On the Equivalence Between Temporal and Static Equivariant Graph Representations

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Contribution

- We summarize existing temporal graph neural networks (TGNNs) into **two main categories** and study their **expressivity** power.

- We propose a simple but effective framework which
  - Is **theoretically more expressive** than existing works;
  - Achieve **similar or even better** performance;
  - Can be **extremely efficient** in certain tasks.

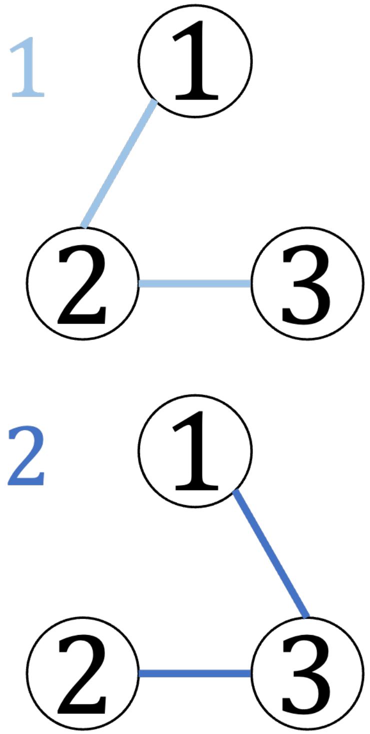
Temporal Graph

- A collection of dynamically changing nodes and edges.

- Temporal graph is common in real-world scenario:
    - Social
    - Communication
    - Transportation/Traffic
    - Biological/Medical
    - ……

Temporal Graph

Snapshotted



- A sequence of snapshots.

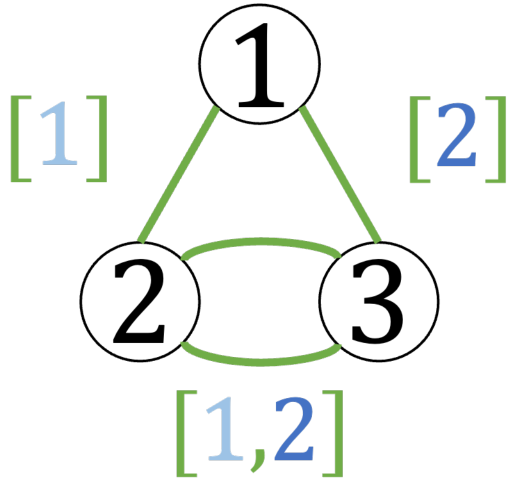
$$\left[G_{t_1}, G_{t_2}, \cdots\right]$$

Temporal Graph

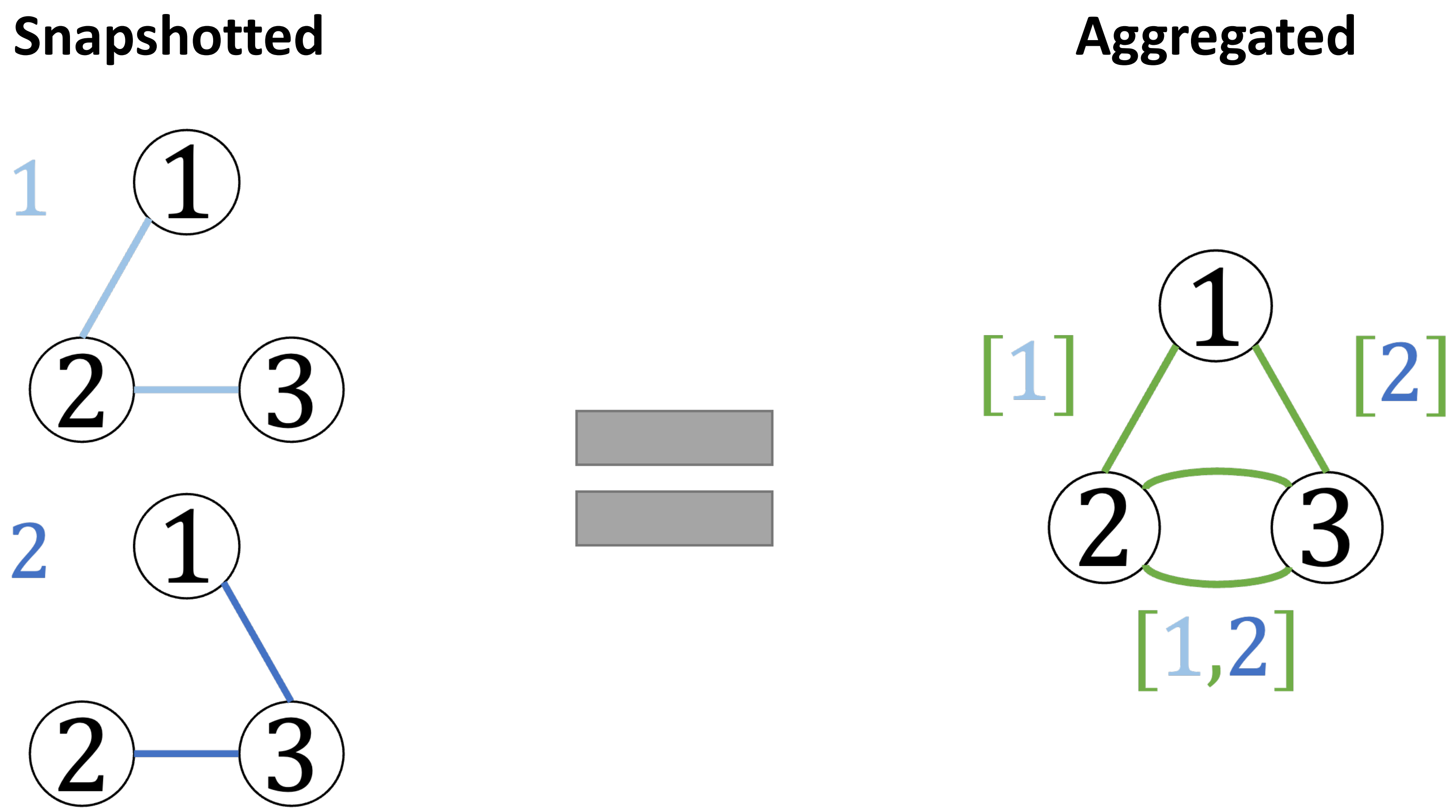
- A multi-graph aggregation of all history snapshots.

$$G^*_{\mathrm{agg}}$$

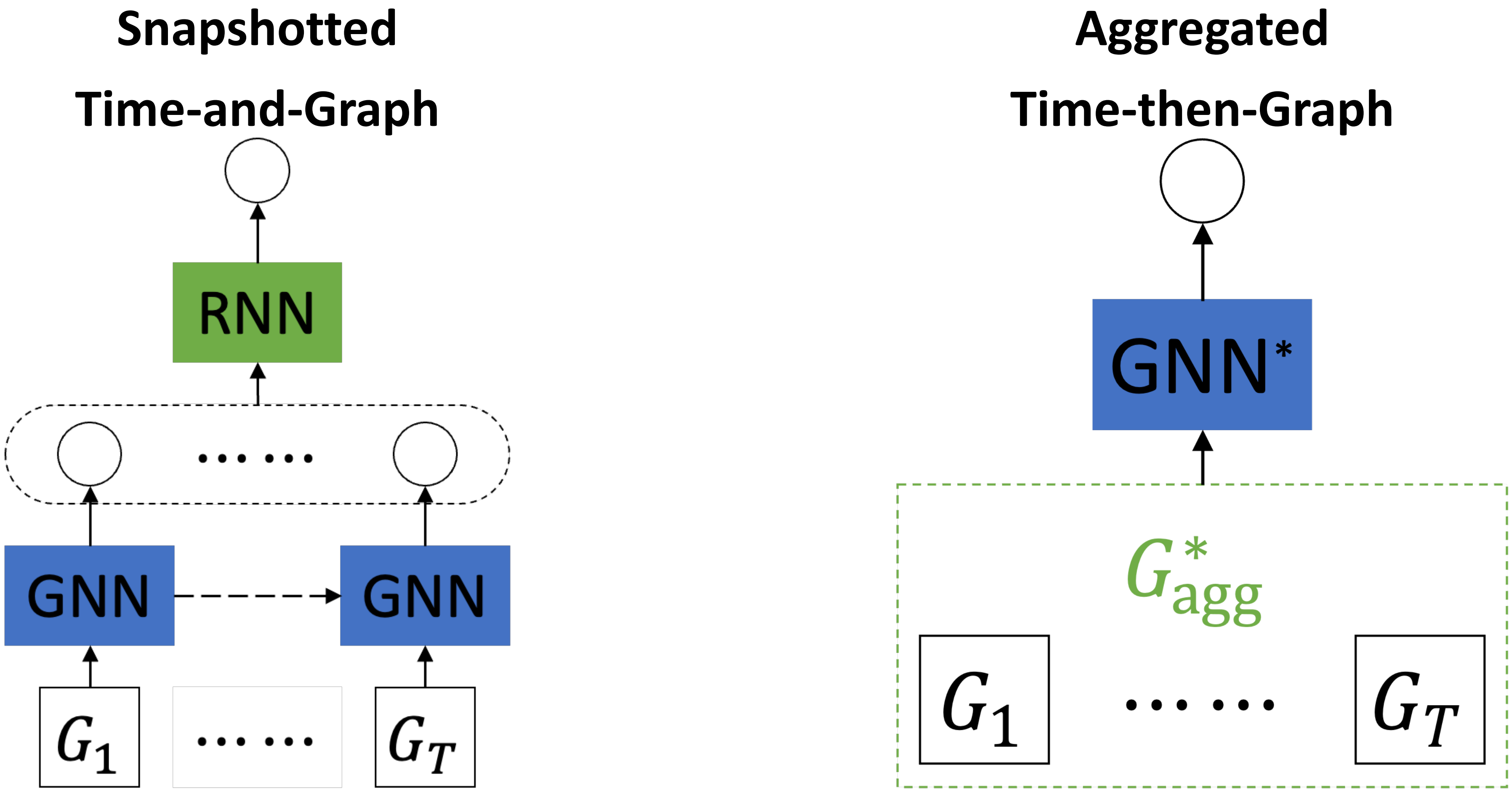
Aggregated



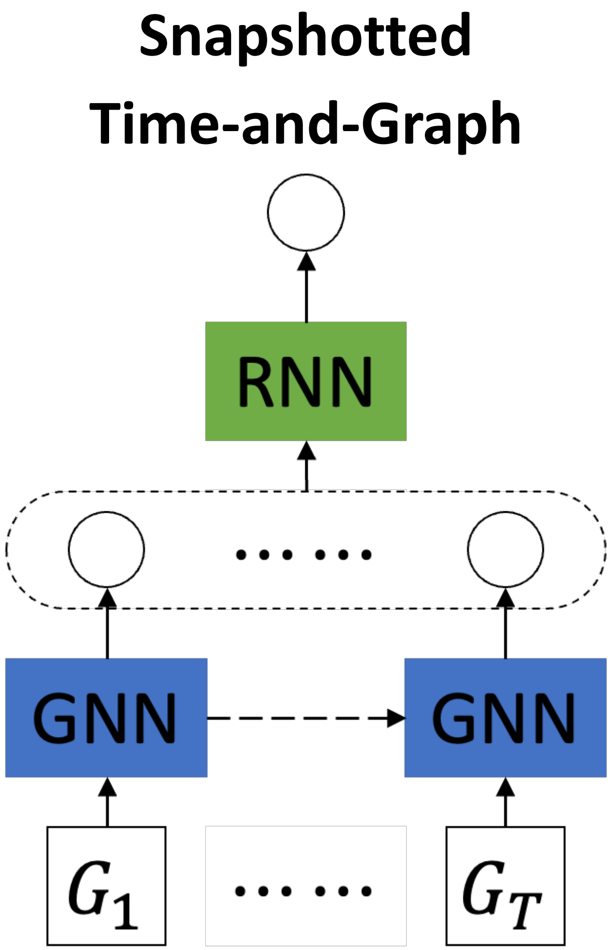
Temporal Graph



Temporal Graph Neural Network



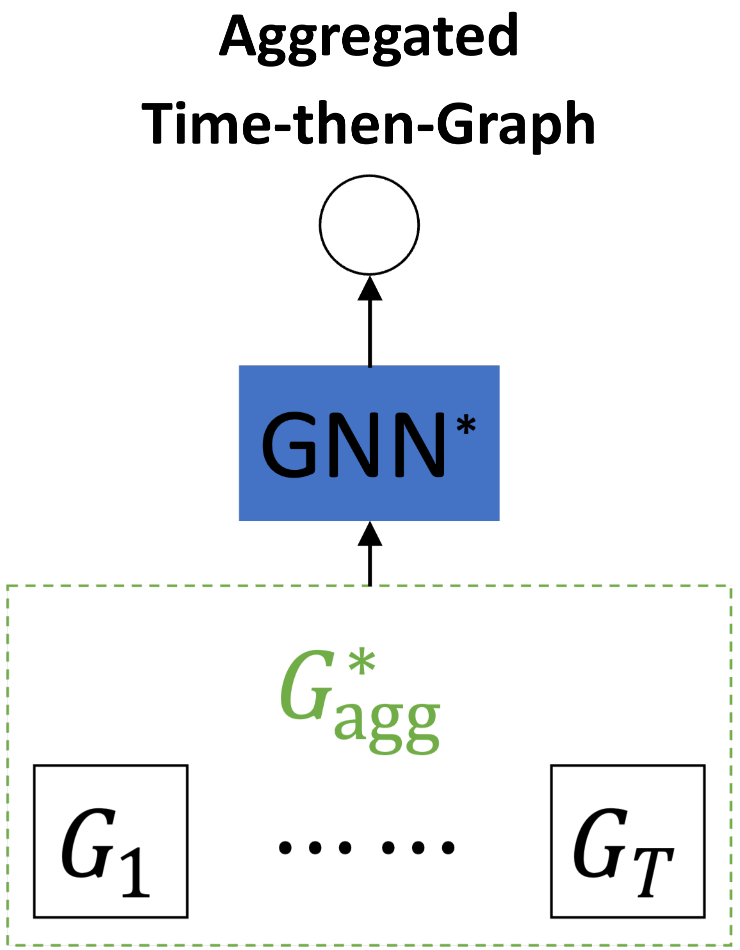
Temporal Graph Neural Network



1. GNN is independently applied to each snapshot;
2. A sequence modeling is used to map GNN embeddings into final representation.

Temporal Graph Neural Network

1. Aggregate all history graphs together into a new graph;
2. Feed new graph into GNN to get final representation.



Expressivity[1]

- Theorem 3.5 (Informal)

  If use only 1WLGNNs, time-then-graph is strictly more expressive than time-and-graph.

  (1WL means *1-Weisfeiler-Lehman*[2,3].)

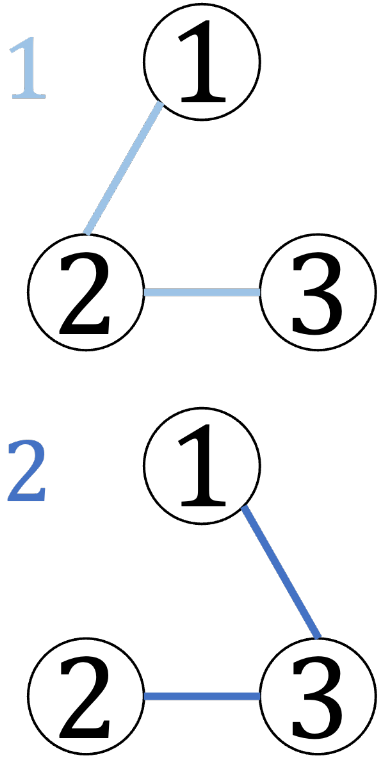
- Theorem 3.6 (Informal)

  With more expressive GNNs[4], the expressivity gap between time-and-graph and time-then-graph become less, and eventually becomes the same with the most expressive GNNs[5].

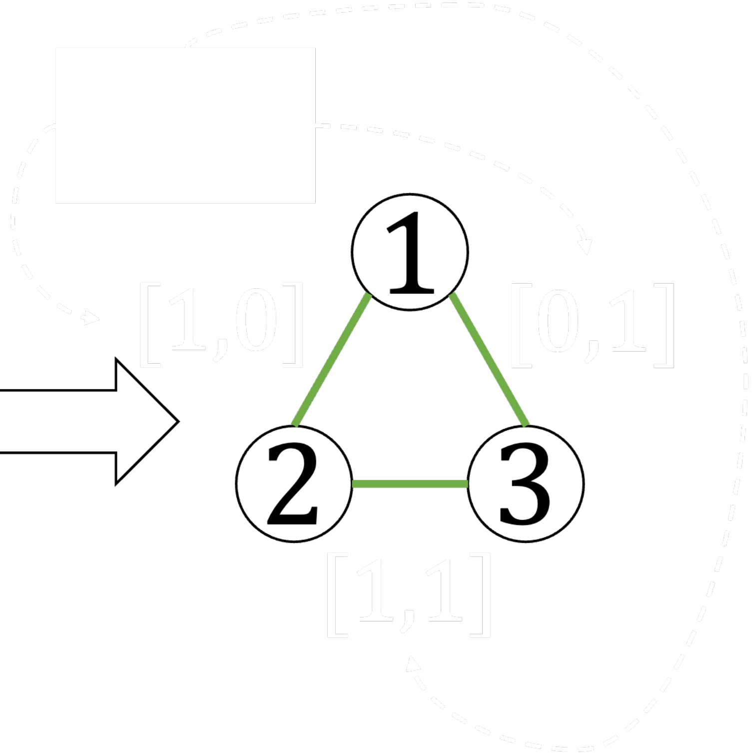
1. See paper.

2. Weisfeiler, B., & Leman, A. (1968). The reduction of a graph to canonical form and the algebra which appears therein. NTI, Series, 2(9), 12-16.
3. Xu, K., Hu, W., Leskovec, J., & Jegelka, S. (2018). How powerful are graph neural networks?. arXiv preprint arXiv:1810.00826.
4. Morris, C., Ritzert, M., Fey, M., Hamilton, W. L., Lenssen, J. E., Rattan, G., & Grohe, M. (2019). Weisfeiler and leman go neural: Higher-order graph neural networks.
5. Maron, H., Fetaya, E., Segol, N., & Lipman, Y. (2019, May). On the universality of invariant networks.

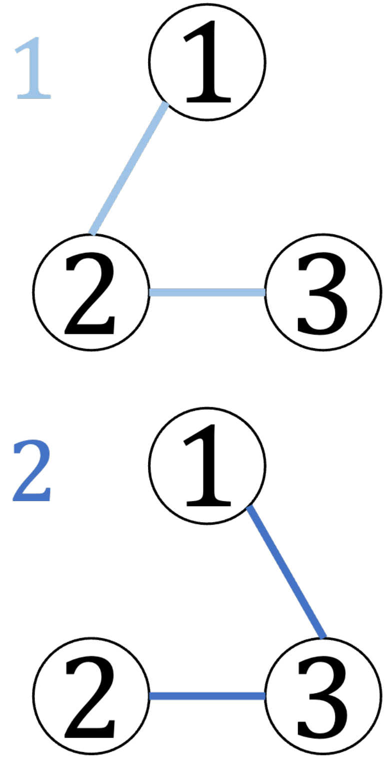
Proposal: GRU-GCN



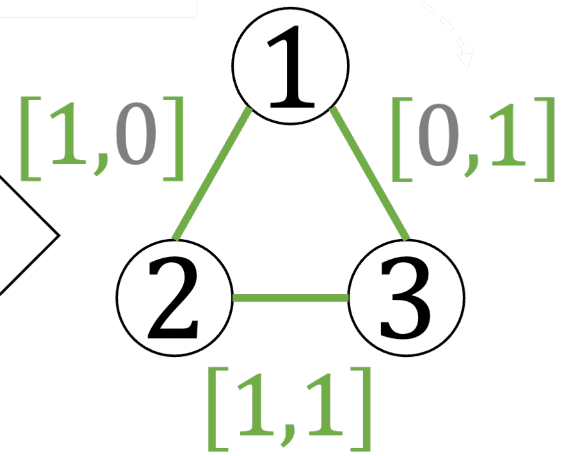
Aggregate attributes
of the same edge over
all times as one edge



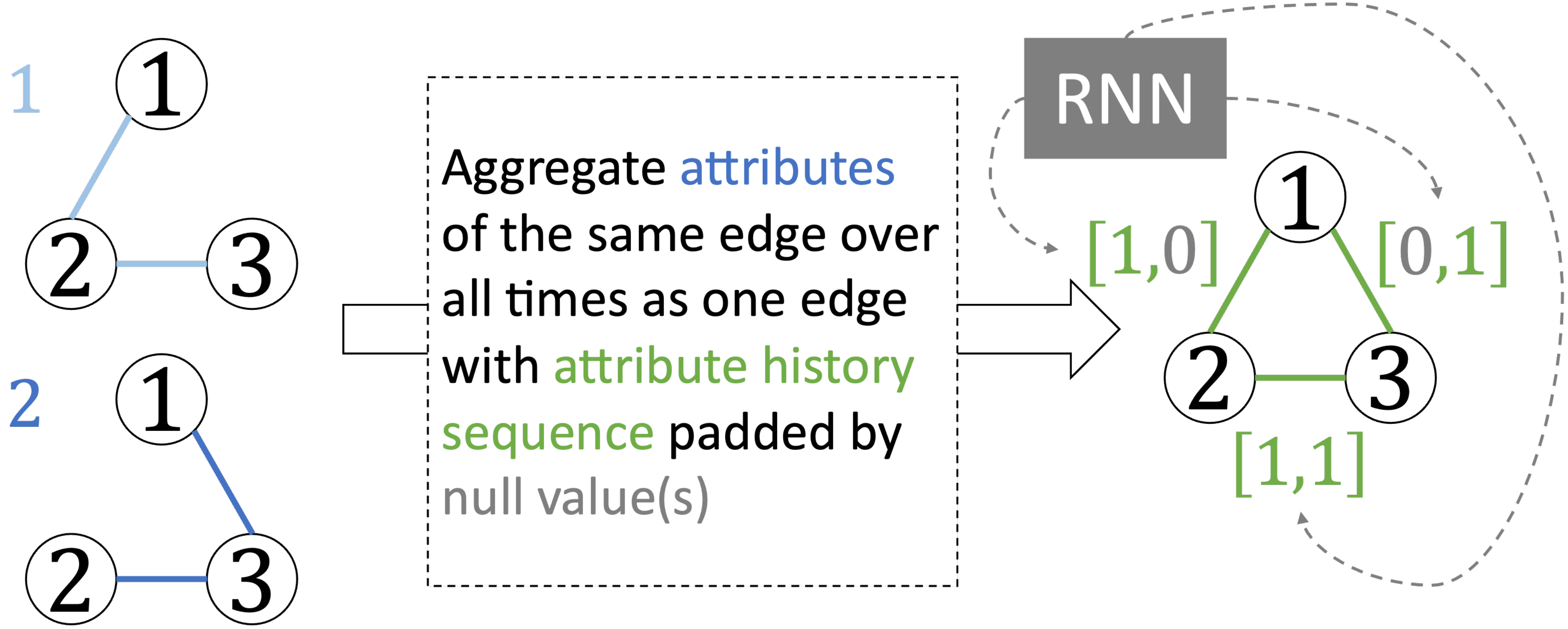
Proposal: GRU-GCN



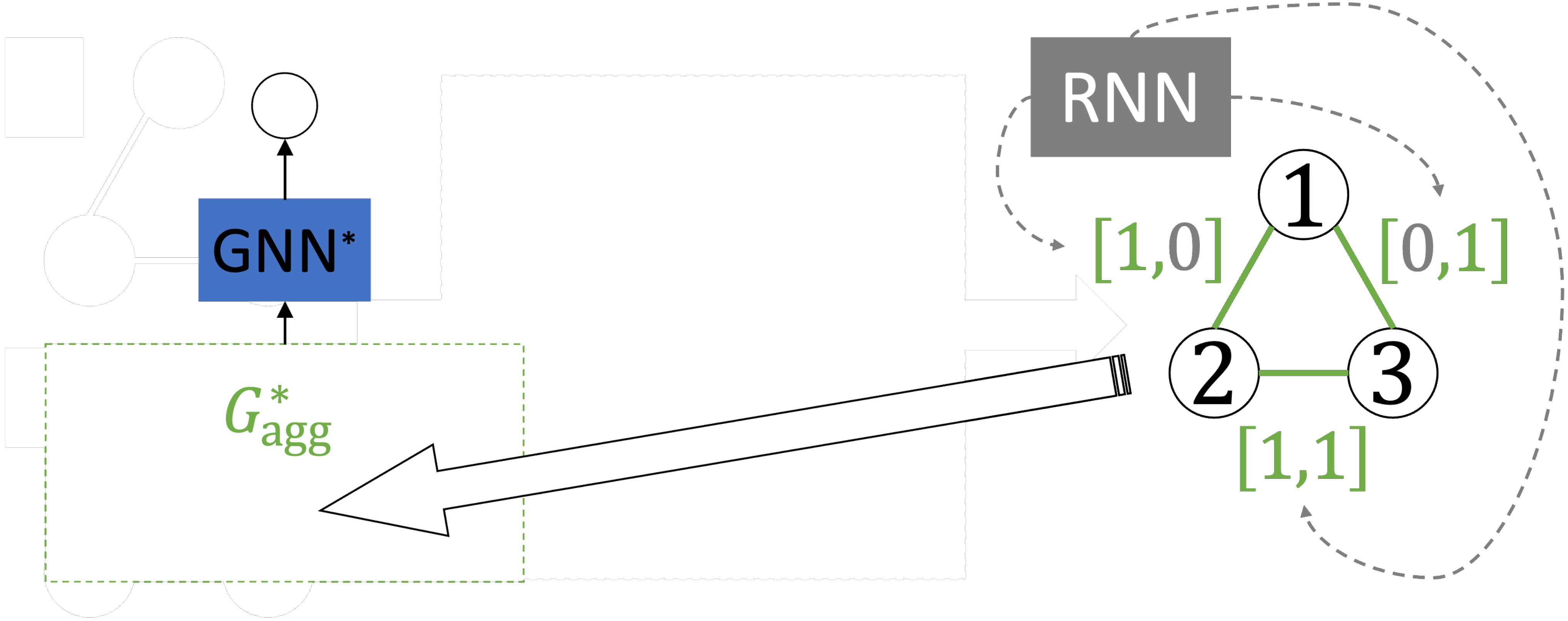
Aggregate attributes of the same edge over all times as one edge with attribute history sequence padded by null value(s)



Proposal: GRU-GCN



Proposal: GRU-GCN



Result

- GRU-GCN can achieve **far better** performance over existing methods in tasks satisfying hypothesis made in proves.

Representation	Model	DynCSL	Brain-10
graph-then-time	EvolveGCN-O	$0.50_{\pm 0.00}$	$0.58_{\pm 0.10}$
	EvolveGCN-H	$0.50_{\pm 0.00}$	$0.60_{\pm 0.11}$
	GCN-GRU	$0.50_{\pm 0.00}$	$0.87_{\pm 0.07}$
	DySAT	$0.50_{\pm 0.00}$	$0.77_{\pm 0.07}$
time-and-graph	GCRN-M2	$0.52_{\pm 0.04}$	$0.77_{\pm 0.04}$
	DCRNN	$0.51_{\pm 0.03}$	$0.84_{\pm 0.02}$
time-then-graph	TGAT	$0.48_{\pm 0.03}$	$0.80_{\pm 0.03}$
	TGN	$0.51_{\pm 0.04}$	$\underline{\mathbf{0.91}_{\pm 0.03}}$
	GRU-GCN	$\underline{\mathbf{1.00}_{\pm 0.00}}$	$\underline{\mathbf{0.91}_{\pm 0.03}}$

Result

- GRU-GCN can achieve **similar or slightly better** performance against existing methods in real-world applications.

Representation	Model	PeMS04		PeMS08		Spain-COVID		England-COVID	
		Transductive	Inductive	Transductive	Inductive	Transductive	Inductive	Transductive	Inductive
graph-then-time	EvolveGCN-O	3.20±0.25%	2.61±0.42%	2.65±0.12%	2.40±0.27%	2.64±0.12%	2.02±0.11%	4.07±0.73%	3.88±0.47%
	EvolveGCN-H	3.34±0.14%	2.84±0.31%	2.81±0.28%	2.81±0.23%	2.62±0.33%	2.09±0.30%	4.14±1.14%	3.50±0.42%
	GCN-GRU	**1.60±0.14**%	1.28±0.04%	1.40±0.26%	1.07±0.03%	2.39±0.06%	1.22±0.66%	**3.56±0.26**%	**2.97±0.34**%
	DySAT	1.86±0.08%	1.58±0.08%	1.49±0.08%	1.34±0.03%	2.15±0.18%	**0.89±0.44**%	3.67±0.15%	3.32±0.76%
time-and-graph	GCRN-M2	1.70±0.20%	1.20±0.06%	**1.30±0.17**%	1.00±0.10%	1.94±0.54%	1.54±0.50%	3.85±0.39%	3.37±0.27%
	DCRNN	1.67±0.19%	1.27±0.06%	1.32±0.19%	1.07±0.03%	2.12±0.33%	0.90±0.21%	3.58±0.53%	3.09±0.24%
time-then-graph	TGAT	3.11±0.50%	2.25±0.27%	2.66±0.27%	2.34±0.19%	2.46±0.04%	1.81±0.14%	5.44±0.46%	5.13±0.26%
	TGN	1.79±0.21%	**1.19±0.07**%	1.49±0.26%	**0.99±0.06**%	**1.62±0.33**%	1.25±0.48%	4.15±0.81%	3.17±0.23%
	GRU-GCN	**1.61±0.35**%	**1.13±0.05**%	**1.27±0.21**%	**0.89±0.07**%	**1.66±0.63**%	**0.65±0.16**%	**3.41±0.28**%	**2.87±0.19**%

Result

- GRU-GCN can achieve **similar or slightly better** performance against existing methods in real-world applications.
- But GRU-GCN will be **far more efficient** on those real-world tasks in both time and memory costs.

Representation	Model	PeMS04 Peak GPU Memory	PeMS04 Average Training Time per Minibatch	PeMS08 Peak GPU Memory	PeMS08 Average Training Time per Minibatch	Spain-COVID Peak GPU Memory	Spain-COVID Average Training Time per Minibatch	England-COVID Peak GPU Memory	England-COVID Average Training Time per Minibatch
graph-then-time	EvolveGCN-O	86 MB	19ms	55 MB	17 ms	221 MB	14 ms	3MB	9 ms
	EvolveGCN-H	205 MB	40 ms	130 MB	31 ms	512 MB	21 ms	4 MB	15 ms
	GCN-GRU	1089 MB	17 ms	602 MB	15 ms	140 MB	12 ms	6 MB	8 ms
	DySAT	1911 MB	26 ms	1060 MB	24 ms	137 MB	18 ms	7 MB	14 ms
time-and-graph	GCRN-M2	3099 MB	195 ms	1871 MB	159 ms	5423 MB	124 ms	22 MB	84 ms
	DCRNN	1730 MB	83 ms	1024 MB	65 ms	2460 MB	50 ms	13 MB	34 ms
time-then-graph	TGAT	7945 MB	101 ms	5680 MB	72 ms	7300 MB	94 ms	96 MB	21 ms
	TGN	3963 MB	25 ms	2908 MB	19 ms	5205 MB	29 ms	73 MB	16 ms
	GRU-GCN	859 MB	**7 ms**	574 MB	**5 ms**	1538 MB	**10 ms**	52 MB	**3 ms**

Conclusion

- We theoretically study expressivity power of temporal graph neural networks.
- And accordingly propose a simple but efficient GRU-GCN framework which lights a new direction in temporal graph representation learning.