Hot Topics in Graph Neural Networks

Graphs in Artificial Intelligence and Neural Networks

Josephine Thomas, Silvia Beddar-Wiesing, Clara Holzhüter, Alice Moallemy-Oureh

25th of October 2022

- The Research Center for Information System Design (ITeG) at the University of Kassel focuses on socially responsible IT design.
- We promote responsible, socially sustainable digitisation through interdisciplinary research.
- 12 research groups from different disciplines (computer science, IT and privacy law, information systems, psychology, sociology, human-machine systems engineering).

Main areas of mutual research

- Methods of socio-technical IT Design to increase digital self-determination and souvereignty
- Privacy and the dynamics of the information society
- AI and Hybrid Intelligence and their embedding in the social system

The Team

Josephine Thomas

Silvia Beddar-Wiesing

Alice Moallemy-Oureh

Clara Holzhüter

Bernhard Sick

Christoph Scholz

Eric Alsmann

Rüdiger Nather

Till-Mattis Nebel

Björn-André Schröder

Workshop Agenda

Time	Speaker	Topic
10:00 - 11:15	GAIN	Expressivity and Dynamic of GNNs in theory and applications to the power grid
11:20 - 12:05	Petar Veličković	Algorithmically-aligned GNNs
Lunch Break		
13:15 - 13:40	Fabian Jogl	Do we need to Improve Message Passing?
13:45 - 14:10	Maximilian Thiessen	Expectation Complete Graph Representations using Graph Homomorphisms
14:15 - 15:00	Massimo Perini	Graph Streams
Coffee Break		
16:00 - 16:45	Antonio Longa	Explaining the explainers in GNNs: a comparative study
16:50 - 17:35	Hannes Stärk	Geometric ML for Molecules

Content

Graph Neural Networks for different Graph Types: A Survey

Josephine M. Thomas*, Alice Moallemy-Oureh*, Silvia Beddar-Wiesing*, Clara Holzhüter*: *Graph Neural Networks Designed for Different Graph Types: A Survey*, `https://arxiv.org/abs/2204.03080`

What can GNNs achieve nowadays and where is work to be done?

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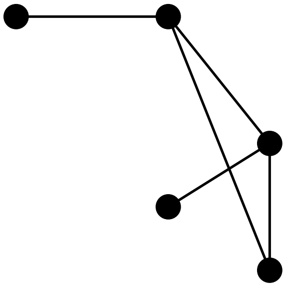
- Graph properties yield graph types $\rightarrow$ Which graph types are there?
- Which graph types can be handled by GNN models?

GNNs for different Graph Types: The graph types

- static undirected graph
- static structural properties
- semantic graph properties
- dynamic structural properties



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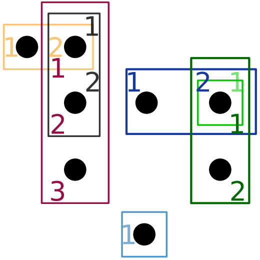

directed hypergraph

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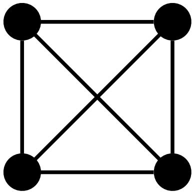

complete graph

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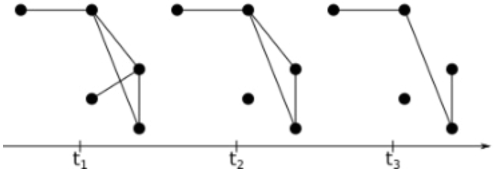

strictly shrinking graph

GNNs for different Graph Types: The representation of dynamic graphs

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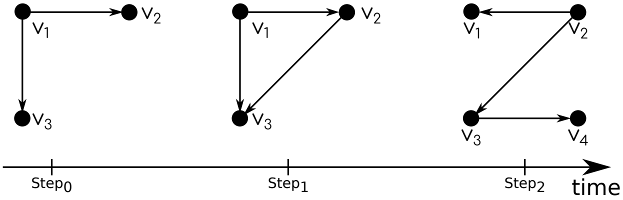
- discrete-time dynamic



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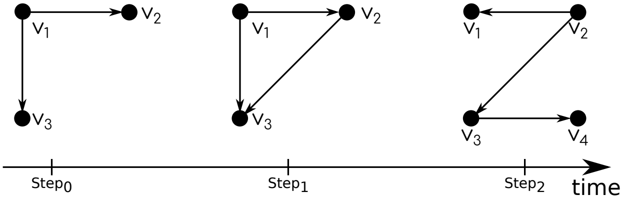
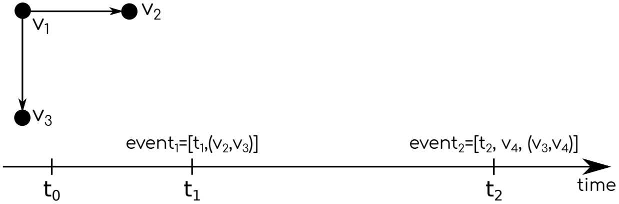


- continuous-time dynamic



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  - Dynamic attributes, especially if data-type is complex

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  - Multiple nodes/eges

The Modeling Power of different Graph Types

Josephine M. Thomas*, Silvia Beddar-Wiesing*, Alice Moallemy-Oureh*, Rüdiger Nather: *Graph type expressivity and transformations*, `https://arxiv.org/abs/2109.10708`

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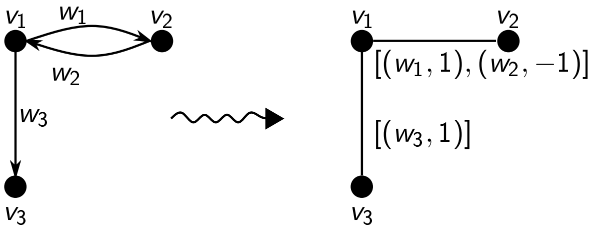
How do we assess the ability of different graph types to represent information?

A graph type $\mathcal{G}_2$ is **at least as expressive** as a graph type $\mathcal{G}_1$, if and only if $\mathcal{G}_2$ encodes at least as many graph properties as $\mathcal{G}_1$ denoted as $\mathcal{G}_1 \preccurlyeq \mathcal{G}_2$. In case both types encode the same graph properties it is denoted as $\mathcal{G}_1 \approx \mathcal{G}_2$.

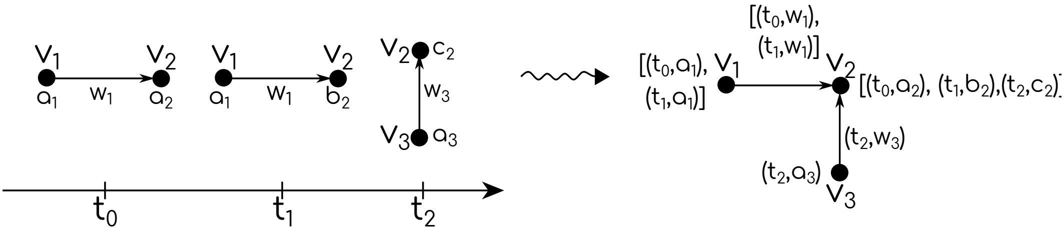
The Modeling Power of different Graph Types: Expres. relation examples



$$\mathcal{G}_{directed} \preccurlyeq \mathcal{G}_{undirected}$$

Transformation directed to undirected graph:
Storing the directions and multiple attributes in the new attributes.

The Modeling Power of different Graph Types: Expres. relation examples



$\mathcal{G}_{dynamic} \preccurlyeq \mathcal{G}_{static}$

Transformation dynamic to static graph:
Cummulating the structural information in one entire graph and storing the corresponding attribute time series as the new attributes.

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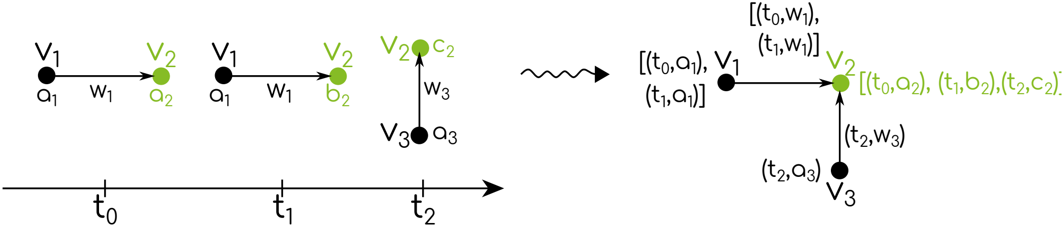

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The Modeling Power of different Graph Types: Results

All attributed graph types can be transformed into a **static attributed undirected homogeneous graph (SAUHG)**.

All attributed graph types are equally expressive.

$\rightarrow$ We can transform graph data to be able to use an arbitrary GNN.
$\rightarrow$ We are free to choose a graph type that models our problem best.

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Weisfeiler–Lehmann goes Dynamic: An Analysis of the Expressive Power of Graph Neural Networks for Attributed and Dynamic Graphs

Weisfeiler-Lehman goes dynamic

Motivation: Expressivity of GNNs

Which **graphs/nodes** can a GNN **distinguish**?

Scarselli et. al (2009)
GNNs cannot distinguish nodes having the **same unfolding trees.**

Xu et. al (2018)
GNNs are **as powerful as** the Weisfeiler-Lehman graph isomorphism test (1-WL, 1968).

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→ static node-attributed graphs only!

Weisfeiler-Lehman goes dynamic

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Which **functions** can a GNN **approximate**?

D'Inverno et. al (2021)
Message Passing GNNs can **approximate** in probability **any measurable function** that respects the unfolding equivalence.

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Contributions

[1] Beddar-Wiesing, D'Inverno, Graziani, Lachi, Moallemy-Oureh, Scarselli, Thomas: *Weisfeiler–Lehman goes Dynamic: An Analysis of the Expressive Power of Graph Neural Networks for Attributed and Dynamic Graphs*, arxiv preprint

Contributions

- **Extension** of WL-Tests and unfolding trees to (edge-)attributes and dynamics
- **Proof of Extended Approximation Theorems:** GNNs can approximate to any precision and probability any measurable function on attributed and dynamic graphs

[1] Beddar-Wiesing, D'Inverno, Graziani, Lachi, Moallemy-Oureh, Scarselli, Thomas: *Weisfeiler–Lehman goes Dynamic: An Analysis of the Expressive Power of Graph Neural Networks for Attributed and Dynamic Graphs*, arxiv preprint

Recap: WL-Test and Unfolding Trees

Weisfeiler-Lehman goes dynamic

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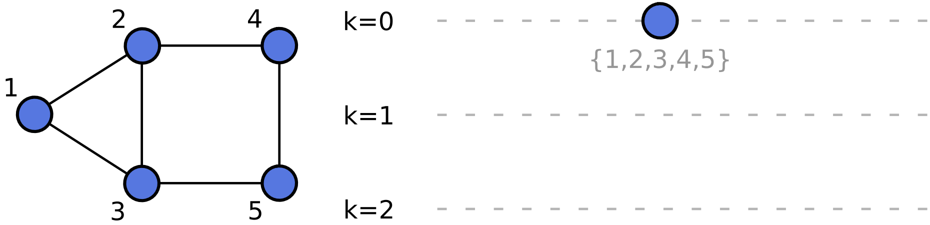

Weisfeiler-Lehman goes dynamic

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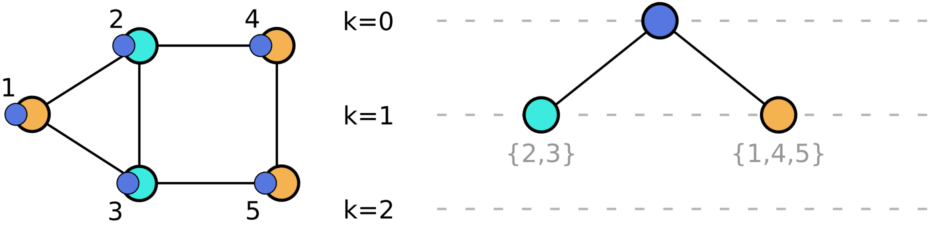

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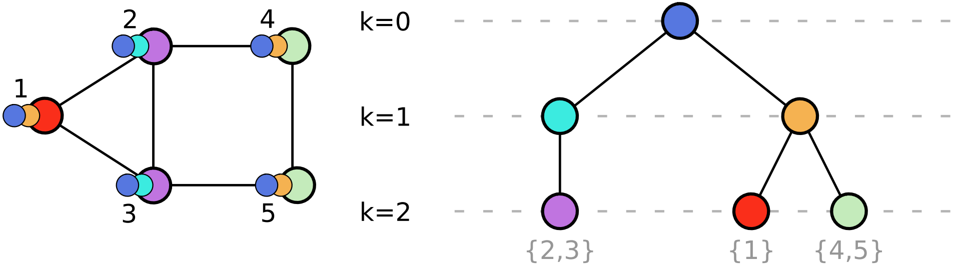

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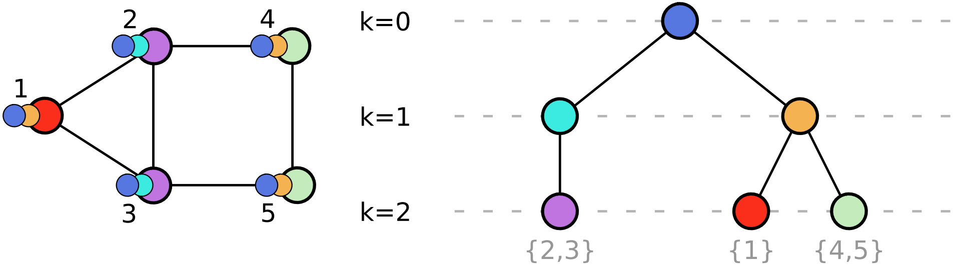
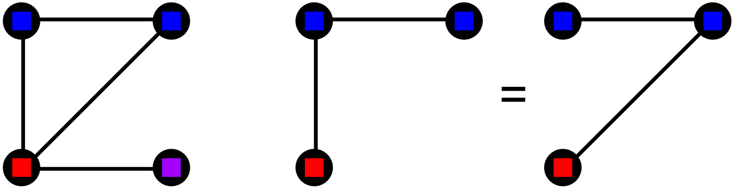


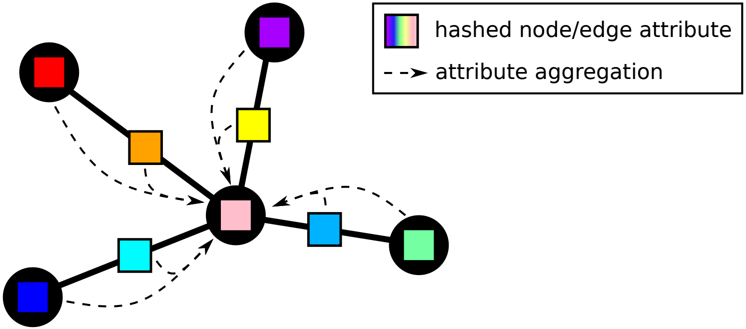
(Thank you Nils Kriege for the wonderful illustration!)

Unfolding Trees

Unfolding Trees of both blue nodes



WL Coloring for Attributed Graphs



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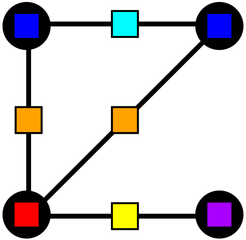

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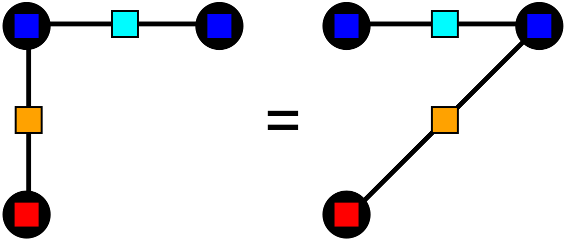
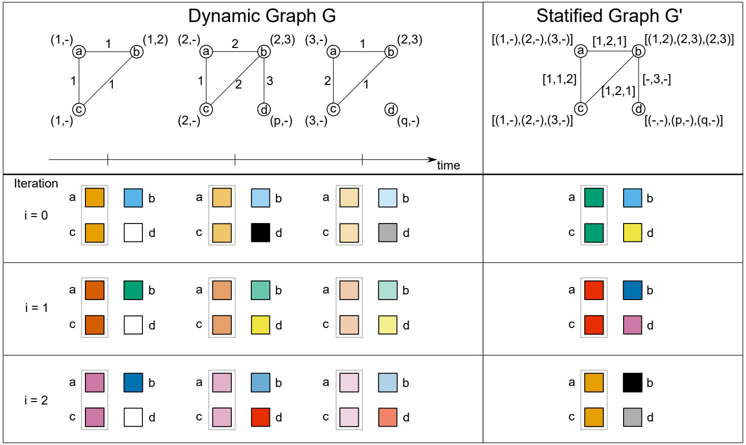


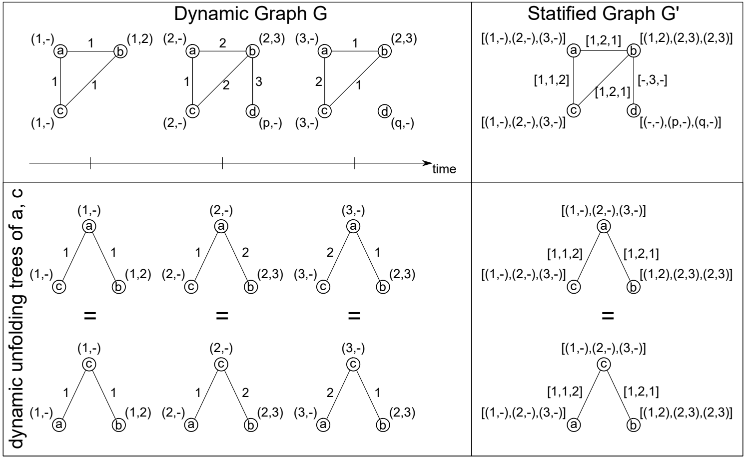
WL Coloring for Dynamic Graphs



Weisfeiler-Lehman goes dynamic

Extension of WL-Test and Unfolding Trees

Unfolding Trees for Dynamic Graphs



Proposition

For all nodes u, v holds:

1. in the attributed case:

$$u \sim_{AWL} v \Leftrightarrow u \sim_{AUT} v.$$

2. in the dynamic case:

$$u \sim_{DWL} v \Leftrightarrow u \sim_{DUT} v.$$

Weisfeiler-Lehman goes dynamic

Generic GNNs: GNN for SAUHGs (SGNN) and dynamic graphs (MP-DGNN)

For a SAUHG $G = (\mathcal{V}, \mathcal{E}, \alpha, \omega)$, let $v \in \mathcal{V}$. The **propagation scheme of the SGNN** for one iteration $k \in [K]$ is defined as

$$\boldsymbol{h}_v^k = \mathrm{COMBINE}\left(\underbrace{\boldsymbol{h}_v^{k-1}}_{\text{history}}, \underbrace{\mathrm{AGGREGATE}\left(\{\boldsymbol{h}_u^{k-1}\}_{u \in \mathcal{N}(v)}, \{\omega(\{u, v\})\}_{u \in \mathcal{N}(v)}\right)}_{\text{neighborhood aggregation}}\right).$$

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For a discrete dynamic graph $G' = (G_t)_{t\in I}$, let $v \in \mathcal{V}_t$. The **propagation scheme of the MP-DGNN** for one iteration $k \in [K]$ at timestamp $t \in [T]$ is defined as

$$h_v^k(t) = \text{COMBINE}_t^{(k)}\left(\underbrace{h_v^{k-1}(t)}_{\text{history}}, \underbrace{\text{AGGREGATE}_t^k\left(\{h_u^{k-1}(t)\}_{u\in\mathcal{N}_t(v)}, \{\omega_{\{u,v\}}(t)\}_{u\in\mathcal{N}_t(v)}\right)}_{\text{temporal neighborhood aggregation}}\right)$$

Weisfeiler-Lehman goes dynamic

Universal Approximation of SGNN and MP-DGNN

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For

- Domain of SAUHGs $\mathcal{G}$ and $r = \max\limits_{g\in\mathcal{G}} diam(G)$;
- any measurable function f preserving $\sim_{AUT}$;
- any norm $||\cdot||$ on $\mathbb{R}$ and probability measure P on $\mathcal{G}$;
- $\epsilon, \lambda \in \mathbb{R}$, **precision** $\epsilon > 0$, **probability** $\lambda \in (0, 1)$.

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There exists an SGNN s.t. the function φ realized by the SGNN, computed after $r + 1$ steps for all $G \in \mathcal{G}$ and $v \in G$, satisfies:

$$P\left(\|f(G, v) - \varphi(G, v)\| \leq \epsilon\right) \geq 1 - \lambda.$$

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There exists an SGNN s.t. the function φ realized by the SGNN, computed after $r+1$ steps for all $G \in \mathcal{G}$ and $v \in G$, satisfies:

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For

- Domain of discrete dyn. graphs $G' = (G_t)_{t \in I} \in \mathcal{G}'$ and $r_t = \max_{G_t \in \mathcal{G}'} diam(G_t)\ \forall t \in I$;
- any measurable dynamic system $dyn(t, G', v)$ preserving $\sim_{DUT}$;
- any norm $\|\cdot\|$ on $\mathbb{R}$ and probability measure P on $\mathcal{G}$;
- $\epsilon, \lambda \in \mathbb{R}$, $\epsilon > 0$, $\lambda \in (0, 1)$.

There exists an MP-DGNN s.t the function ψ realized by the MP-DGNN, computed after $r_t + 1$ steps satisfies:

$$P\left(\|dyn(t, G', v) - \psi(G', v)\| \leq \epsilon\right) \geq 1 - \lambda.$$

Conclusion

[2] Beddar-Wiesing, D'Inverno, Graziani, Lachi, Moallemy-Oureh, Scarselli, Thomas: *Weisfeiler–Lehman goes Dynamic: An Analysis of the Expressive Power of Graph Neural Networks for Attributed and Dynamic Graphs*, arxiv preprint

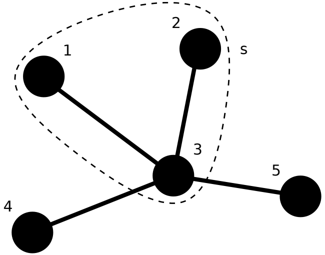
- There **exist** SGNNs and MP-DGNNs to **approximate any measurable function** on attributed and dynamic graphs to any precision and probability.
- The **proof** is based on attributed and dynamic WL- and UT- equivalence.

[2] Beddar-Wiesing, D'Inverno, Graziani, Lachi, Moallemy-Oureh, Scarselli, Thomas: *Weisfeiler–Lehman goes Dynamic: An Analysis of the Expressive Power of Graph Neural Networks for Attributed and Dynamic Graphs*, arxiv preprint

On the Extension of the Weisfeiler-Lehman Hierarchy by WL Tests for Arbitrary Graphs

S. Beddar-Wiesing, G.A. D'Inverno, C. Graziani, V. Lachi, A. Moallemy-Oureh, F: Scarselli *On the Extension of the Weisfeiler-Lehman Hierarchy by WL Tests for Arbitrary Graphs*, 18th International Workshop On Mining and Learning with Graphs, 2022,
`https://openreview.net/forum?id=Qt6GrgDz2y5`

Higher dimensional WL test



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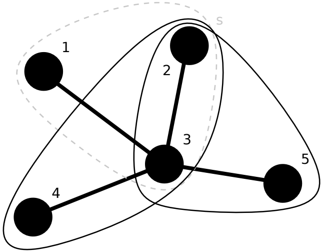

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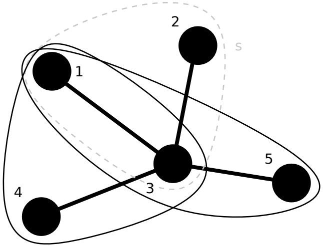

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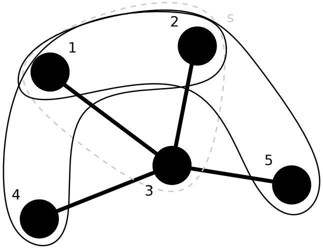

Extension of the WL Hierarchy

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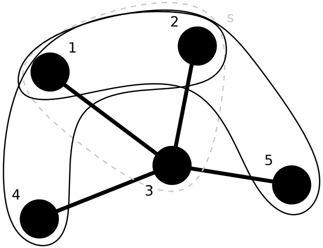

Extensions to k-AWL/DWL are analogously.

Extension of the WL Hierarchy

The WL Hierachy

$$\textbf{1-WL} = \textbf{2-WL} \subsetneq \textbf{3-WL} \subsetneq \ldots \subsetneq k - \textbf{WL} \subsetneq \ldots \subsetneq \textbf{GI}$$

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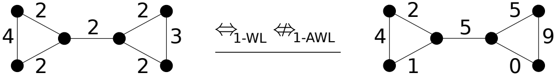
How do the *k*-AWL and *k*-DWL fit there?

Extension of the WL Hierarchy

Some trivial observations are:

- 1-WL $\subsetneq$ 1-AWL
- $\Rightarrow$ k-WL $\subsetneq$ k-AWL
- 2-WL $\subsetneq$ 1-AWL
- k-AWL/DWL $\subseteq$ $(k+1)$-AWL/DWL
- k-AWL $=$ k-DWL



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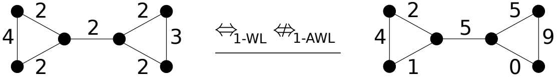
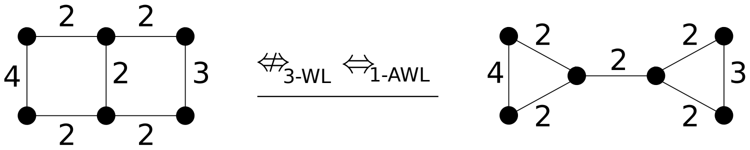


- $1\text{-WL} \subsetneq 1\text{-AWL}$
- $\Rightarrow k\text{-WL} \subsetneq k\text{-AWL}$
- $2\text{-WL} \subsetneq 1\text{-AWL}$
- $k\text{-AWL/DWL} \subseteq (k+1)\text{-AWL/DWL}$
- $k\text{-AWL} = k\text{-DWL}$

Nevertheless, the hierarchy can just induce a partial order:

- $3\text{-WL} \not\subseteq 1\text{-AWL}$
- $3\text{-WL} \not\supseteq 1\text{-AWL}$
- ...

3-WL $\not\subseteq$ 1-AWL



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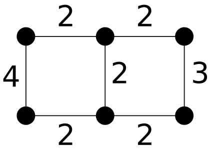
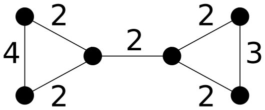


$\not\Leftrightarrow_{3\text{-WL}} \; \Leftrightarrow_{1\text{-AWL}}$



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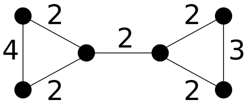

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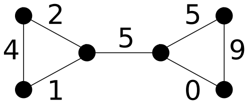

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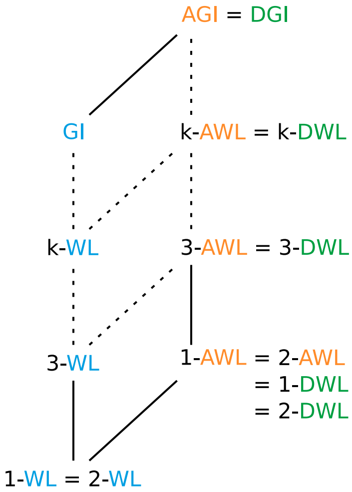

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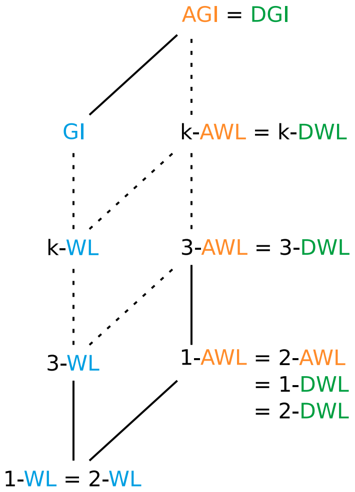

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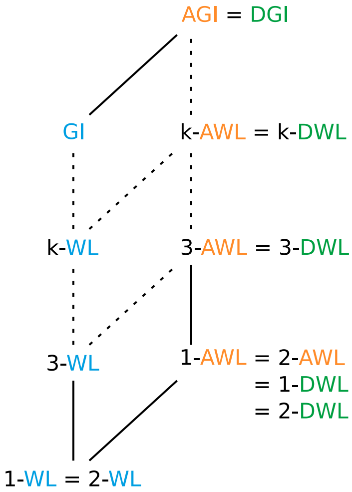

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- Lattice is complete, infinite, bounded, distributive and modular.

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Since this is future work, **feel free to share your expertise!**

Graph Neural Networks for Power Grids

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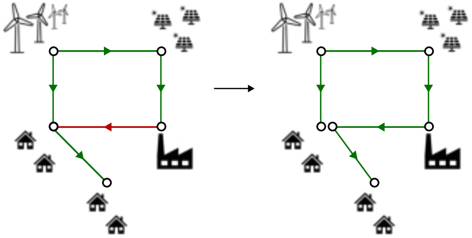

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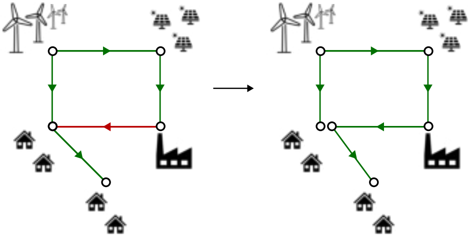

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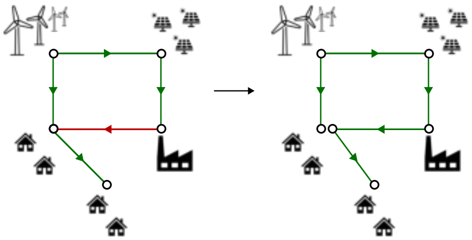

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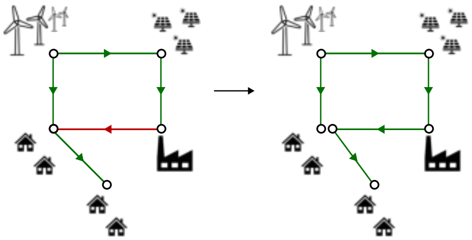

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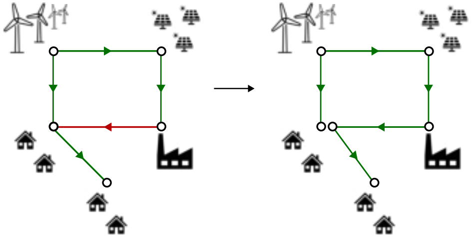
$\Rightarrow$ Deep Learning Models



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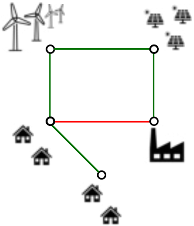
Goal: Design a GNN to predict a suitable topology

Approach

- Input: power grid at a specific time stamp
- Construct Graph
- Apply GNN
- Output: Encoded Graph indicating the splitting candidates
- Change topology according to prediction



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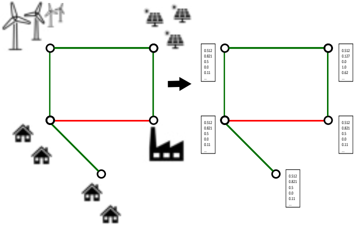

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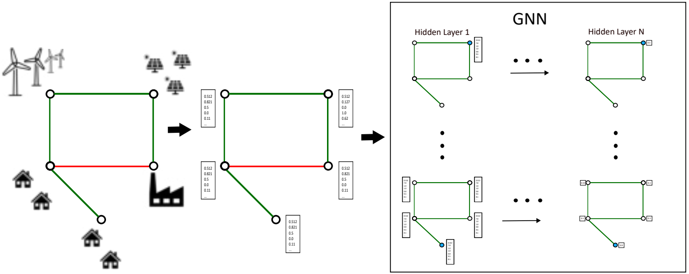

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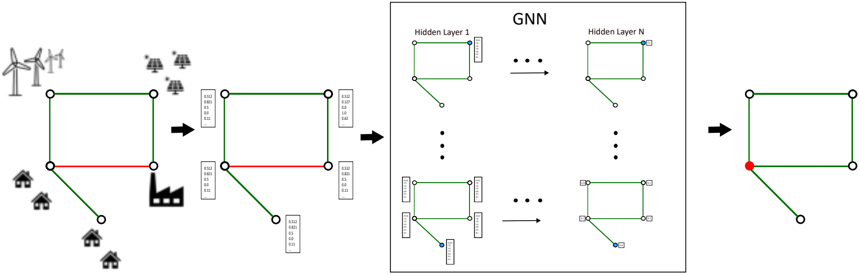

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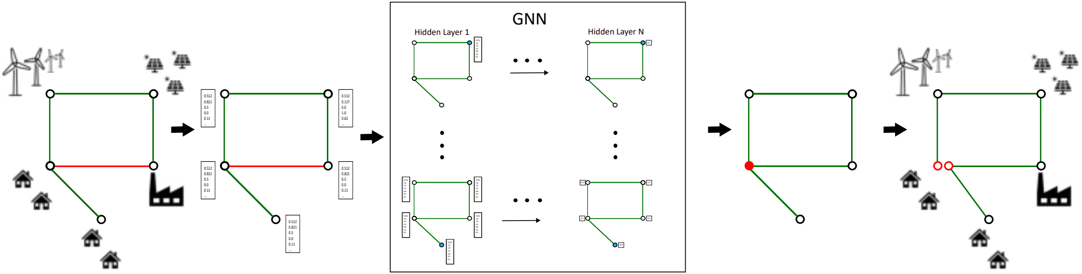

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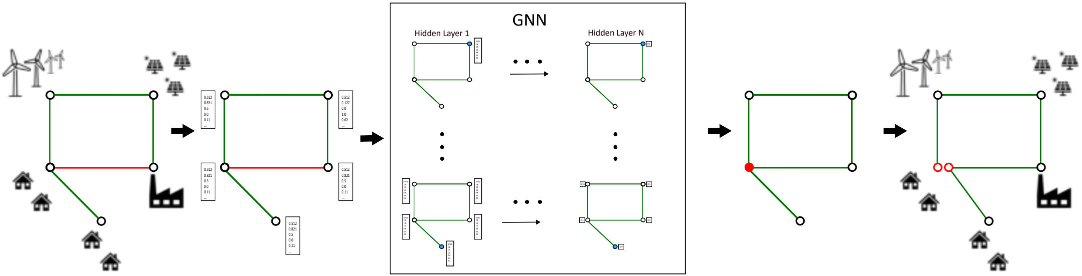

→ Node Classifcation Task to identify the candidates for node splitting

Further Considerations

- Hardly any approaches for this specific use case

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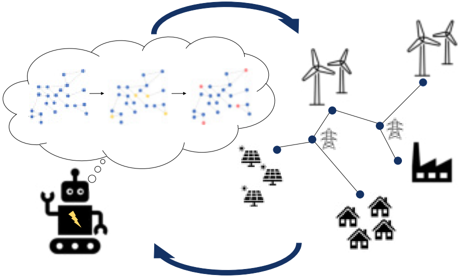
  - Time Series Embedding
  - Dynamic GNN

Ultimate Goal

- Combine the GNN Approach with a Reinforcement Learning Algorithm



Learning to Run a Power Network

[3] Marot, Antoine and Donnot, Benjamin and Romero, Camilo and Donon, Balthazar and Lerousseau, Marvin and Veyrin-Forrer, Luca and Guyon, Isabelle: *Learning to run a power network challenge for training topology controllers*, Electric Power Systems Research vol. 189, Elsevier

Learning to Run a Power Network

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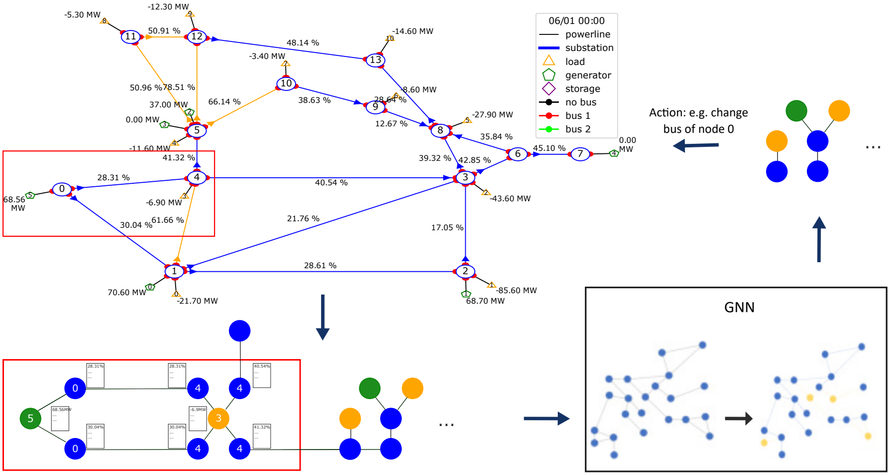
[3] Marot, Antoine and Donnot, Benjamin and Romero, Camilo and Donon, Balthazar and Lerousseau, Marvin and Veyrin-Forrer, Luca and Guyon, Isabelle: *Learning to run a power network challenge for training topology controllers*, Electric Power Systems Research vol. 189, Elsevier

GNN Pipeline with the Gri2Op[4] Virtual Power Grid



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[4] B. Donnot, Grid2op- A testbed platform to model sequential decision making in power systems.
`https://GitHub.com/rte-france/grid2op`

Ongoing Research

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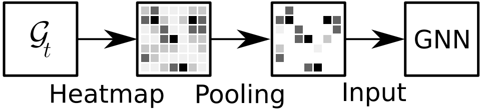
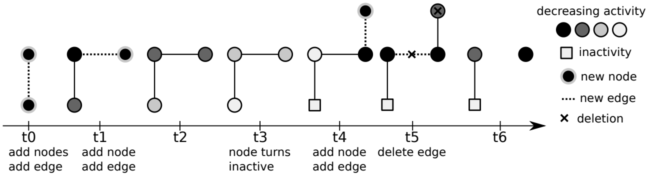
- Local Activity Encoding for Dynamic Graph Pooling in Structure Dynamic Graphs
- Continuous-Time Generative GNN for Attributed Dynamic Graphs
- FDGNN: Fully Dynamic GNN

Local Activity Encoding for Dynamic Graph Pooling in Structure Dynamic Graphs[5]

- **graph compression algorithm** for processing structural dynamic graphs
- includes local **activity encoding** with subsequent **pooling**
- generates important graph sequence of **equal sizes** in $\mathcal{O}(T)$



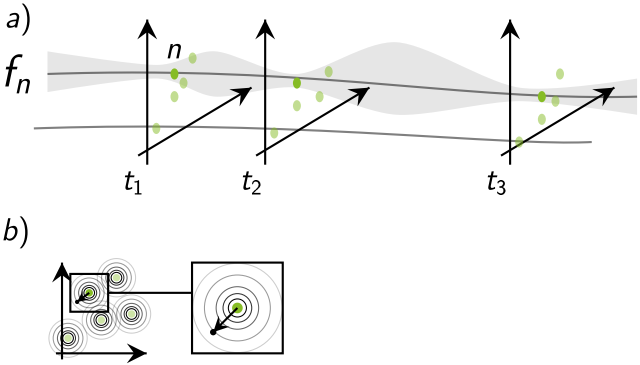


[5] Beddar-Wiesing: *Using local activity encoding for dynamic graph pooling in stuctural-dynamic graphs*, SAC '22: Proceedings of the 37th ACM/SIGAPP Symposium on Applied Computing

Continuous-Time Generative GNN for Attributed Dynamic Graphs[6]

Let $G = (g_{t_0}, \mathbb{E})$ be a dynamic graph in continuous-time.
The approach is determined by:

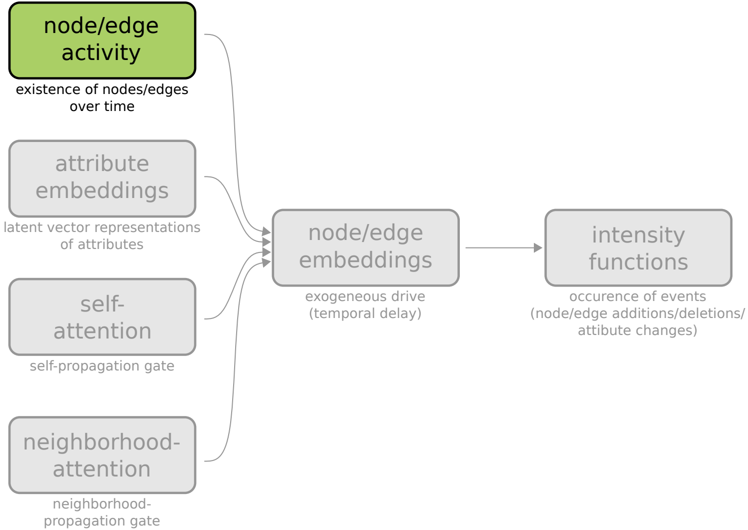
1. Discretization of G
2. Embedding via vGAE
3. Interpret timestamps as another embedding space scaling axis and fit Gaussian regression functions



- emb. coord. of node n at time t_i
- emb. forecast coord. of node n at time t_{i+1}
- → polynomial regression function $f_n(t)$

[6] Moallemy-Oureh: *Continuous-time generative graph neural network for attributed dynamic graphs*, SAC '22: Proceedings of the 37th ACM/SIGAPP Symposium on Applied Computing, `https://doi.org/10.1145/3477314.3508018`

FDGNN: Fully Dynamic Graph Neural Network[7]



[7] Moallemy-Oureh, Beddar-Wiesing, Nather, Thomas: *FDGNN: Fully Dynamic Graph Neural Network*, arXiv:2206.03469

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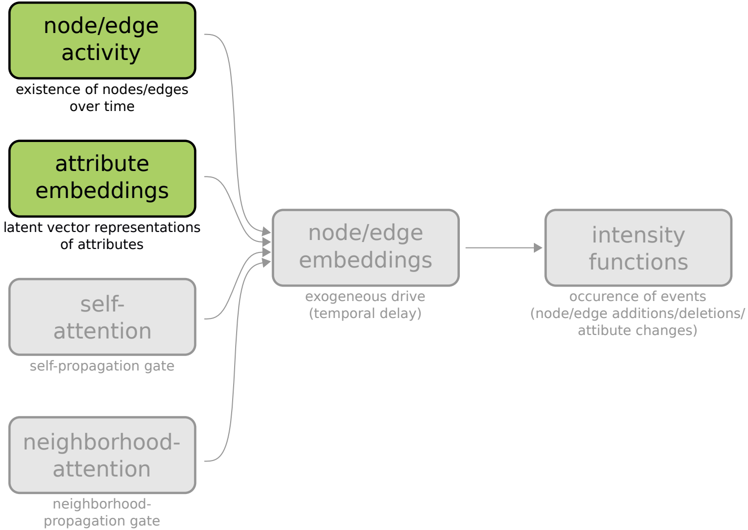

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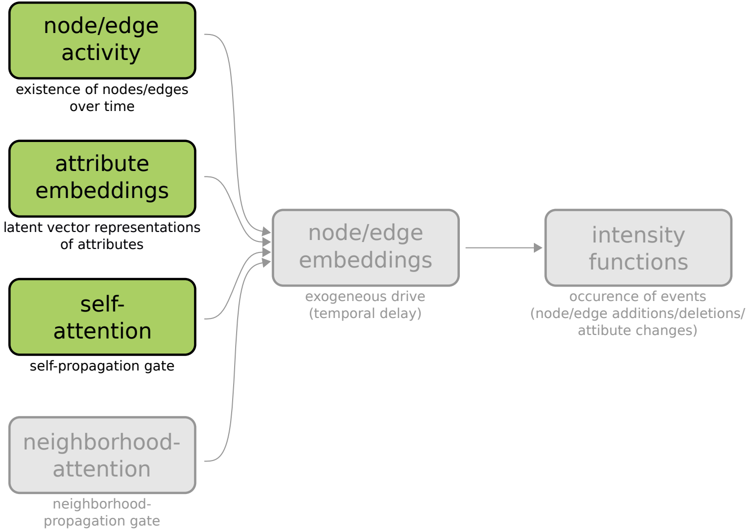

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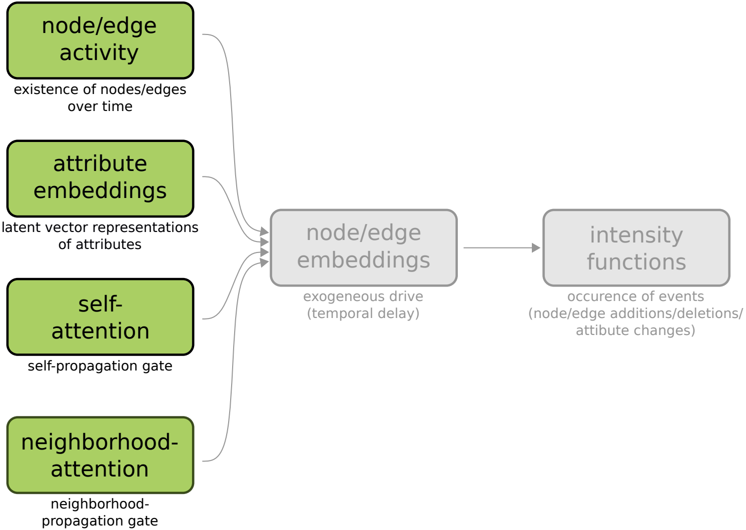

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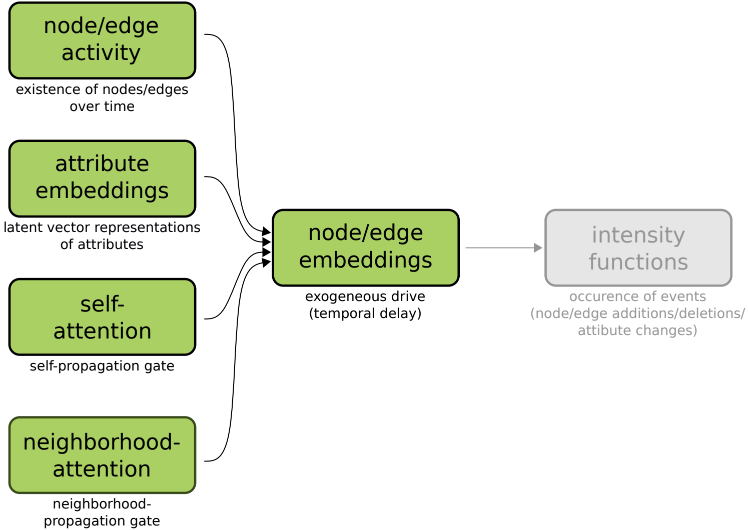

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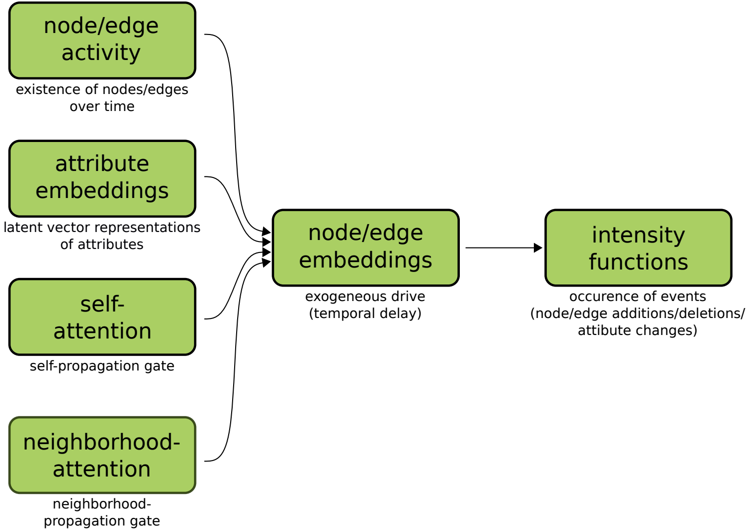

[7] Moallemy-Oureh, Beddar-Wiesing, Nather, Thomas: *FDGNN: Fully Dynamic Graph Neural Network*, arXiv:2206.03469

Contact

Thank you for your attention!
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