FAIR SPOKE WORKSHOPS 2024
SPOKE 9 - GREEN-AWARE AI

Graph Deep Learning for Green-aware Knowledge

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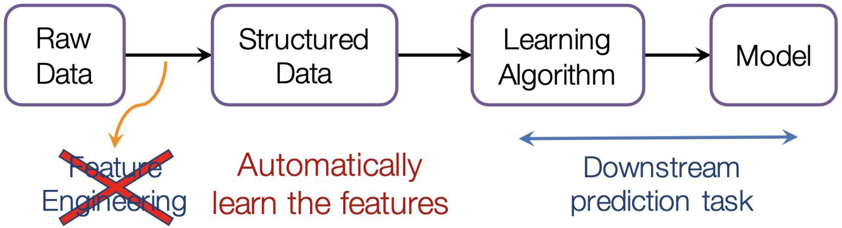
WP9.4

- *Knowledge Representation & Reasoning* and *Machine/Deep Learning* methodologies, and their novel combinations, for dealing with green-aware agents and systems and providing explanations to distinguish the role played in the decisions by domain-specific features and by hard/soft sustainability and green constraints
- Core paradigms: Abstract Argumentation, Ontology-mediated Query Answering, and Graph/Language Neural Network models
- Focus of Task 9.4.4: Graph representation learning for
  - modeling and analyzing real-world scenarios represented by attributed, multilayer/dynamic, and heterogeneous graph data
  - by leveraging both structural and semantic relationships among graph entities that are relevant to green-aware facts and events

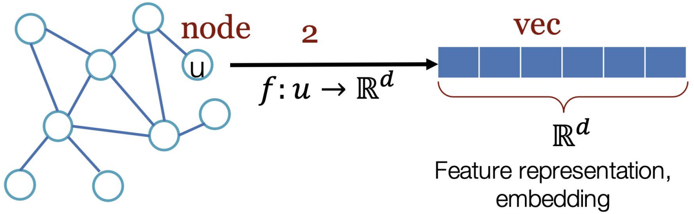
Graph Representation Learning

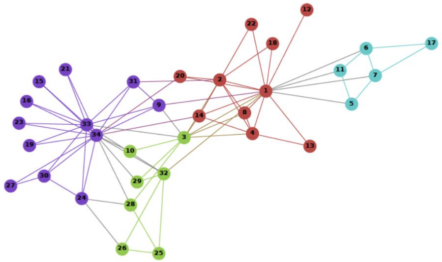
(Supervised) Machine Learning lifecycle requires feature engineering - every time

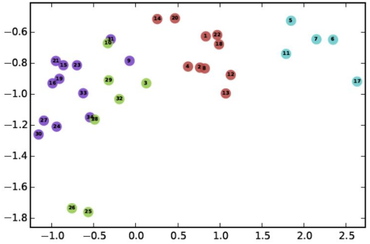


Efficient (task-independent) **feature learning** for machine learning in graphs

Leskovec et al., Representation Learning on Networks, WWW 2018

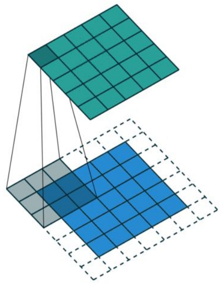






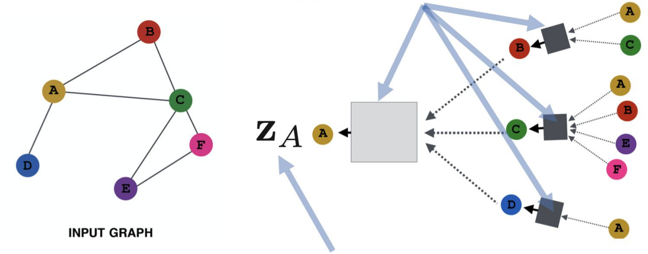
Graph Neural Networks

- Networks are not grids or sequences!
- Both structural information and additional features may be taken into account
- Key idea: aggregation schemes on neighborhood properties
- GNNs are now SOTA in several tasks
  - Node classification, link prediction, graph classification
- Popular approaches:
  - Graph Convolutional Network (GCN) [Kipf and Welling, 2017]
  - Graph Attention Network (GAT) [Velickovic et al., 2018]



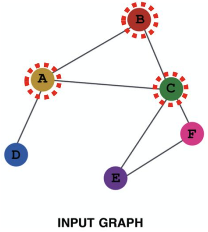
Graph Neural Networks

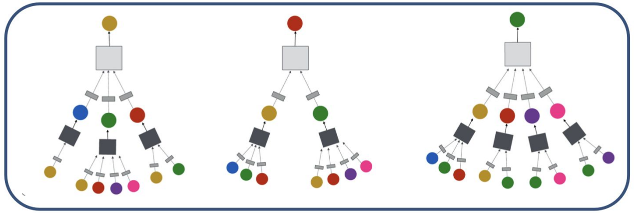
1) Define a neighborhood aggregation function.

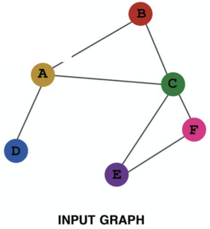


2) Define a loss function on the embeddings, $\mathcal{L}(z_u)$

3) Train on a set of nodes, i.e., a batch of compute graphs

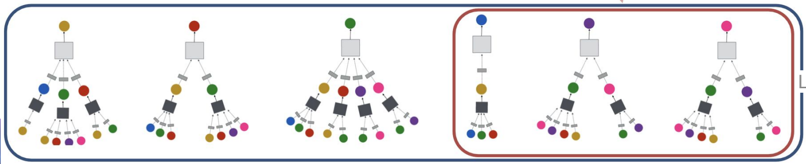






4) Generate embeddings nodes as needed

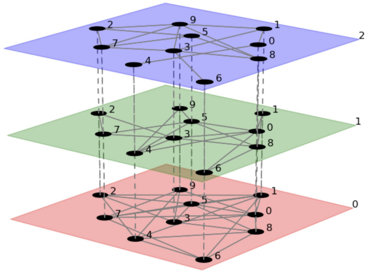
Even for nodes we never trained on!!!!

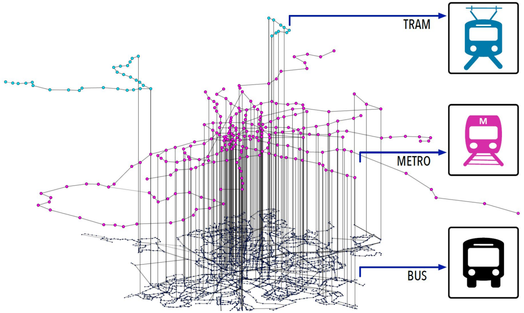


Leskovec et al., Representation Learning on Networks, WWW 2018

Challenges on complex networks

- Handling complexity in graph data through the **multilayer** network model, and the **heterogeneous** network model



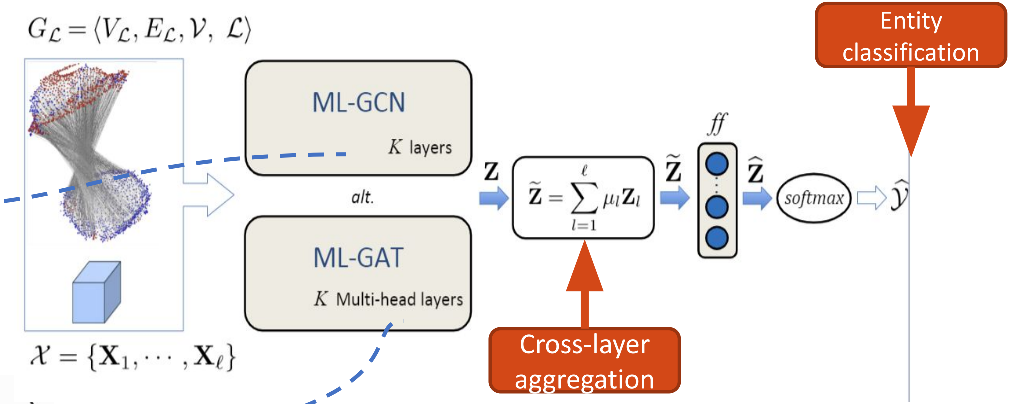


- Multiplicity of node type and/or edge type
- Network-of-networks system: layers (not to be confused w
NN layers…)
- Entity/node duality
- Intra-layer/type and inter-layer/type interactions
- Layer/Type-specific features (external information)

Graph convolutional and attention models for entity classification in multilayer networks

How to consider a node's neighborhood in the multilayer network to properly generate the embeddings?

$$\mathbf{h}^{(k+1)}_{(i,l)} = \sigma\left(\sum_{(j,m)\in\Gamma(i,l)\cup\Psi(i,l)} \frac{1}{\sqrt{\widetilde{\mathbf{D}}_{ii}\widetilde{\mathbf{D}}_{jj}}} \mathbf{W}^{(k)\,\mathrm{T}} \mathbf{h}^{(k)}_{(j,m)} \right)$$

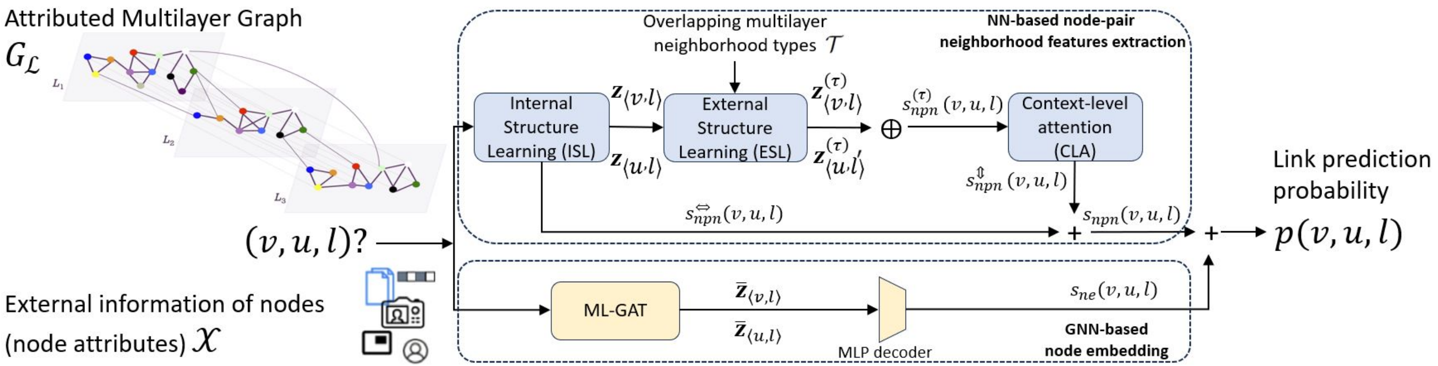


$$\mathbf{h}^{(k+1)}_{(i,l)} = \Big\Vert_{q=1\ldots Q}\, \sigma\left(\sum_{(j,m)\in\Gamma(i,l)\cup\Psi(i,l)} \alpha^{(q)}_{(i,l),(j,m)} \mathbf{W}^{(q,k)\,\mathrm{T}} \mathbf{h}^{(q,k)}_{(j,m)} \right)$$

Link prediction on multilayer networks

How to enhance the (simplistic) approach to link prediction based on pairwise node similarity?

- Combine similarities between multilayer-node embeddings, with
- node-pair neighborhood feature learning



GNNs for multilayer heterogeneous networks

- How to effectively learn from networks that are simultaneously **multilayer**, **heterogeneous** and attributed?

- How to exploit the structural, semantic and external information of each heterogeneous graph?
- How to integrate across-layer information and meta-type information?

GNNs for multilayer heterogeneous networks

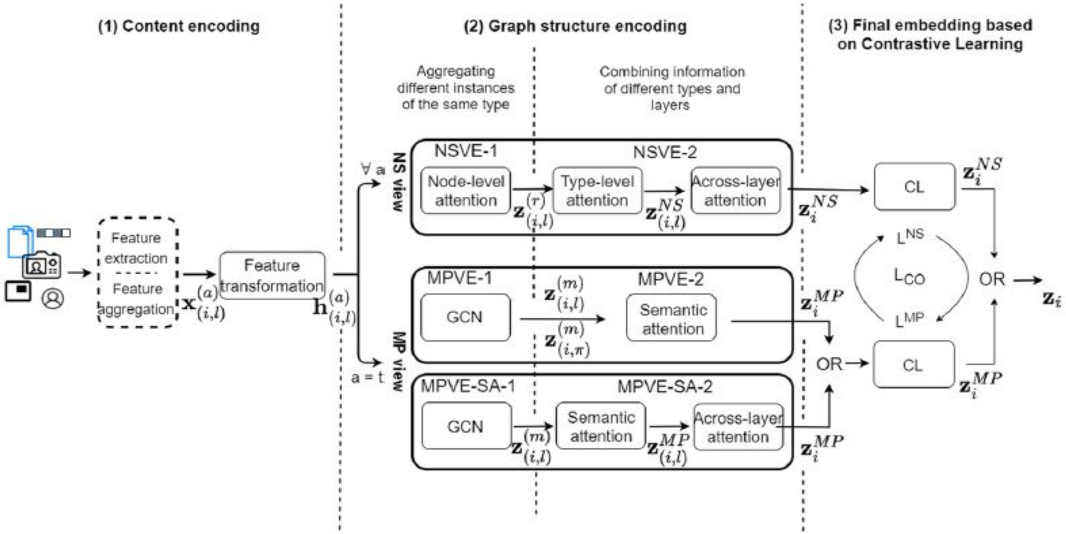
Unsupervised, general and flexible framework based on cooperative **contrastive learning**

Multi-view paradigm

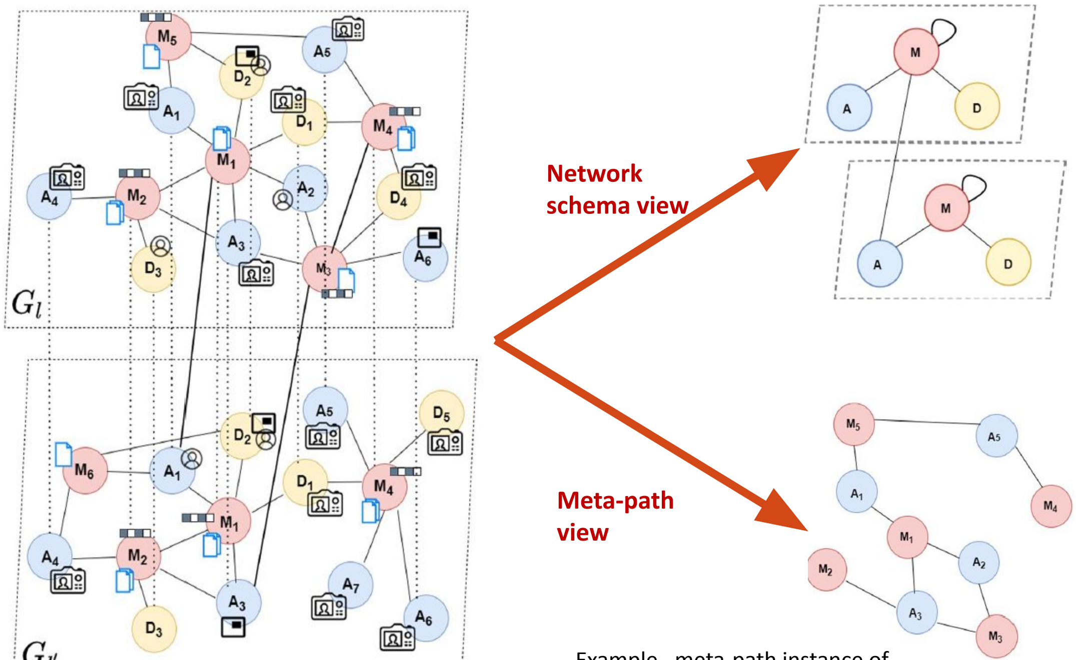
- Local and high-order structure
- Two views collaboratively supervise each other

The learned embeddings can be used to support different downstream tasks

- Entity classification
- Node regression
- Link prediction



GNNs for multilayer heterogeneous networks



Example, meta-path instance of type M-A-D

Network schema graph

- Encodes local structure of nodes
- Handles heterogeneity

Meta-path based graph

- Encodes global structure of nodes
- Handles information from distant nodes

Green-Aware Applications of Graph Representation Learning

- Intelligent Transportation Systems (ITS)
  - nodes: transportation entities such as intersections, road segments, and traffic signals
  - edges: relationships between transportation entities, such as roads or traffic flow
  - node/edge features include geographical information, traffic characteristics, infrastructure details etc.
- Energy and Power Systems
  - nodes: such as gas regulators, power grid components
  - edges: relationships between energy entities such as physical connections, regulators that are mutually connected
  - node/edge features include inlet/outer gas pressure, characteristics of the underlying components etc.

Intelligent Transportation Systems

- Traffic Forecasting
- Demand Prediction
- Intersection Management
- Vehicle Control Systems

Traffic Forecasting & Demand Prediction

Problem: predict the most likely traffic measurements $\{X_{t+1}, \dots, X_{t+T}\}$ (e.g. flow, demand, time) in the next *T* time steps after time *t*, given the previous *M* time steps' traffic measurements $\{X_{t-1}, \dots, X_{t-M+1}\}$ as observations. The goal is to find the optimal prediction values $\{X^*_{t+1}, \dots, X^*_{t+T}\}$ accurate as possible:

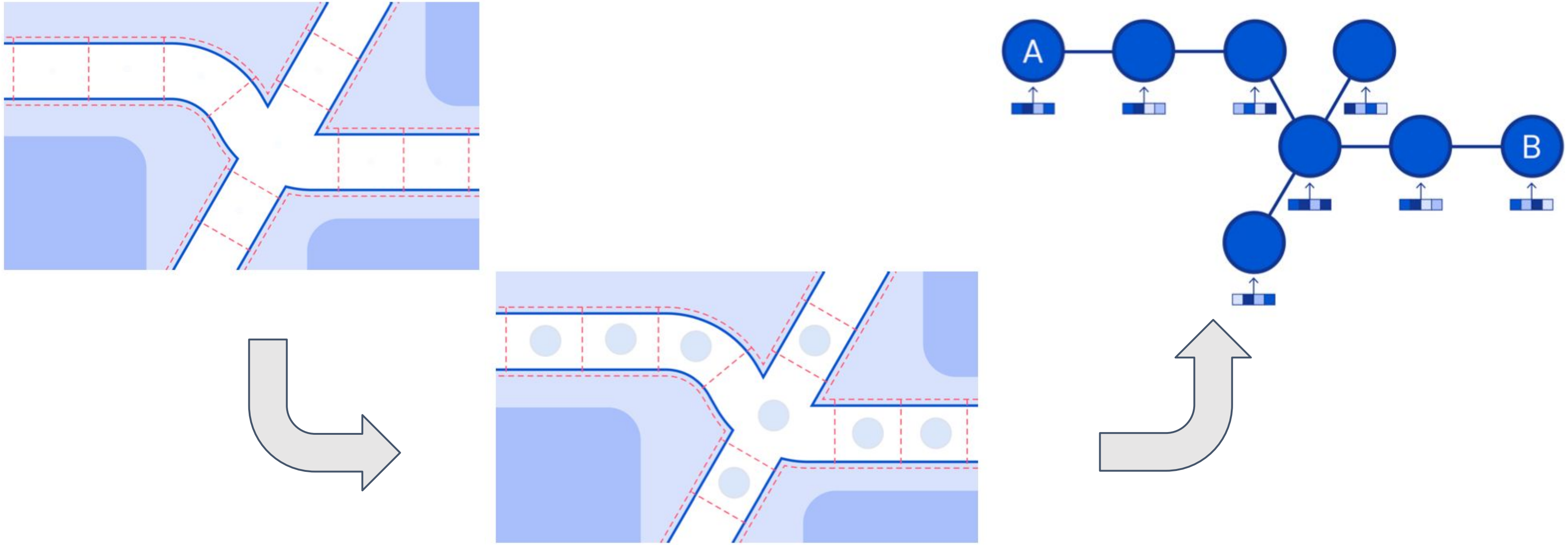
$$X^*_{t+1}, \dots, X^*_{t+T} = argmax_{X_{t+1},\dots,X_{t+T}} \log P(X_{t+1}, \dots, X_{t+T} | X_{t-1}, \dots, X_{t-M+1})$$

where $X_t \in R^{N \times D}$ is the *D*-dimensional traffic measurements of all *N* road segments at time *t*.

GNNs for Traffic/Demand Forecasting

https://deepmind.google/discover/blog/traffic-prediction-with-advanced-graph-neural-networks

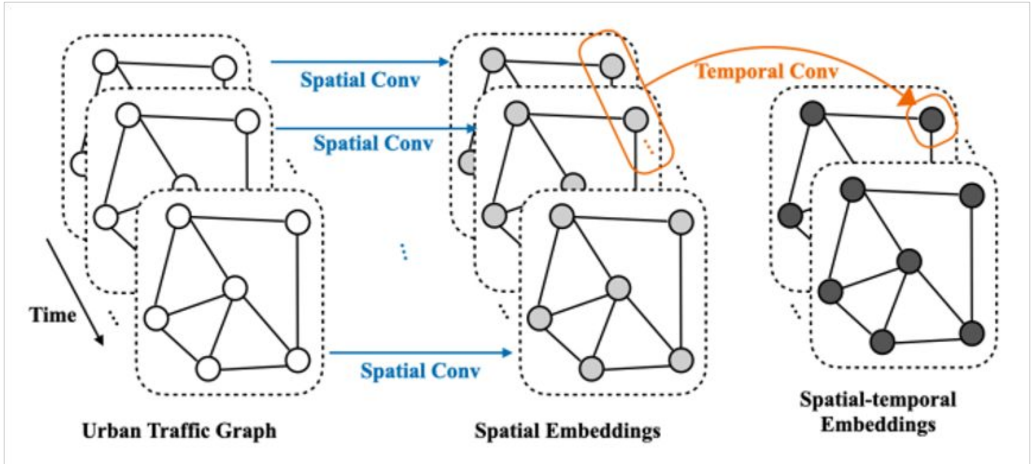
GNNs for Traffic/Demand Forecasting



https://deepmind.google/discover/blog/traffic-prediction-with-advanced-graph-neural-networks

Spatio-Temporal GNNs

Idea: addressing spatial aspects (e.g. the connectivity of roads) and temporal factors (e.g. traffic flow variations over time).



Demand Prediction

GNNs opened doors for considering complex and dynamic non-Euclidean spatial-temporal dependencies in large-scale travel demand prediction

- Ride-Hailing Services
- Bike Sharing Systems
- Passenger Flow Prediction
- Multi-Modal Demand Prediction Studies

Table. A Comprehensive Overview of Most Related Studies for Demand Prediction

Model	Article	Year	Prediction Task	Graph Views	GNN Module	Temporal Module
PGDRT	[82]	2023	Taxi Passenger	Neighborhood, Function, Connectivity	GCN	ConvLSTM
MSTGNN	[211]	2023	Bus, Metro, Taxi	Neighborhood, Connectivity	GCN	Temporal GCN
STGMT	[165]	2023	Taxi & Highway	Traffic Network	Node2Vec	Multi-head Attention
PAG-TSN	[87]	2023	Ride-hailing	Distance, POI relation	BAT-GCN	PA-GRU
HetGNN-LSTM	[117]	2023	Taxi	Decentralized taxi graph	HetGNN	LSTM
MFGCN	[97]	2023	Ride-hailing	OD network	MODGCN	TAS-LSTM
SGCNPM	[182]	2023	Dockless Bike-Sharing	Distance, Function, Interconnectio	MGCN	LSTM
DSTGNN	[56]	2022	Taxi & Bike	Spatial dependency	DCNN	Multi-head Attention
DMVST-VGNN	[72]	2022	Ride-hailing	Multi-view Graph Generation	GAT	Multi-head Attention
ST-MGCN	[38]	2019	Ride-hailing	Neighborhood, Function, Connectivity	ChebNet	RNN

Li, Hourun, et al. "A Survey on Graph Neural Networks in Intelligent Transportation Systems." *arXiv preprint arXiv:2401.00713* (2024).

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Intersection Management

Benefits: alleviate urban traffic congestion, reduce vehicle emissions etc.

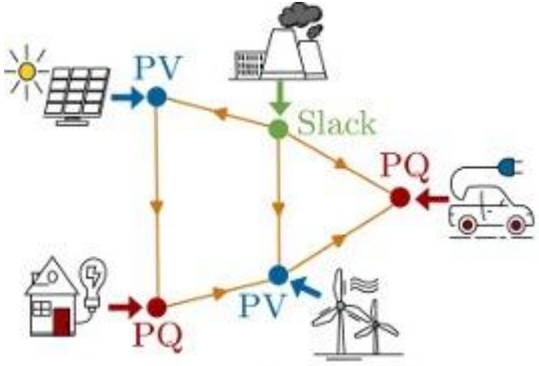
- **Attention Mechanism for Multi Intersections**: the intersections on the main traffic road may have a more significant effect on the target intersection than those on the side road
- **Spatial and Temporal Dependency**: it is essential to consider the historical states of surrounding intersections when predicting the future signal of a target intersection
- **Multi-agent Reinforcement Learning and GNNs**: each signal with an RL agent and creates policies for every intersection by obtaining neighboring intersections information through GNNs

Vehicle Control Systems

- **Perception**: detecting and classifying objects (sets of pixels or cloud points) surrounding the ego vehicle through GNN modeling
- **Motion/Trajectory Prediction**: predicting the future trajectories for the surrounding objects (e.g. vehicles, cyclists and pedestrians) of an autonomous vehicle by unraveling complex interrelations between objects
- **Motion Planning**: responsible for the safe and smooth maneuvers of the ego vehicle while avoiding the static and dynamic obstacles and agents in the scene

Energy and Power Systems

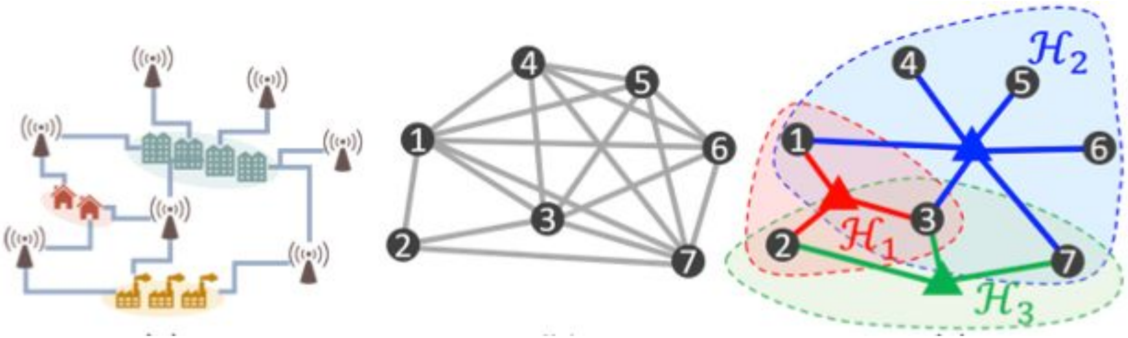
- Fault Scenario Application
- Time Series Prediction
- Power Flow Calculation



Power grid example

Hypergraph Modeling

Core idea: modeling higher-order interactions among grid components and integrating the hypergraph convolution to RNN, so as to model correlated multivariate sequential data from real-world sensor networks



(a) Physical system with interconnected nodes (b) Graph representation of the network (c) Hypergraph representation of the network

Yi, Jaehyuk, and Jinkyoo Park. "Hypergraph convolutional recurrent neural network." *Proceedings of the 26th ACM SIGKDD* 2020.

Conclusions

Takeaway Message: Graph representation learning is an effective tool to address learning problems in Intelligent Transportation Systems and Energy/Power Systems

Ongoing Work:

- Focus on the development of GNN models for Green-aware attributed multilayer heterogenous networks
- Consider explainability aspects of the developed models

Conclusions

Intra-spoke collaborations:
Task 9.4.3 – Explainable ontology-mediated query answering on environmental knowledge bases
Task 9.4.5 – Social network and user behavior analysis for understanding the citizens' attitude to the green transition

Focus on combination with NLP methods for identifying behavioral aspects in social contents and analyzing opinion dynamics (emotions and sentiments) and shaping polarization phenomena in Green-aware social debates