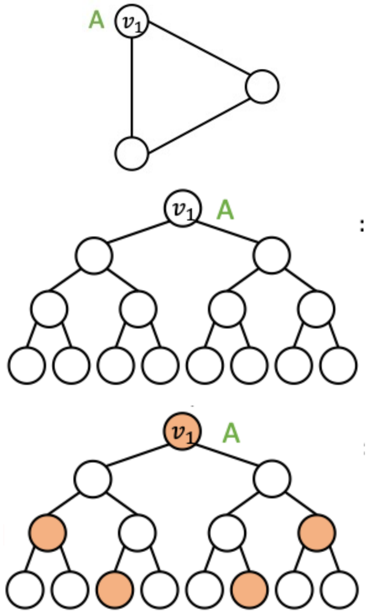
Limitations of Existing Solutions for Multigraphs

2. Multi-GNN (Egressy et al. [2]) Introduce three multigraph adaptations on the base GNN model.

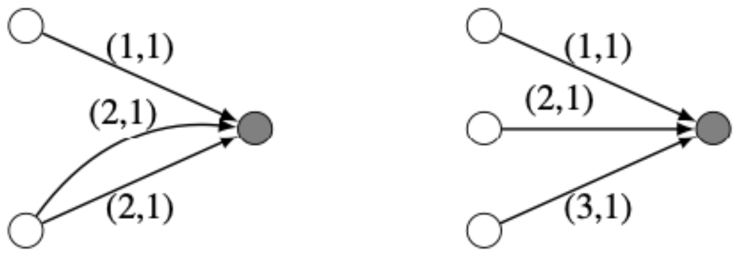
Reverse MP



EgoIDs



Multigraph Port Numbering



Port numbers are added to **distinguish** between edges from the same neighbor and those from different neighbors.

[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Related Work

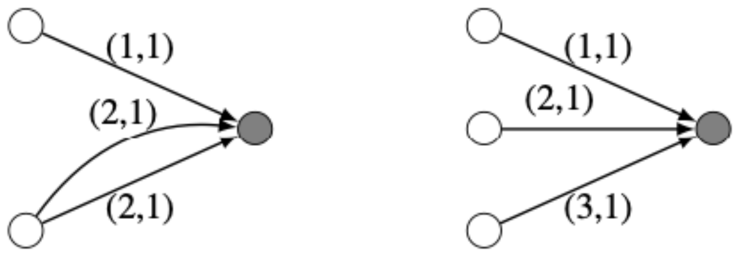
Limitations of Existing Solutions for Multigraphs

2. Multi-GNN (Egressy et al. [2]) Introduce three multigraph adaptations on the base GNN model.

The assignment of port numbers is arbitrary.

- Breaks **permutation equivariance.**
- Inconsistent model predictions under arbitrary permutations of node/edges.

Multigraph Port Numbering



Port numbers are added to **distinguish** between edges from the same neighbor and those from different neighbors.

[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

- Introduction
  - Motivation for Multigraph Neural Networks
- Related Work
  - Limitations of Existing Solutions for Multigraphs.
- MEGA-GNN: Our Proposed Solution
  - Motivation
  - Multigraph Message Passing with Multi-edge Aggregations
  - Why does a Two-stage Aggregation Make Sense?
  - Bi-directional Message Passing
  - Properties
- Experiments & Results
- Conclusion

MEGA-GNN

Motivation

- New message-passing framework for multigraphs.
  - Two-stage message aggregation schema.

[6] Xu, Keyulu, et al. How powerful are graph neural networks?. 2019 ICLR
[7] Corso, Gabriele, et al. Principal neighborhood aggregation for graph nets. 2020 NeurIPS

MEGA-GNN

Motivation

- New message-passing framework for multigraphs.
  - Two-stage message aggregation schema.
- It can extend baseline GNN models, GIN (Xu et al. [6]), or PNA (Corso et al. [7]), etc.

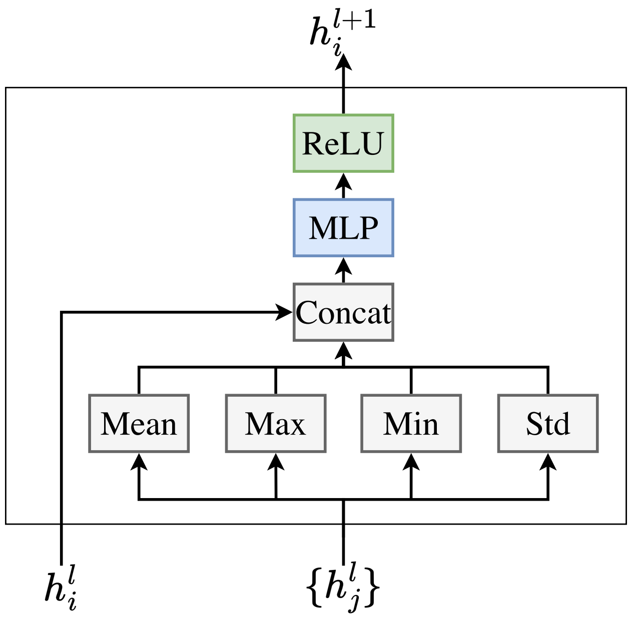
[6] Xu, Keyulu, et al. How powerful are graph neural networks?. 2019 ICLR
[7] Corso, Gabriele, et al. Principal neighborhood aggregation for graph nets. 2020 NeurIPS

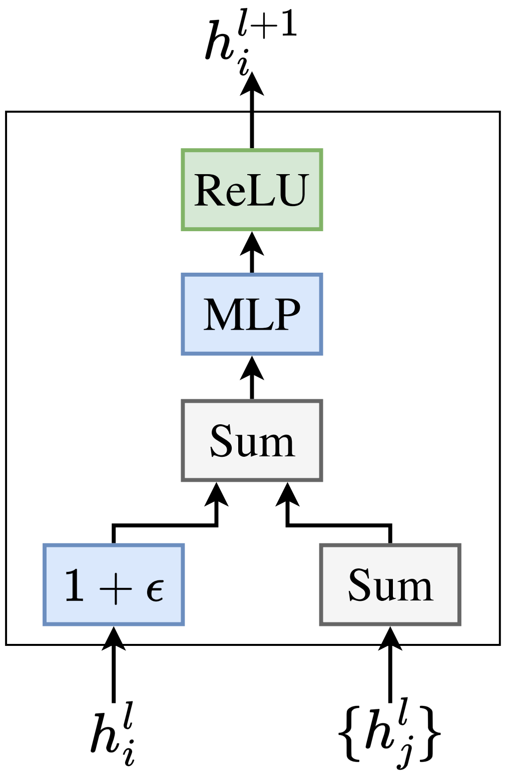
MEGA-GNN

Motivation

- New message-passing framework for multigraphs.
  - Two-stage message aggregation schema
- It can extend baseline GNN models, GIN (Xu et al. [6]), or PNA (Corso et al. [7]), etc.

PNA Layer





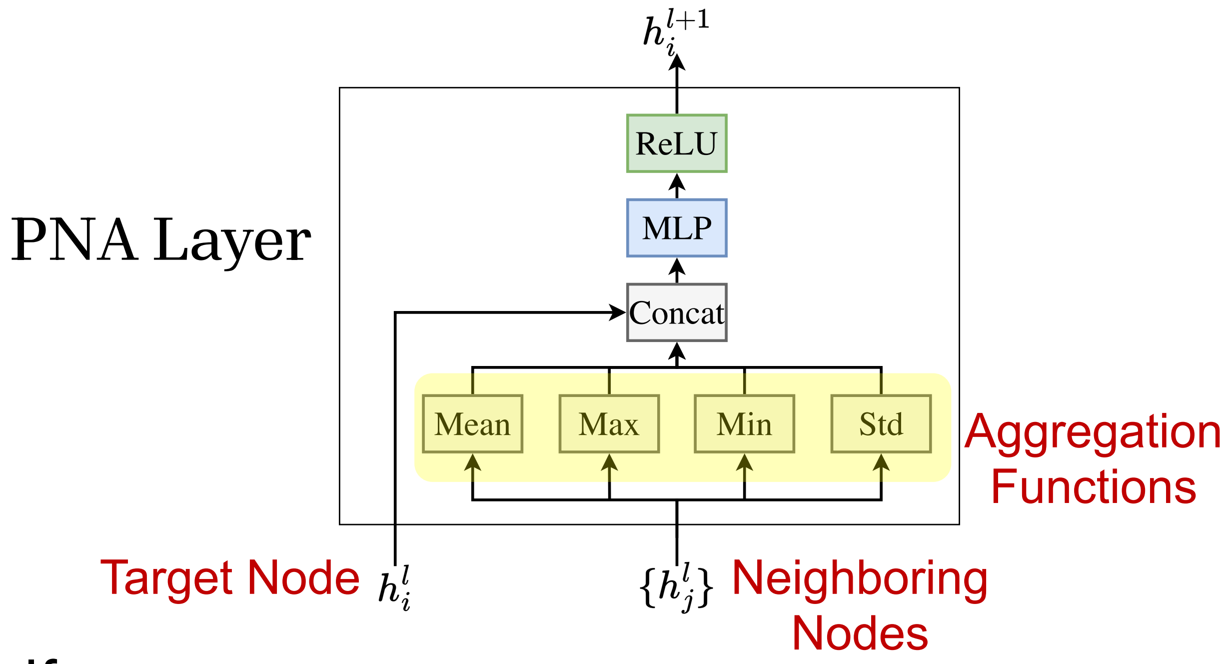
GIN Layer

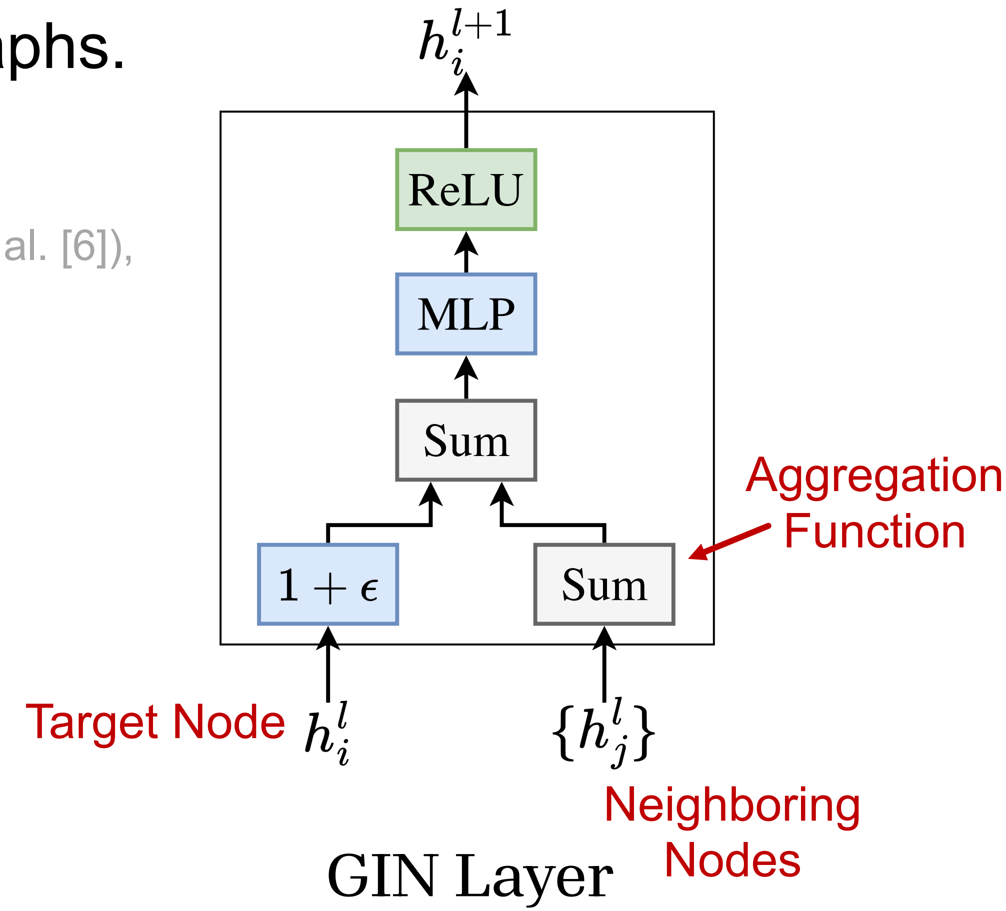
[6] Xu, Keyulu, et al. How powerful are graph neural networks?. 2019 ICLR
[7] Corso, Gabriele, et al. Principal neighborhood aggregation for graph nets. 2020 NeurIPS

MEGA-GNN

Motivation

- New message-passing framework for multigraphs.
  - Two-stage message aggregation schema
- It can extend baseline GNN models, GIN (Xu et al. [6]), or PNA (Corso et al. [7]), etc.



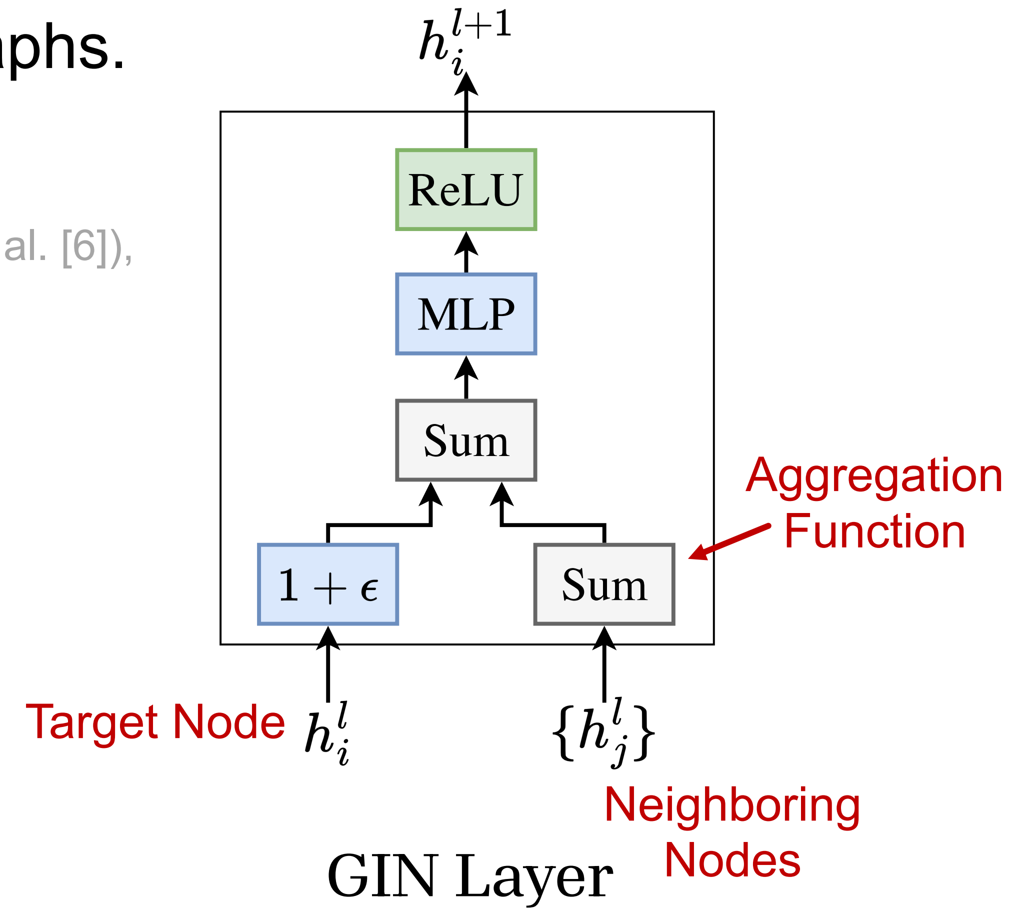


[6] Xu, Keyulu, et al. How powerful are graph neural networks?. 2019 ICLR
[7] Corso, Gabriele, et al. Principal neighborhood aggregation for graph nets. 2020 NeurIPS

MEGA-GNN

Motivation

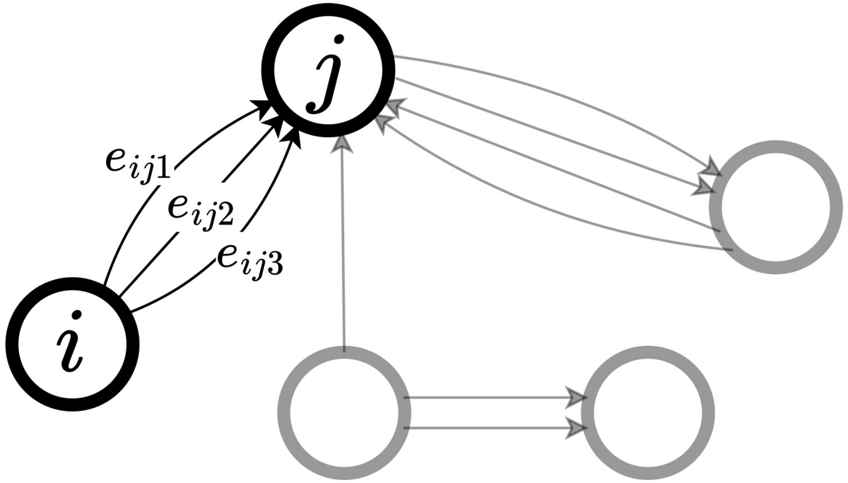
- New message-passing framework for multigraphs.
  - Two-stage message aggregation schema
- It can extend baseline GNN models, GIN (Xu et al. [6]), or PNA (Corso et al. [7]), etc.
- GenAgg (Kortvelesy et al. [8]), learnable aggregation function.



[6] Xu, Keyulu, et al. How powerful are graph neural networks?. 2019 ICLR
[7] Corso, Gabriele, et al. Principal neighborhood aggregation for graph nets. 2020 NeurIPS
[8] Kortvelesy, Ryan, et. al. Generalised f-mean aggregation for graph neural networks. 2023 NeurIPS

MEGA-GNN

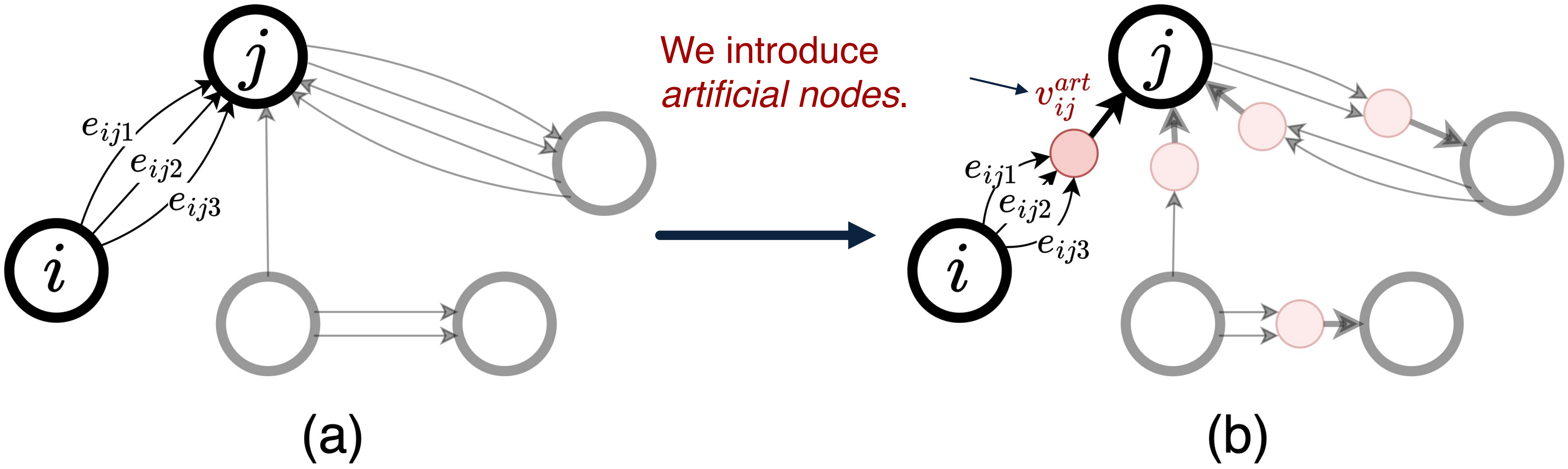
Multigraph Message Passing with Multi-edge Aggregations



(a)

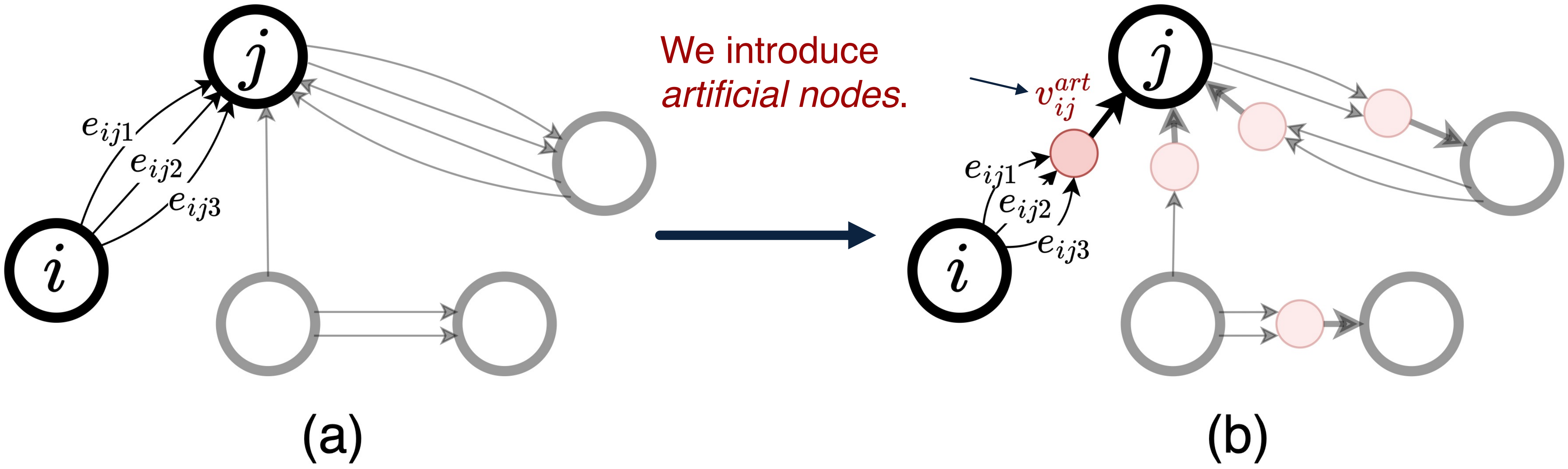
MEGA-GNN

Multigraph Message Passing with Multi-edge Aggregations



MEGA-GNN

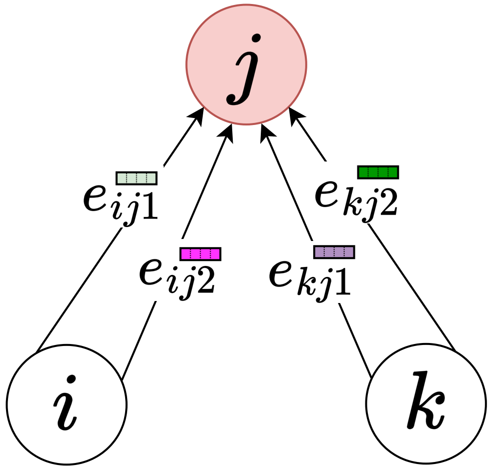
Multigraph Message Passing with Multi-edge Aggregations



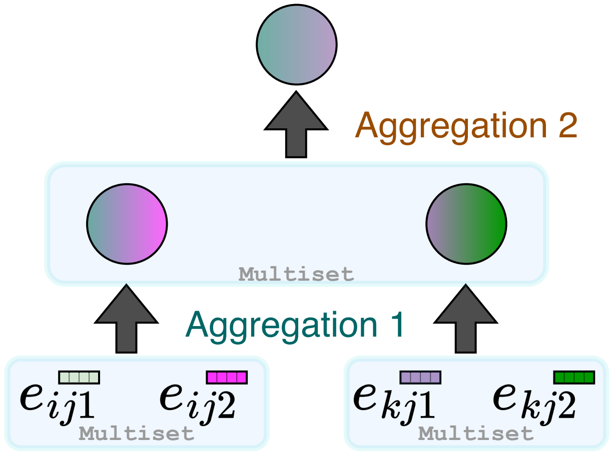
- Message passing for multigraphs with two-stage aggregation
  1. Multi-edge aggregation; aggregates multi-edges on artificial nodes.
  2. Node-level aggregation, aggregates messages from distinct neighbors.

MEGA-GNN

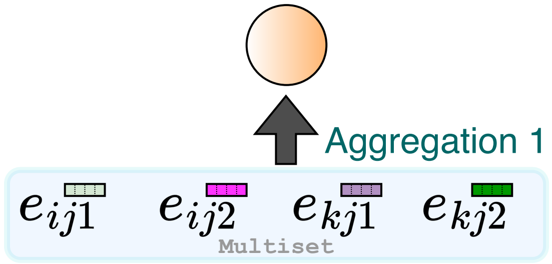
Why a Two-stage Aggregation Makes Sense?



Graph



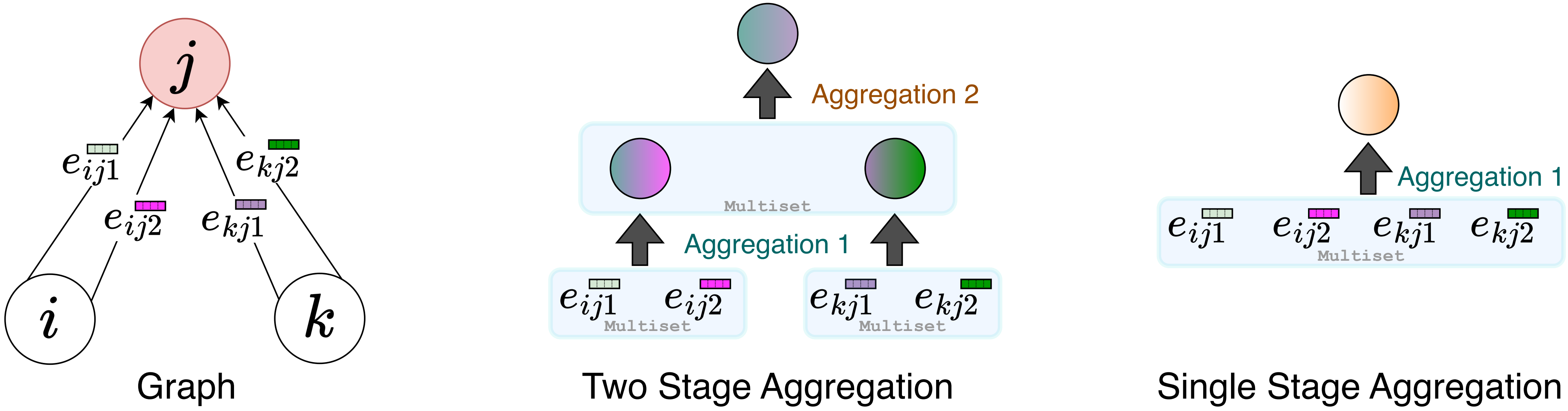
Two Stage Aggregation



Single Stage Aggregation

MEGA-GNN

Why a Two-stage Aggregation Makes Sense?

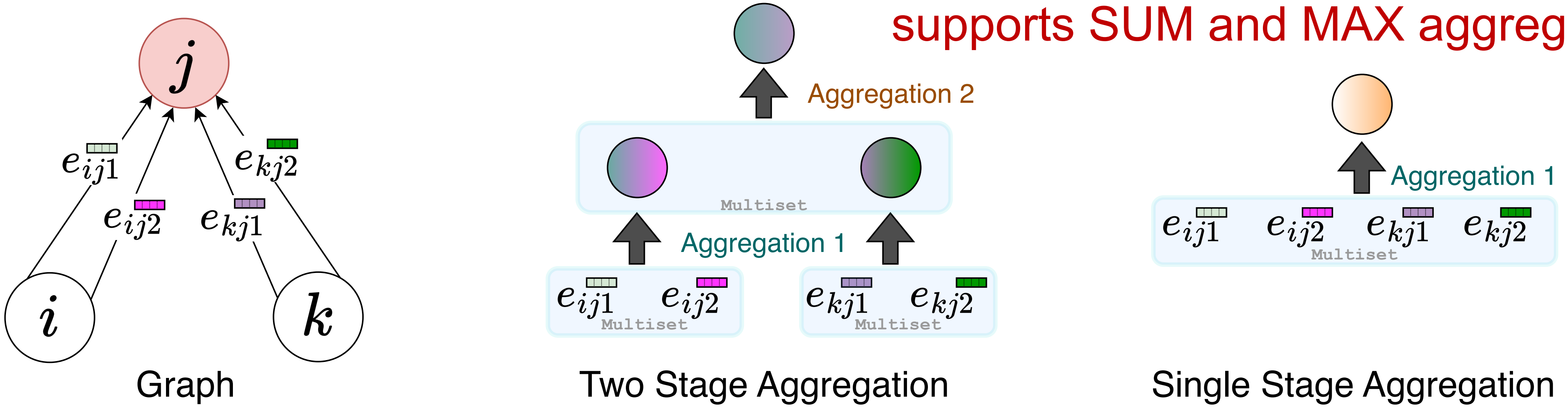


- **Two Stage:** Multi-edges are aggregated first followed by a node-level aggregation.
- **Single Stage:** All edges are aggregated at once.

MEGA-GNN

Advantage of Two-stage Aggregation

Assume the baseline GNN model supports SUM and MAX aggregations.

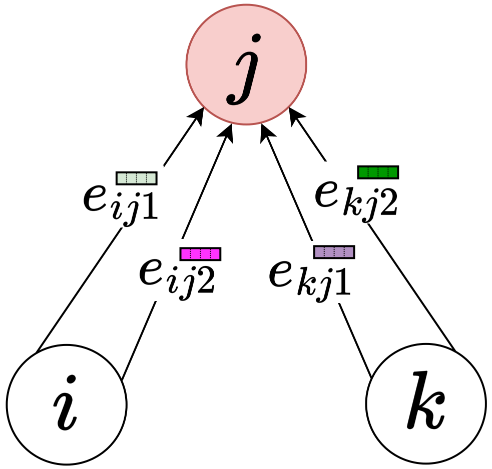


$$\mathrm{SUM}\Big\{\mathrm{SUM}\{e_{ij1}, e_{ij2}\}, \mathrm{SUM}\{e_{kj1}, e_{kj2}\}\Big\},$$
$$\mathrm{MAX}\Big\{\mathrm{MAX}\{e_{ij1}, e_{ij2}\}, \mathrm{MAX}\{e_{kj1}, e_{kj2}\}\Big\}$$

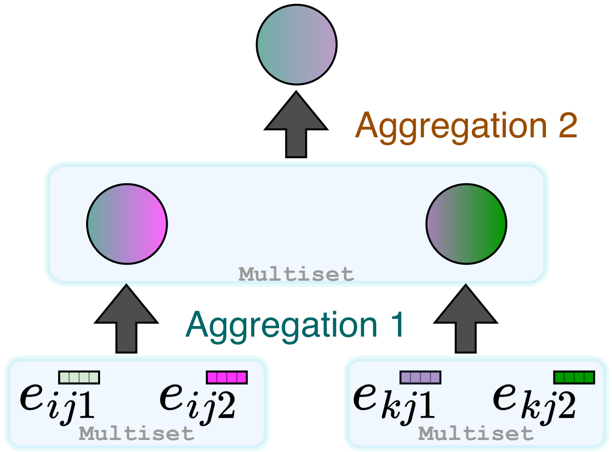
$$\mathrm{SUM}\{e_{ij1}, e_{ij2}, e_{kj1}, e_{kj2}\},\ \mathrm{MAX}\{e_{ij1}, e_{ij2}, e_{kj1}, e_{kj2}\}.$$

MEGA-GNN

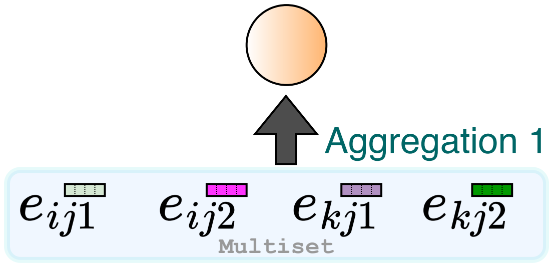
Advantage of Two-stage Aggregation



Graph



Two Stage Aggregation



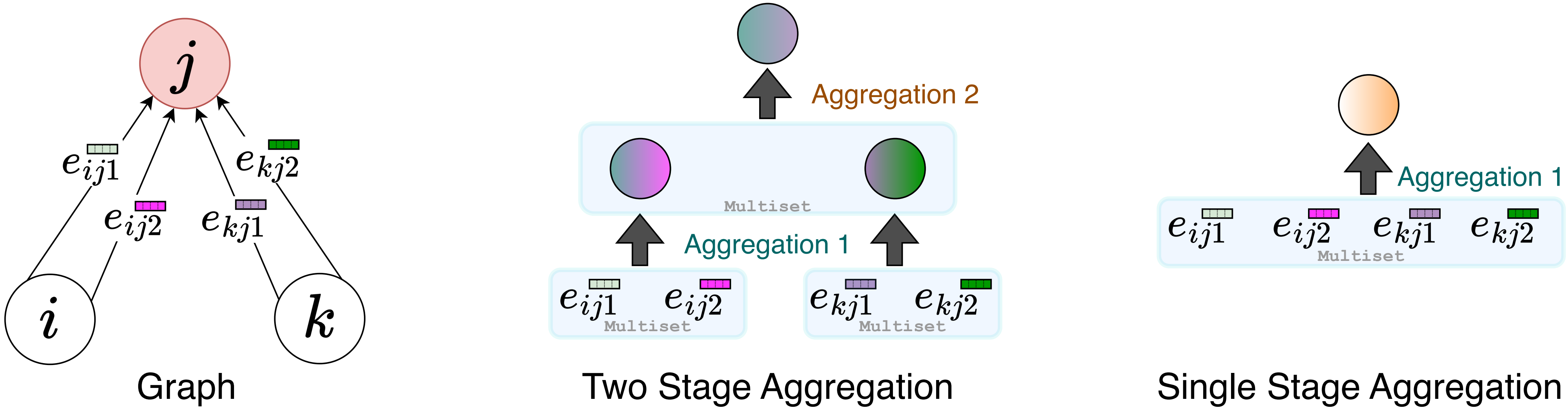
Single Stage Aggregation

$$\mathrm{SUM}\{\mathrm{MAX}\{e_{ij1}, e_{ij2}\}, \mathrm{MAX}\{e_{kj1}, e_{kj2}\}\}, \quad \mathrm{MAX}\{\mathrm{SUM}\{e_{ij1}, e_{ij2}\}, \mathrm{SUM}\{e_{kj1}, e_{kj2}\}\}$$

$$\mathrm{SUM}\{e_{ij1}, e_{ij2}, e_{kj1}, e_{kj2}\}, \ \mathrm{MAX}\{e_{ij1}, e_{ij2}, e_{kj1}, e_{kj2}\}.$$

MEGA-GNN

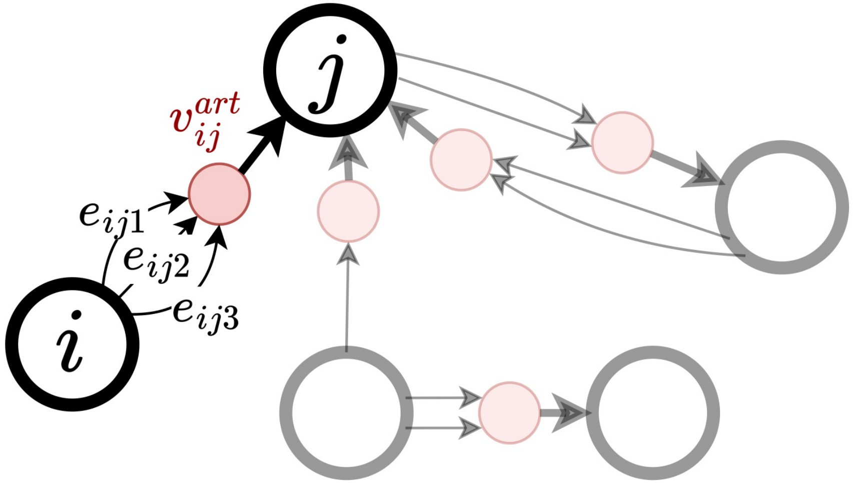
Advantage of Two-stage Aggregation



- The two-stage aggregation captures edge statistics per neighbor.
  - **Example:** Detects maximum sum of payments per sender.

MEGA-GNN

Reverse Message Passing with Multi-Edge Aggregations

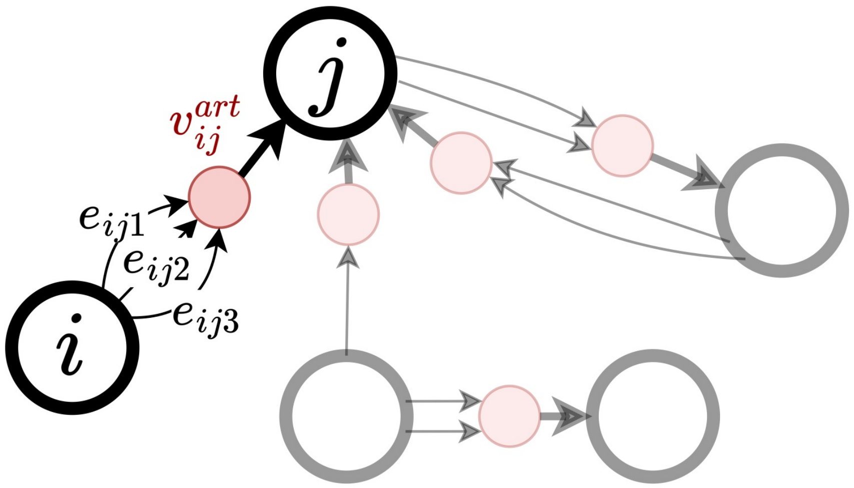


(b)

- Enhances model expressivity by handling incoming and outgoing neighbors separately.
- Enables computation of both **in-degree** and **out-degree**, unlike undirected or single-direction models.

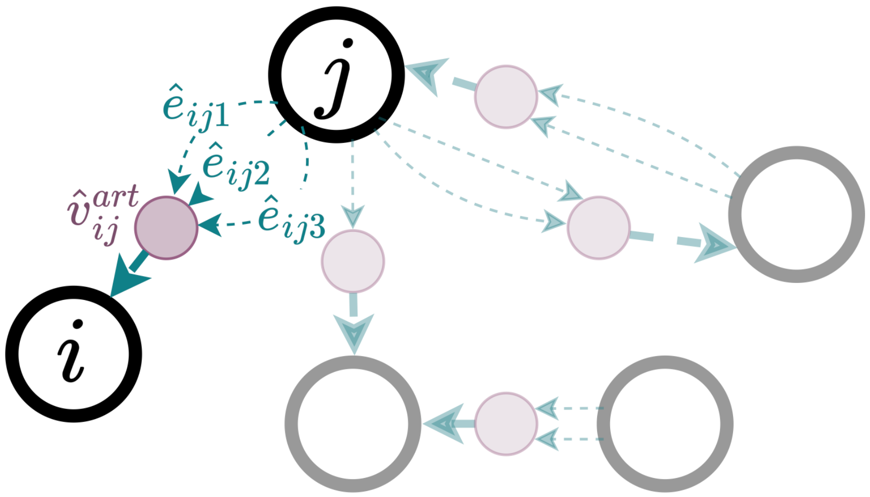
MEGA-GNN

Reverse Message Passing with Multi-Edge Aggregations



(b)

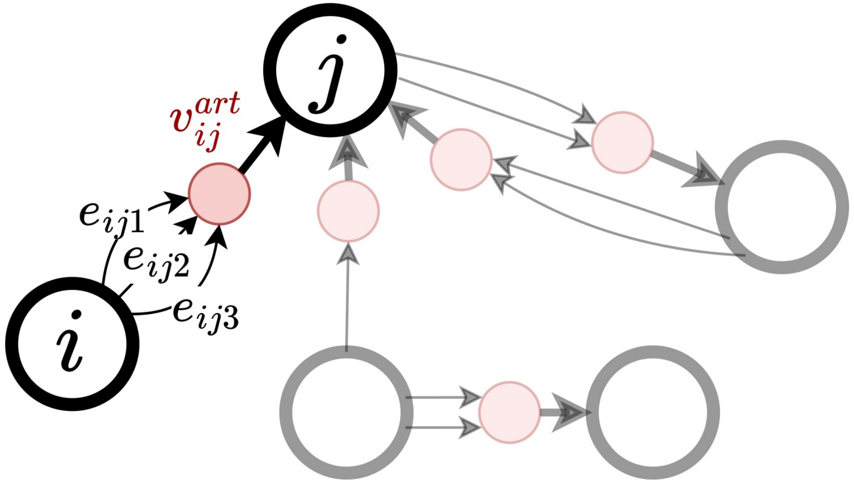
Reversed edges are also added to the Graph



(c)

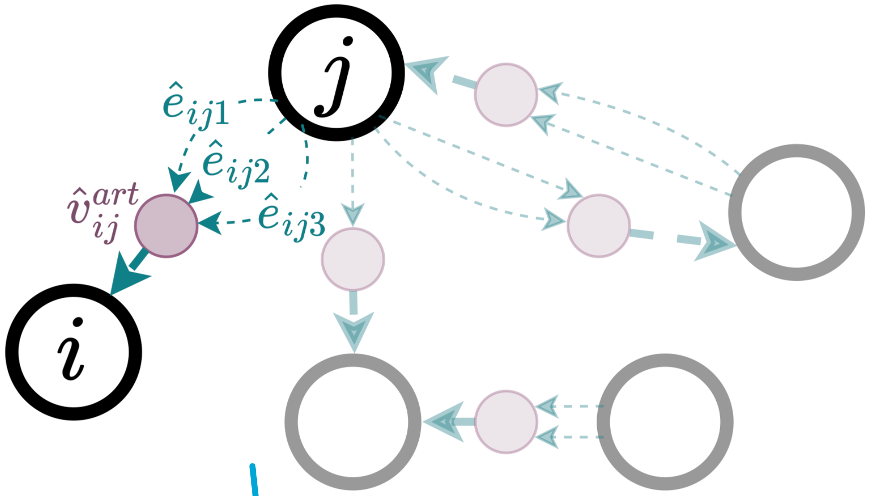
MEGA-GNN

Reverse Message Passing with Multi-Edge Aggregations



(b)

Reversed edges are also added to the Graph



(c)

- Messages from incoming and outgoing neighbors are separately aggregated.

$$\mathbf{x}_j^{(l)} = g_v^{(l-1)}\left(\mathbf{x}_j^{(l-1)}, \mathbf{a}_j^{(l-1)}, \hat{\mathbf{a}}_j^{(l-1)}\right)$$

MEGA-GNN

Properties

Permutation Equivariance:

- As a message passing based model, MEGA-GNN is permutation equivariant.

Universality:

- If there is a strict total order on the edges, then MEGA-GNN is universal.
  - Financial transaction networks exhibit this property, e.g., in the form of timestamps.

MEGA-GNN

Properties

Permutation Equivariance:

- As a message passing based model, MEGA-GNN is permutation equivariant.

Universality:

- If there is a strict total order on the edges, then MEGA-GNN is universal.
  - Financial transaction networks exhibit this property, e.g., in the form of timestamps.

How about Multi-GNN (Egressy et. al. [2])?

- Not permutation equivariant when the port numbering is arbitrary.
- Multi-GNN is always universal.

[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

- Introduction
  - Motivation for Multigraph Neural Networks
- Related Work
  - Limitations of Existing Solutions for Multigraphs.
- MEGA-GNN: Our Proposed Solution
  - Motivation
  - Multigraph Message Passing with Multi-edge Aggregations
  - Why does a Two-stage Aggregation Make Sense?
  - Bi-directional Message Passing
  - Properties
- Experiments & Results
- Conclusion

Experiments & Results

Datasets

1. Anti-Money Laundering (AML)
   - **Task:** Edge classification.
2. Ethereum Phishing Transaction (ETH)
   - **Task:** Node classification.

Dataset	# Nodes	# Edges	Illicit Rate	Split [%]
AML Small HI	515,088	5,078,345	0.102%	64/19/17
AML Small LI	705,907	6,924,049	0.051%	64/19/17
AML Medium HI	2,077,023	31,898,238	0.110%	61/17/22
AML Medium LI	2,032,095	31,251,483	0.051%	61/17/22
AML Large HI	2,116,168	179,702,229	0.124%	60/20/20
AML Large LI	2,070,980	176,066,557	0.057%	60/20/20
ETH	2,973,489	13,551,303	0.04%	65/15/20

Experiments & Results

Datasets

1. Anti-Money Laundering (AML)
   - **Task:** Edge classification.
2. Ethereum Phishing Transaction (ETH)
   - **Task:** Node classification.

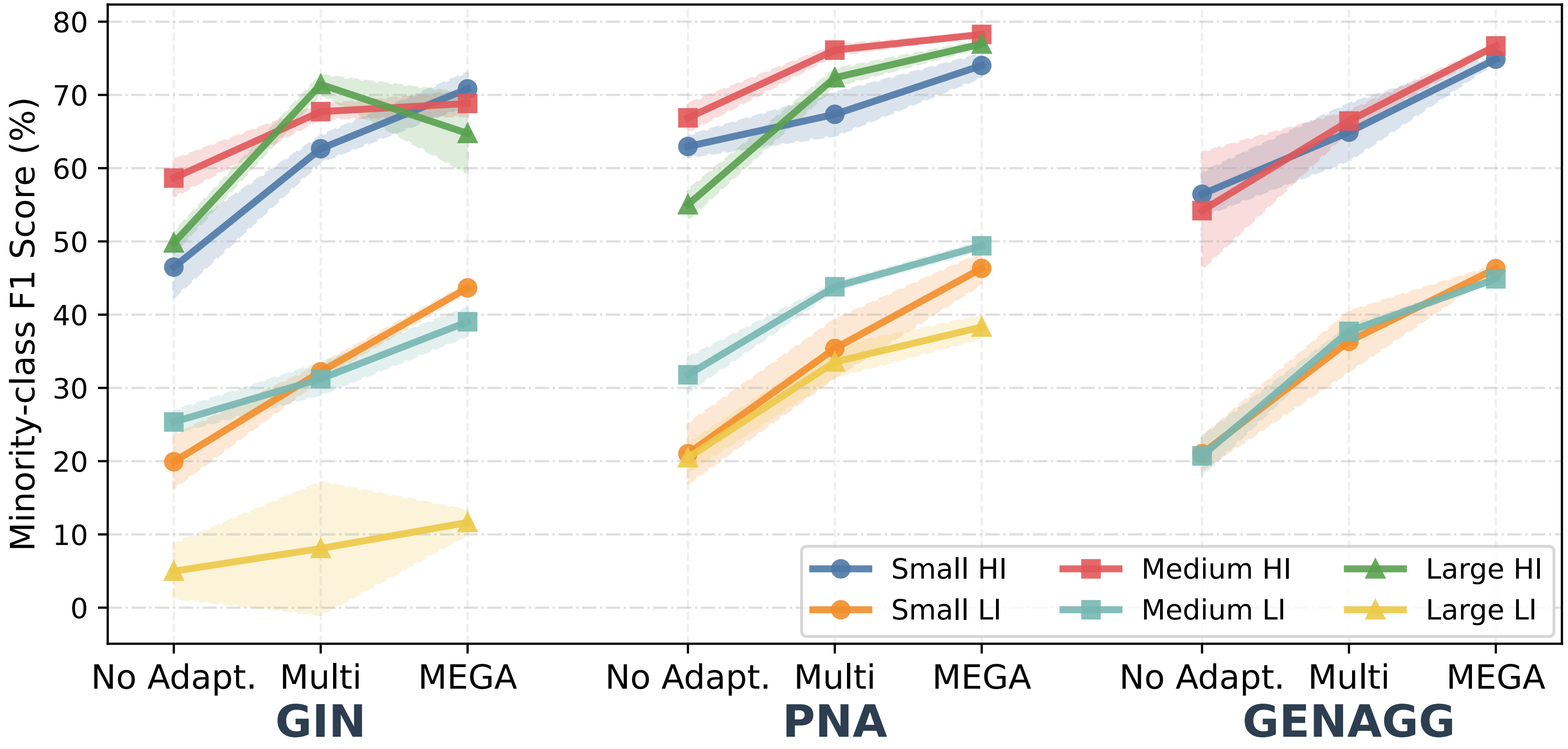
Dataset	# Nodes	# Edges	Illicit Rate	Split [%]
AML Small HI	515,088	5,078,345	0.102%	64/19/17
AML Small LI	705,907	6,924,049	0.051%	64/19/17
AML Medium HI	2,077,023	31,898,238	0.110%	61/17/22
AML Medium LI	2,032,095	31,251,483	0.051%	61/17/22
AML Large HI	2,116,168	179,702,229	0.124%	60/20/20
AML Large LI	2,070,980	176,066,557	0.057%	60/20/20
ETH	2,973,489	13,551,303	0.04%	65/15/20

Baselines

Multigraph Adaptations	GIN	PNA	GenAgg
No adaptations	✓	✓	✓
Multi (Egressy et al., 2024)	✓	✓	✓
ADAMM (Sotiropoulos et al., 2023)	✓	✓	✓
MEGA (ours)	✓	✓	✓

Experiments & Results

AML Edge Classification Results

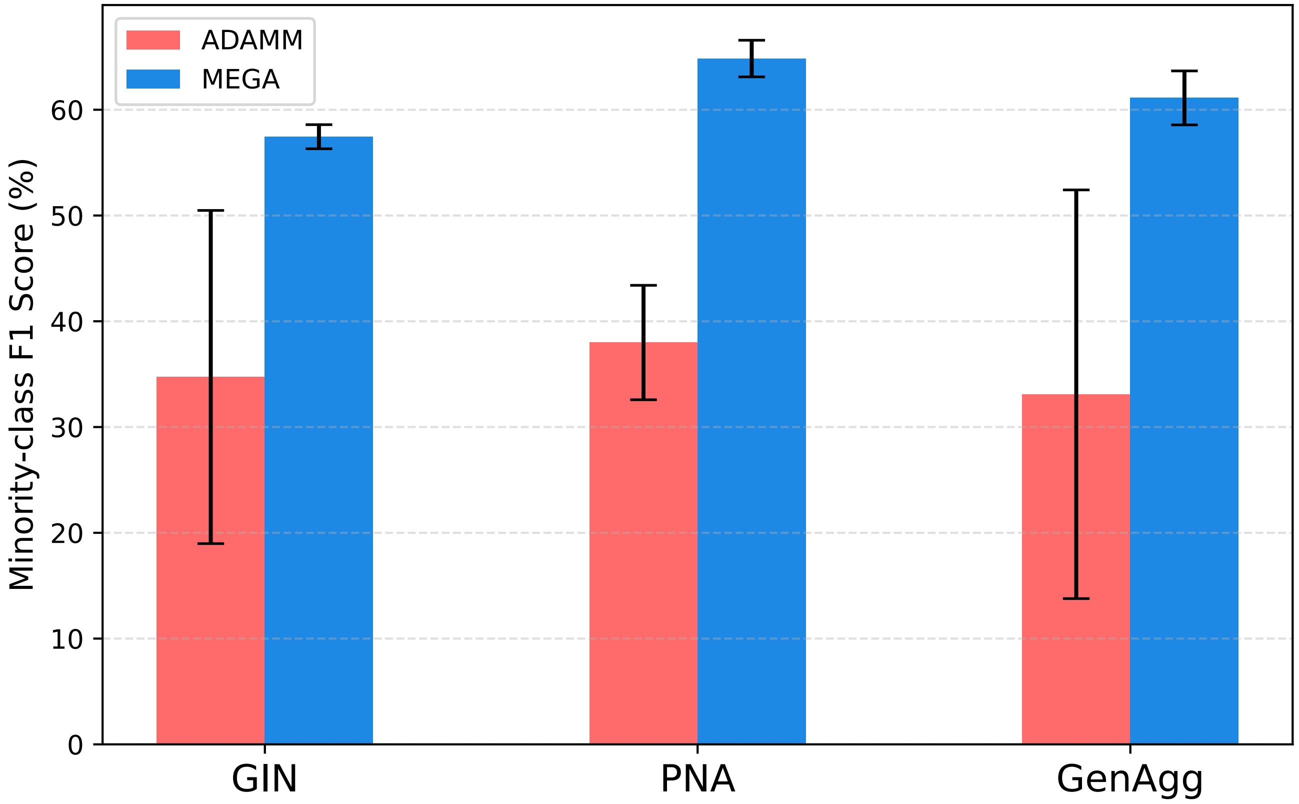


- On average, MEGA-GNN improves minority-class F1 scores by 4.75% on HI datasets and 6.77% on LI datasets compared to Multi-GNN (Egressy et al. [2]).

[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Experiments & Results

ETH Node Classification Results

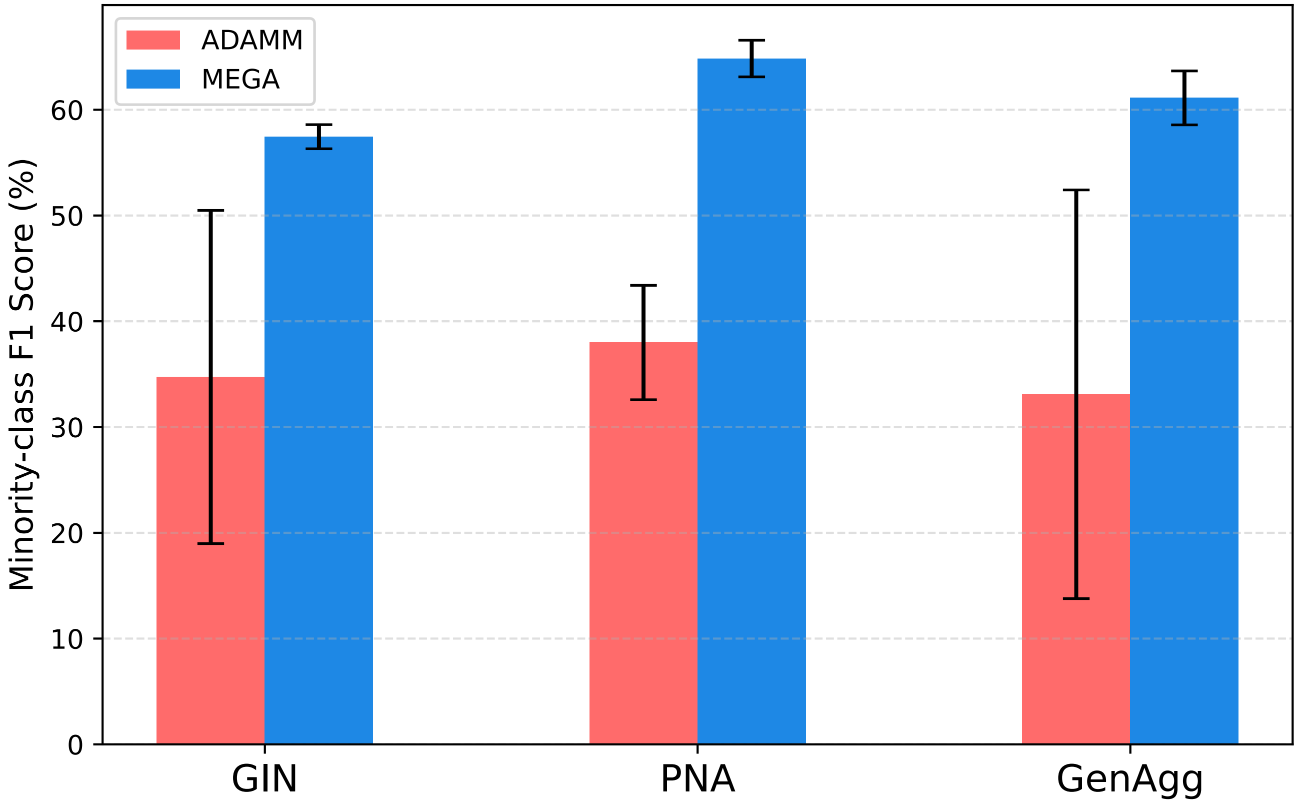


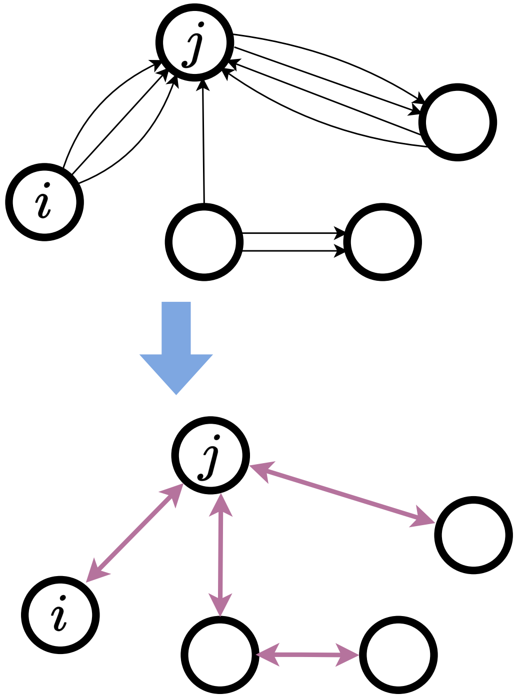
- Compared to the ADAMM (Sotiropoulos et. al. [1]), our MEGA-GNN variants consistently deliver over 20% higher performance across base architectures.

[1] Sotiropoulos K, Zhao L, Liang PJ, Akoglu L. ADAMM: Anomaly Detection of Attributed Multi-graphs with Metadata: A Unified Neural Network Approach. 2023 IEEE International Conference on Big Data.

Experiments & Results

ETH Node Classification Results





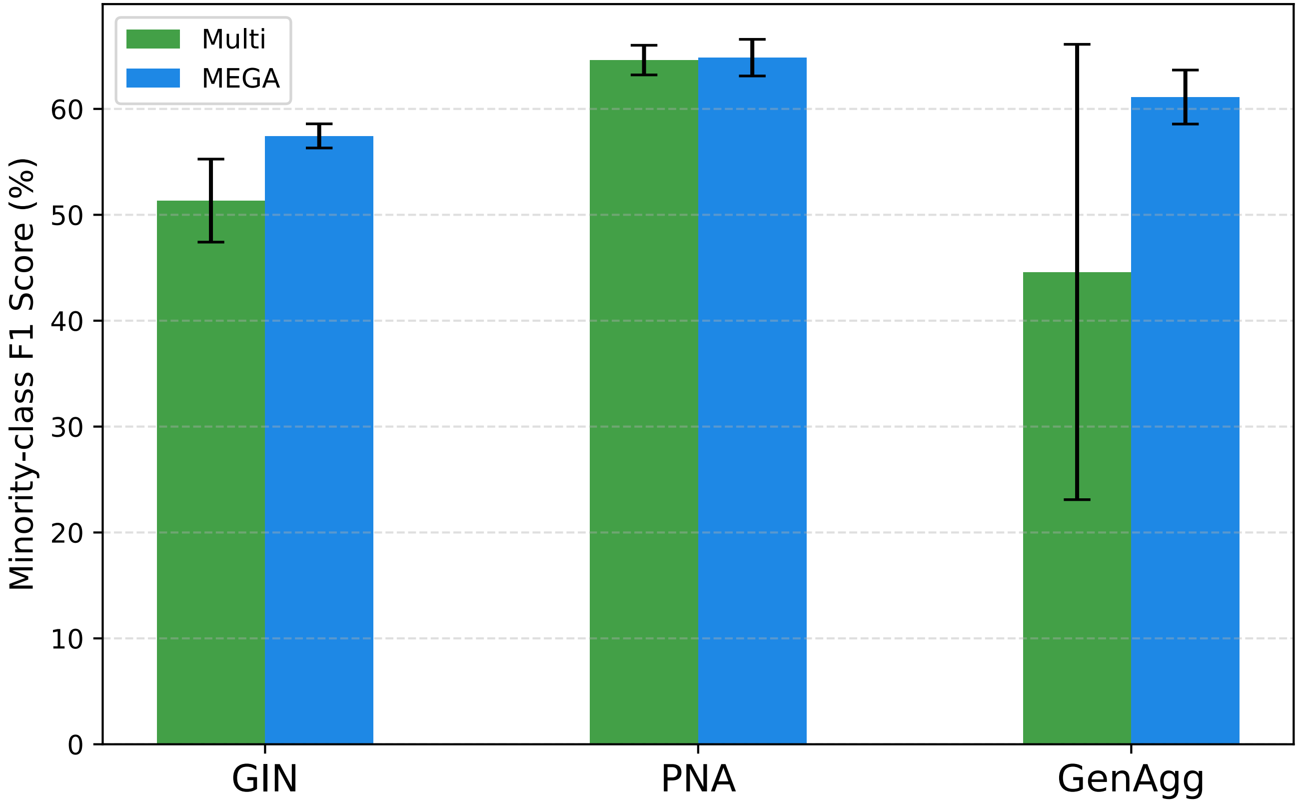
ADAMM
(Sotiropoulos et. al. [1])

- Compared to the ADAMM (Sotiropoulos et. al. [1]), our MEGA-GNN variants consistently deliver over 20% higher performance across base architectures.

[1] Sotiropoulos K, Zhao L, Liang PJ, Akoglu L. ADAMM: Anomaly Detection of Attributed Multi-graphs with Metadata: A Unified Neural Network Approach. 2023 IEEE International Conference on Big Data.

Experiments & Results

ETH Node Classification Results

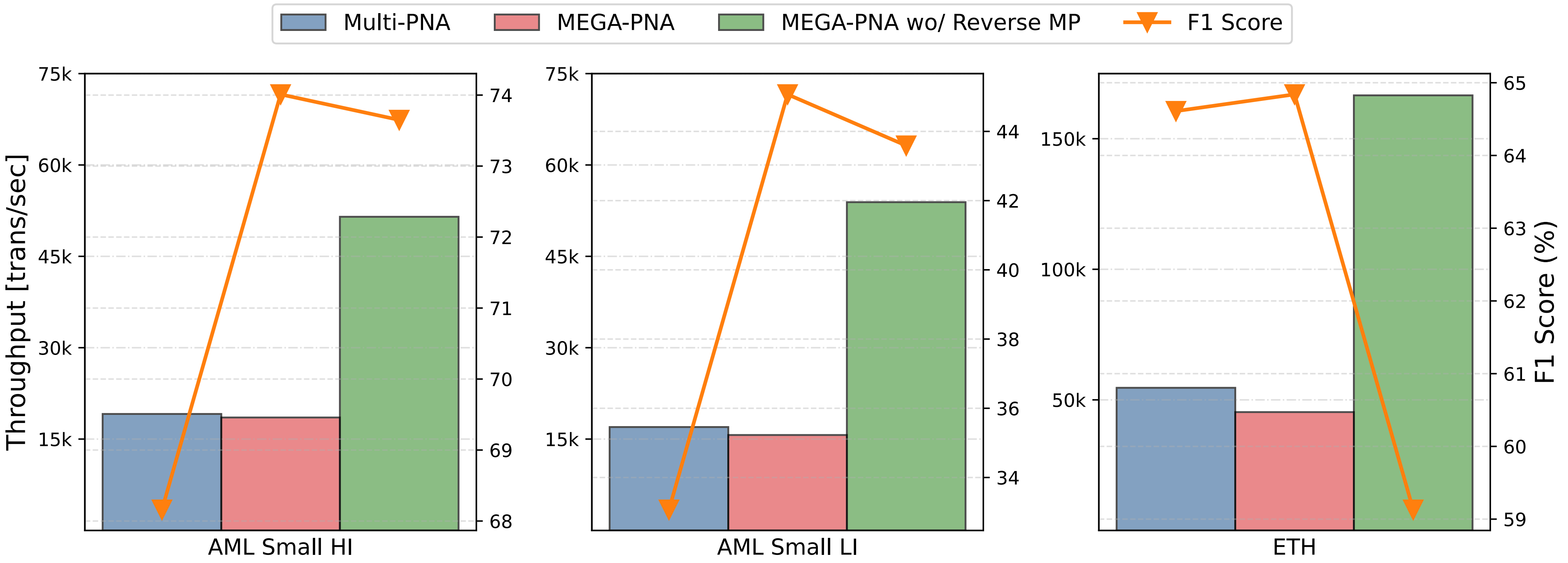


- Compared to the Multi (Egressy et al. [2]), our MEGA variants improve the GIN and GenAgg models and match the performance of PNA.

[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Experiments & Results

Computational Overhead



- **Minimal computational overhead**
- **Boosts** inference speed by disabling reverse message passing.

[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Conclusion

- We addressed the shortcomings of the existing methods.
  - Preserve original topology
  - Permutation Equivariance

- **AML Datasets:**
  - Improvements up to +10.93% F1 (minority-class) over Multi-GNN(Egressy et al. [2]).

- **ETH Dataset**
  - +20% F1 over ADAMM (Sotiropoulos et. al. [1]), matching Multi-GNN (Egressy et al. [2]).

[1] Sotiropoulos K, Zhao L, Liang PJ, Akoglu L. ADAMM: Anomaly Detection of Attributed Multi-graphs with Metadata: A Unified Neural Network Approach. 2023 IEEE International Conference on Big Data.
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Thank you

The pre-print of the MEGA-GNN paper can be found on
https://arxiv.org/pdf/2412.00241

13-02-2025

Experiments & Results

Ablation Study

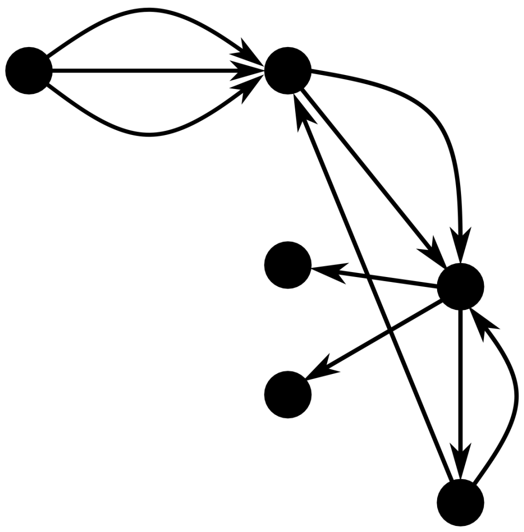
- MEGA-GNN outperforms most baselines using only two-stage aggregation, proving its strength without bi-directional MP or ego IDs.

Ablation	AML Small HI	AML Small LI	ETH
MEGA-GIN w/ Ego-IDs & Bi-directional MP	70.83 ± 2.18	43.66 ± 0.54	55.19 ± 2.33
MEGA-GIN w/ Bi-directional MP	72.50 ± 3.26	41.67 ± 1.51	57.45 ± 1.14
MEGA-GIN w/ Ego-IDs	69.59 ± 1.07	40.79 ± 1.91	42.82 ± 3.34
MEGA-GIN (Unidirectional MP)	69.98 ± 2.02	41.45 ± 2.13	43.56 ± 2.67
MEGA-PNA w/ Ego-IDs & Bi-directional MP	74.01 ± 1.55	46.32 ± 2.07	60.02 ± 5.10
MEGA-PNA w/ Bi-directional MP	74.98 ± 1.59	45.36 ± 1.18	64.84 ± 1.73
MEGA-PNA w/ Ego-IDs	73.61 ± 0.55	44.47 ± 1.53	57.62 ± 1.23
MEGA-PNA (Unidirectional MP)	73.65 ± 0.36	43.77 ± 1.53	59.13 ± 0.51

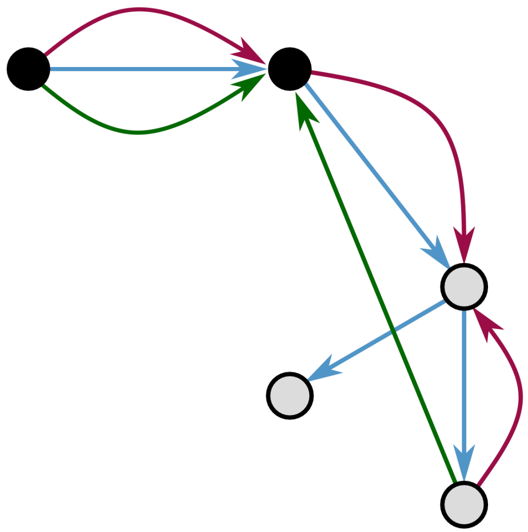
[2] Egressy, B., et. al. Provably Powerful Graph Neural Networks for Directed Multigraphs. 2024 In Proceedings of the AAAI Conference on Artificial Intelligence

Introduction

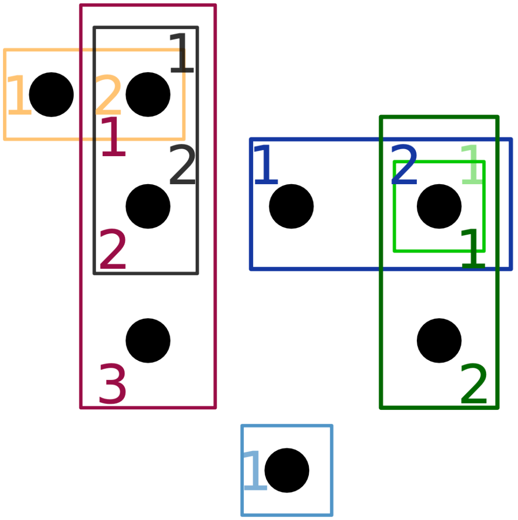
Motivation: Multigraphs



Multigraph



Multi-relational Graph



Hypergraph

Introduction

Motivation: Multigraphs

Feature	Multigraphs	Multi-Relational Graphs	Hypergraphs
Edge Structure	Multiple edges between the same two nodes	Heterogeneous Edge Types	Hyperedges connecting multiple nodes
Edge Features	Each edge has **independent features**	Edge types determine relation semantics	Features assigned to hyperedges
Example	Financial transactions (multiple payments between accounts)	Knowledge graphs (e.g., "Alice works for CompanyX")	Co-authorship networks (one paper connecting multiple authors)
GNN Implication	Requires multi-edge aggregation	Requires different rules for different edge types	Requires hyperedge aggregation