

Project Kick-Off



Graphs in Artificial Intelligence and Neural Networks

Josephine Thomas, Silvia Beddar-Wiesing, Alice Moallemy

5th of May 2021

Thank you!



UNIKASSEL
VERSITÄT



Intelligent
Embedded Systems



Fraunhofer
IEE

- 1 Introduction of group members
- 2 What is the purpose of the kick-off?
- 3 What is GAIN all about?
- 4 **Project Overview**
 - Graph Neuronal Networks and Graph Learning Problems
 - Structure-Dynamic Graphs
 - Attribute-Dynamic Graphs
 - Explainability
 - Generation of Graphs with GNNs
- 5 **Strategy**



- Diploma in physics (TU Berlin)
- Doctoral thesis on 'Using non-linear dimension reduction to embed networks into hyperbolic space' (TU Dresden)
- Data Scientist (Fraunhofer IEE)





- B.Sc. in Mathematics
Combinatorial Optimization



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- M.Sc. in Computer Science
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 - Fraunhofer IEE Kassel
 - Intelligent Embedded Systems, University of Kassel



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Computational Intelligence and Data Analytics
- Research Assistant at
 - Fraunhofer IEE Kassel
 - Intelligent Embedded Systems, University of Kassel
- Current Research Topic:
Machine Learning for structure-dynamic Graphs

Introduction: Alice Moallem-Oureh





- M.Sc. Mathematics (University of Kassel)
- Application focus in Computer Science



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Previous experiences cover:

- practice (Fraunhofer IEE)
- teaching (Tutor at University)
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→ **Next personal goal:**

Causing a GNN revolution with GAIN.



- Director Department Intelligent Embedded Systems (IES)
- 24 researchers, 12 external doctoral candidates
- Focus on Machine Learning and Artificial Intelligence
 - Basic research: e.g. uncertainty modeling, active learning, collaborative learning
 - Applications: e.g. autonomous driving, future energy systems, physics and materials
- Mentor of GAIN and HyMeKI

What is the purpose of the kick-off?



We would like ...

- ... you to get to know us and to possibly form **collaborations**,

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- ... you to get to know us and to possibly form **collaborations**,
- ... all of us to be inspired by bringing people from **different topics** and various backgrounds together,
- ... you to give us **feedback** regarding our strategy.

What is GAIN all about?



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- Success of Deep Learning

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- Interesting data in form of graphs

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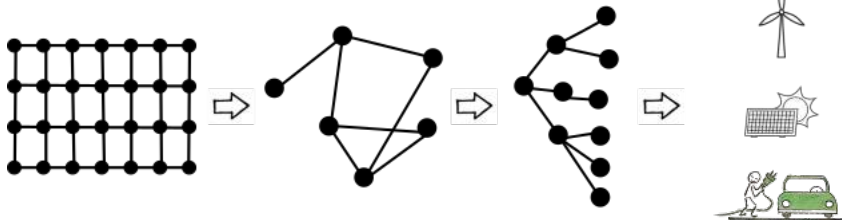


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- Use cases in supply networks

What is GAIN all about?



- Success of Deep Learning
- Interesting data in form of graphs
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0. Survey on dynamic GNN's and analysis of graph types
1. Develop GNN's with different dynamics
 - changing node/link attributes
 - changing numbers of nodes and links
 - fully dynamic model
2. Explainable GNN's
3. Generation of graphs with GNN's

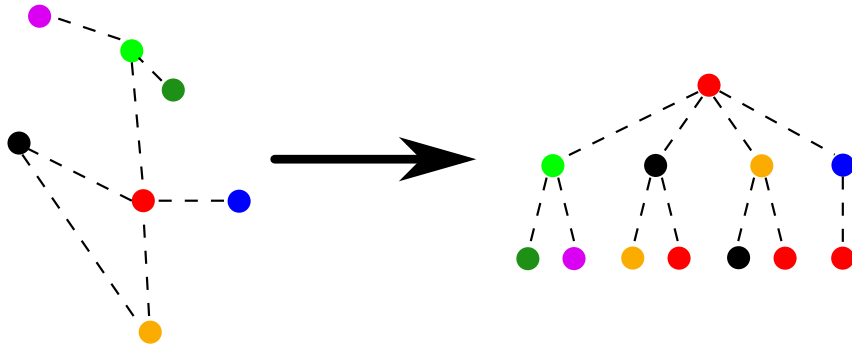
Graph Neural Network (GNN)

Message Passing for Structure Learning



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Node-/Edge-/(Sub-)Graph-Level		
Supervised	Unsupervised	Semi-Supervised
Classification Regression Temporal Predictions ...	Clustering Embedding Temporal Pattern Detection ...	Transductive Class./Regr. Inductive Class./Regr. Temporal Predictions ...

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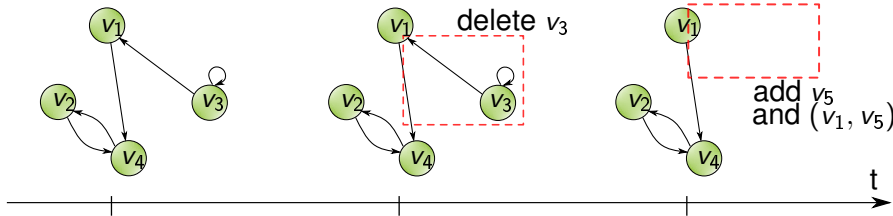
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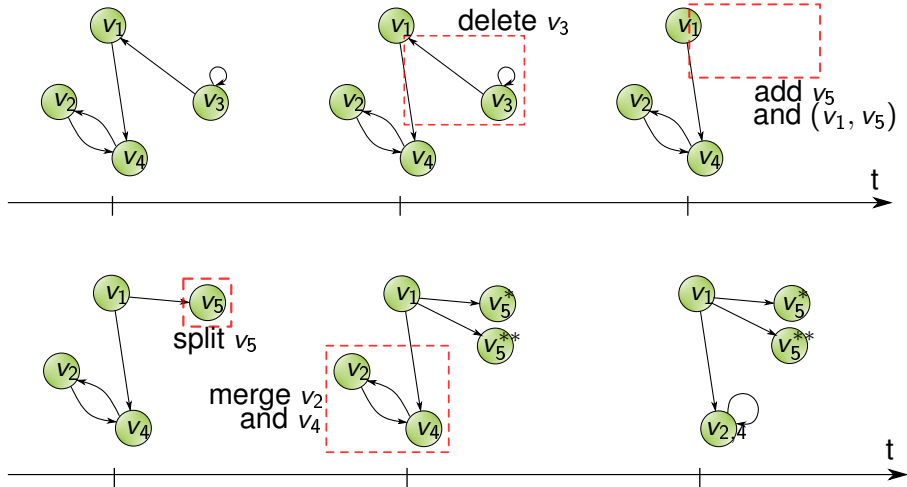
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- *Temporal and Structural Learning: Spatio-Temporal GNN* [Kapoor et al. 2020]



Structure-Dynamic Graphs



Structure-Dynamic Graphs



Challenges in Learning on Structure-Dynamic Graphs





*How to **represent** a struct. dyn. Graph for the Processing with GNN's?*

- Representation of Continuous Dynamics
- Large-Scale Processing



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- Efficient and in Real-Time

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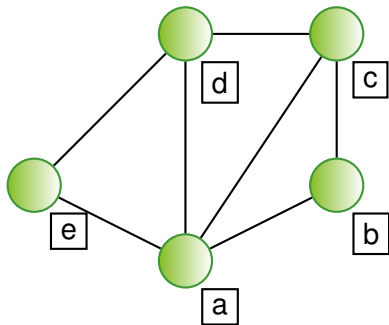
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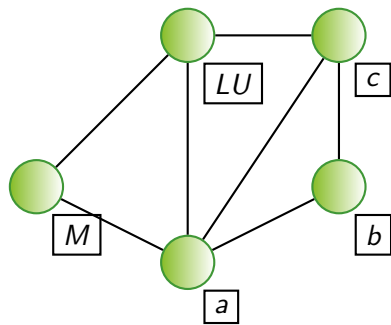
- Addition and Deletion of Information
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*How to consider additional **Properties** for the **Embedding**?*

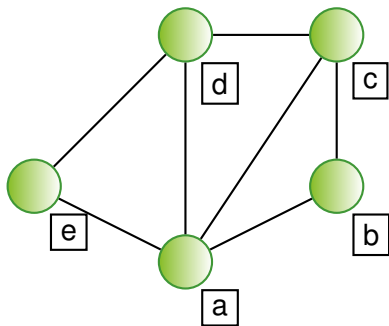
- Graph Property Preservation
- Smoothness
- Efficiency



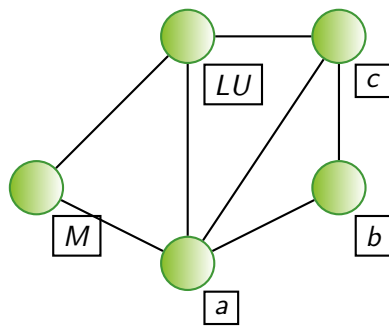
Day 1



Day 2

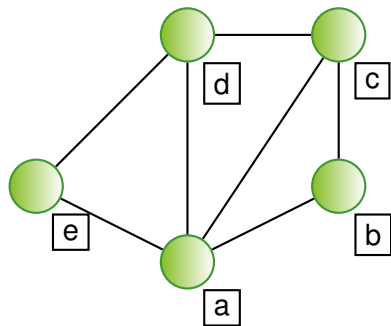


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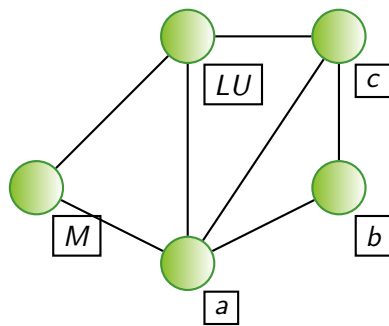


Day 2

- **static** in the structure of their nodes and edges



Day 1



Day 2

- **static** in the structure of their nodes and edges
- **dynamic** in the node and edge attributes.

Representation possibilities:





- **discrete-time dynamic (DTD)**

$\mathcal{G}_d = (g_1, g_2, \dots, g_T)$, where

$i \in \{1, 2, \dots, T\}$ are time **steps** and g_i is some static graph



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Example for an event:

at time **stamp** t ,

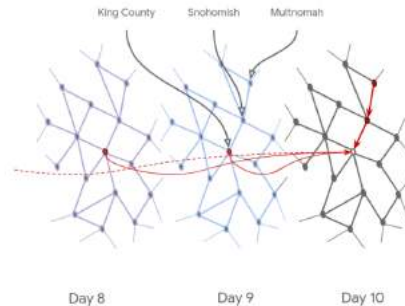
$\epsilon = (t, \text{add}, v)$ that is,
add a node called v into
graph g .

$\epsilon = (t, v, a)$ that is,
the **attribute** of node v in
graph g equals a .



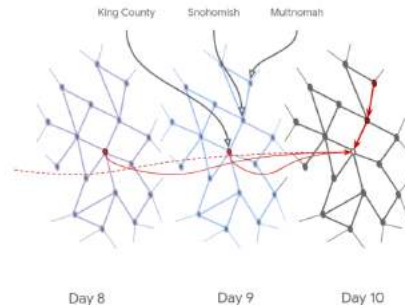
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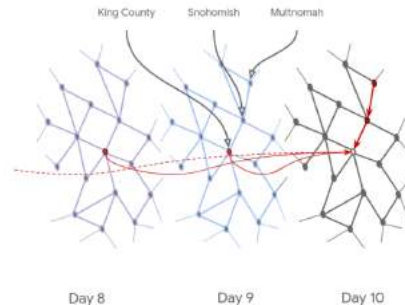
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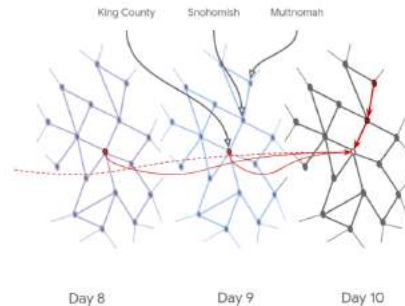
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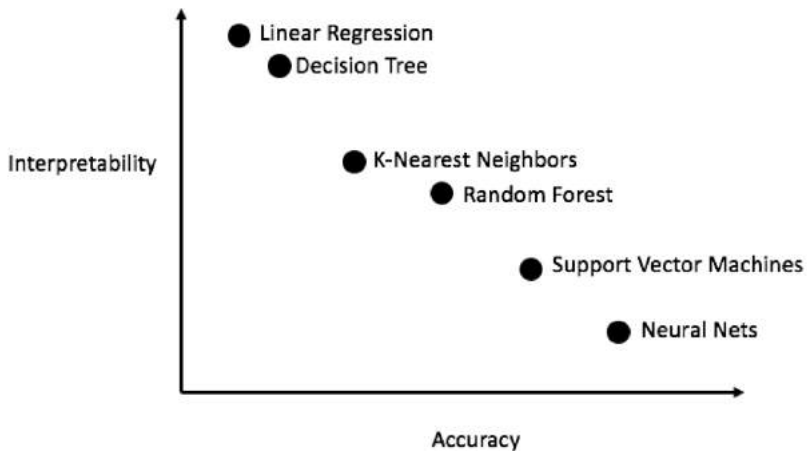


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Explainability: Accuracy-Interpretability Trade-off



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source



- inherent vs post-hoc

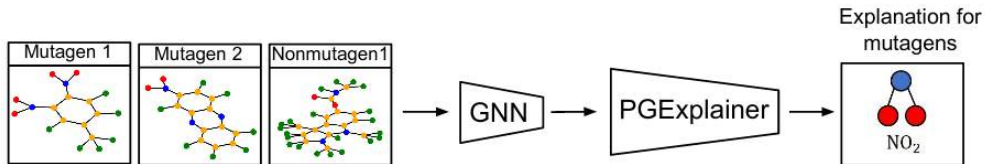


- inherent vs post-hoc
- blackbox vs. whitebox explainer



- inherent vs post-hoc
- blackbox vs. whitebox explainer
- instance-based vs. model based

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source

Generation of Graphs with GNNs

Adding additional instances to an otherwise too small data set

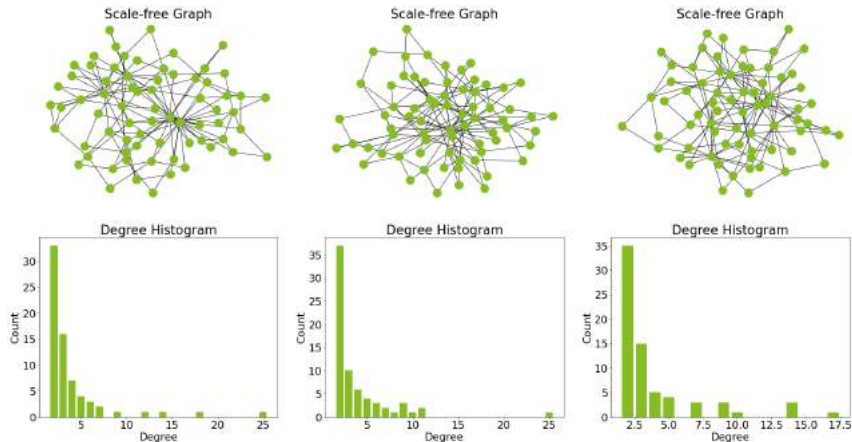
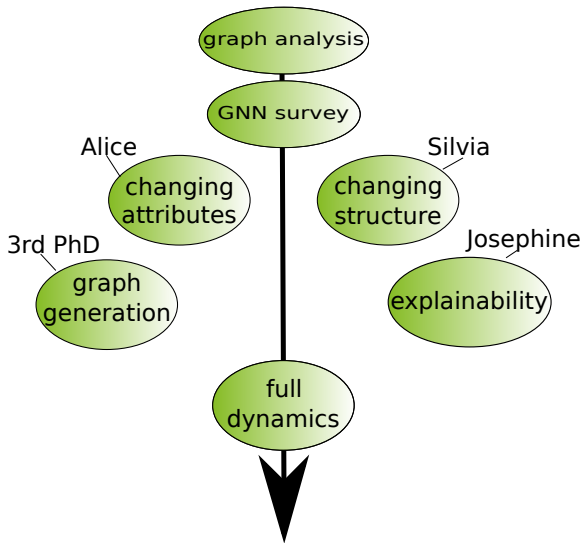


figure is self made





Thank you for your attention!
Questions?

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