

# XAI on Graphs

## Hands-on Tutorial

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# Introduction

These slides aim to explain:

- XAI in General
- Explainers of GNNS, which are implemented by GraphXAI [1]

Additionally, everybody is encouraged to work with explainers for synthetic datasets during the Hands-on Tutorial.

All code is available:

[https://github.com/mathematiger/Hands\\_on\\_GraphXAI](https://github.com/mathematiger/Hands_on_GraphXAI)

# Gliederung

- 1 XAI
  - Overview on XAI
  - What is an Explanation?
- 2 Taxonomy of interpretability
  - Overview of methods
  - Overview of the Explainers
- 3 HoT 1
- 4 Optimization methods
- 5 Evaluation of explanations
- 6 Conclusion and outlook
- 7 HoT 2

# Definitions of XAI

- Interpretability is the degree to which a human can **understand the cause** of a decision. [2]
- Interpretability is the degree to which a human can **consistently predict** the models result. [3]
- The **model itself becomes the source of knowledge** instead of the data. Interpretability makes it possible to extract this additional knowledge captured by the model. [4]

# Goals of XAI

DARPA [5]: XAI program aims to create a suite of ML techniques, that:

- **Produce more explainable models** while maintaining a high level of prediction accuracy
- Enable human users to **understand, appropriately trust, and effectively manage** the emerging generation of AI partners

# Who wants to achieve what in XAI? [6] [7]

## Data Scientists want to Improve

- Did the model use all relevant input?
- Feature Engineering
- Detect flaws: Has the model only learned in the expected way?

## Decision Makers want to Justify & Control

- Develop trust
- Assess regulatory compliance
- Use models appropriately

## Governments want Fairness & Predictability

- DSGVO/GDPR: Citizens have a right to an explanation  
e.g. healthcare, police searches
- Detect discriminatory patterns

## Domain Experts want to Discover

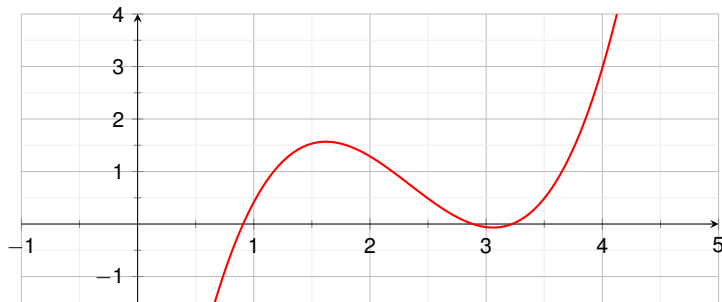
- Has the model detected a connection that was previously missed out?

# What is an explanation?

- Explaining functions in general
- Psychology of explanations
- Why explanations are important

## What is an Explanation?

## Explaining functions: Discussion of curves (binary classification)



- **Extrema:** What are maxima / minima of the model?
- **Zeros:** Where does the model change labels?
- **Monotonous intervals** (for functions in  $\mathbb{R} \rightarrow \mathbb{R}$ )
- **Approximate:**
  - With a simpler function
  - With the same function on restricted input



# Psychology of explanations 1/2 [2] [9]

## ■ People often tend to **abductive reasoning**

- Seeking the simplest & most likely explanation: "Given our theories T of the world: If A where true, the observation O would be a matter of course"
- Explanations are incomplete and could be falsified empirically
- Selecting explanations for correct abductive reasoning is crucial

## ■ **Statistics don't matter**

- People cannot think well about statistics (Kahneman [8])
- People take the most probable explanation always as the best explanation

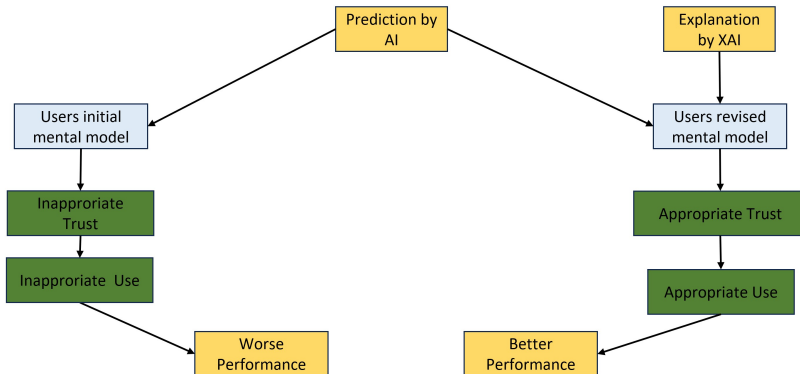
## Psychology of explanations - 2/2

- Explanations should be **contrastive**
  - Why was P predicted and not Q?
- **Social explanations**
  - Only say, what is truly believed, what is necessary and what is relevant
  - Handling already known information as unnecessary

## What is an Explanation?

# How explanations improve performance

Figure inspired by [9]



# End-user explanation issues with AI

- How do we know, if the user has achieved a pragmatic understanding of the AI? [10]
- What is the mental model of end-users of XAI? Is it in line with how XAI works? [11]
- Do users learn to to appropriately use the model, or do they blindly follow / neglect the model? [12]

# Explanator as a function [4] [13]

- Input
- Output
- Method of finding the optimal explanation

# Input

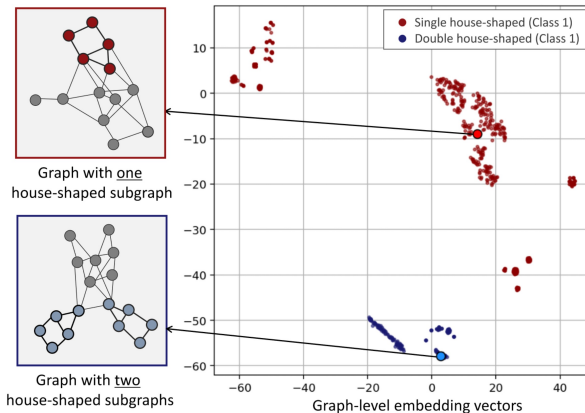
- Post-hoc vs. Intrinsic
  - the model output or the models' input as input
- Locality: Global vs. Instance explanation
  - whole predictions or just one prediction as input
- Portability: Model-specific vs. Model-agnostic
  - The model as input, or just the model output

# Output

- Explanatory subgraph
  - As important input for an instance explanation
  - As a global explanation or prototype explanations
  - As counterfactuals
- Surrogate model
- Logical rules/explanations

# Prototype Explanations

We train a GNN to classify graphs into the number of house-motifs they contain.

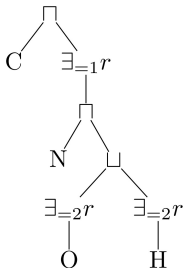


From Figure 3 in [14]



# Logical Expressions

Example: MUTAG for detecting mutagenic molecules [15] [16]



Class Expression for C with a NH<sub>2</sub> group or a NO<sub>2</sub> group.

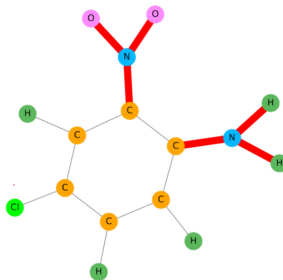
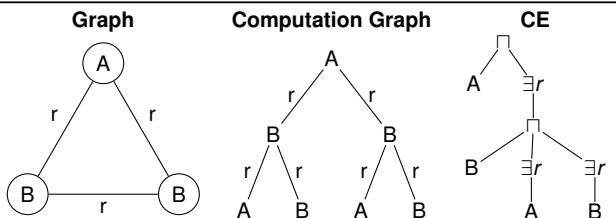


Figure from Figure 5 in [17]

# Motivation for using description logics

The computation graph mainly follows a tree structure  $\rightarrow$  it can better be approximated by a class expression



# Finding the best explanation

- Optimization framework
  - Mutual information
  - GNN-Output
  - Backpropagation / Feature Importance
- Regularization
  - Length of explanation
  - Connected subgraphs
  - . . .

# Explaining a GNN

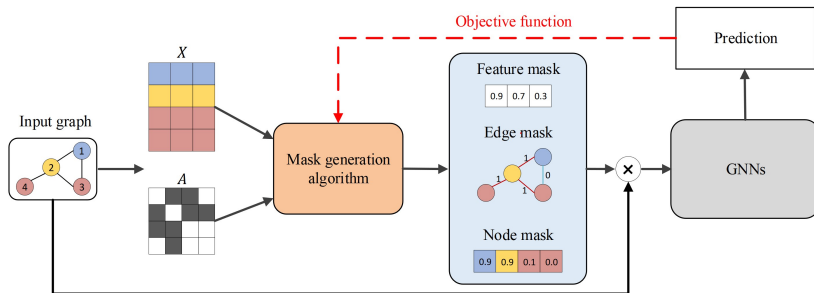
Most common goal: Find a subgraph, which explains a label

- Instance explanations: Masking important input
  - Node masks [16]
  - Edge masks [15]
  - Feature masks [16]
- Global explanations: One explanatory graph for one class/label
  - Select a prototype instance explanation [14]
  - Create synthetic graphs [18]

## Overview of methods

# Masking the input data

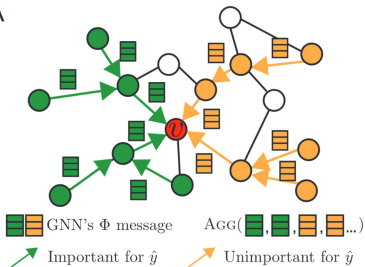
From Figure 2 in [19]:



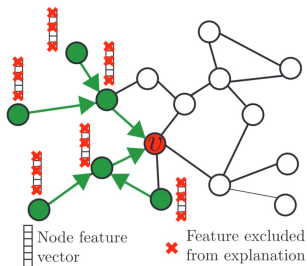
# Node masks: GNNExplainer [16]

From Figure 2 in [16]:

A



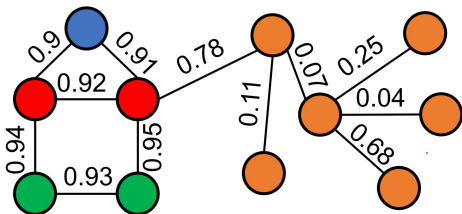
B



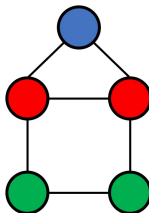
## Edge masks: PGExplainer [15]

From Figure 2 in [16]:

PGExplainer



Ground Truth Explanation



# Obtaining an explanation by removing nodes: SubgraphX [20]

## Notation

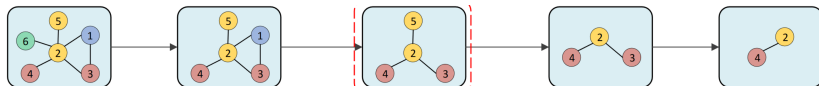
$G_i$  is subgraph after removing one node,  $N$  is the set of nodes not in  $G_i$ ,  $f$  is the GNN

In each step, the least contributive node is removed (measured by shapley values)

$$\phi(G_i) = \sum_{S \subset N} \frac{|S|! (|N| - |S|)!}{|N|!} (f(S \cup G_i) - f(S))$$

This is how the subgraph contributing the most to the GNN prediction can be found.

From Figure 1 in [20]:

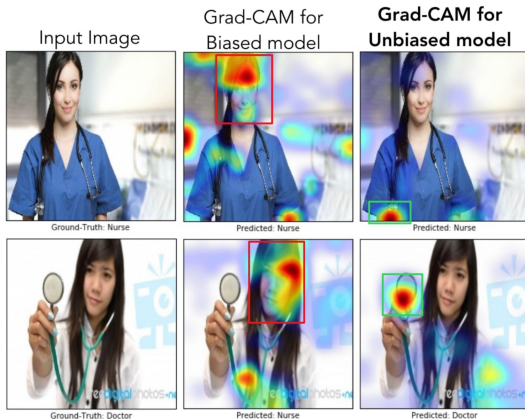




## Overview of the Explainers

# Obtaining a subgraph by gradients: [21] [22] [23]

- Algorithms aggregate gradients in last CNN(GCN)-layer to find relevant input data
- Adopted from GNNs, not specifically tailored to GNNs



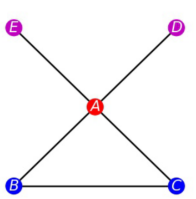
From Figure 8 in [21]

## Overview of the Explainers

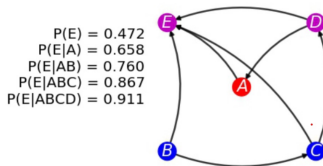
# Probabilistic graph model (PGM): [24]

- Surrogate model for node classification
- Trains a bayesian network to capture statistical dependencies, observed by perturbed input

From Figure 1 in [24]:



to-be-explained motif

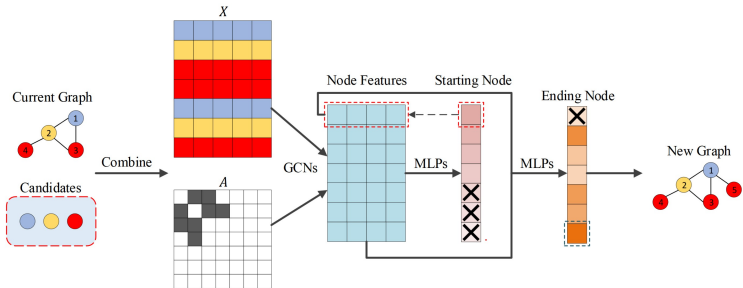


Bayesian network for dependencies

# Generating explanations

- Finding an explanatory subgraph via reinforcement learning [25]
- Synthetically creating a new graph as explanation
  - Reinforcement learning [26]
  - One-shot learning [18]

From Figure 2 in [26]:



- Dataset: 10 different Motif Datasets, with the explainers from above

Setup:

- Link: [https://github.com/mathematiger/Hands\\_on\\_GraphXAI](https://github.com/mathematiger/Hands_on_GraphXAI)
- You can install it yourself or use an available VM
- Time: 15min



# Mutual Information

## Question

- *How many questions are needed to identify  $x$ , if you know  $y$ ?*
- *How predictable is  $x$ , after observing  $y$ ?*

## Definition

*The entropy  $H$  measures the surprise of a random variable  $x$ :*

$$H(x) = E[-\log p(x)] = \sum_x p(x) \log\left(\frac{1}{p(x)}\right)$$

One can identify:

- $p(x)$  as the probability
- $\log\left(\frac{1}{p(x)}\right)$  as the number of needed y/n questions to identify this  $x$

## Definition

*Mutual Information (MI) is measured as:*

$$I(x, y) = H(x) - H(x | y)$$

# MI in XAI

## Reminder

$$H(x) = \sum_x p(x) \log\left(\frac{1}{p(x)}\right)$$

$$I(x, y) = H(x) - H(x | y)$$

If:

- $x$  is the original output of the GNN
- $y$  is the output of the GNN on an explanatory subgraph

we can ask:

## Question

*How predictable is  $x$  after observing  $y$ ?*

In XAI we are interested in maximizing this predictability.

# Difference of MI and GNN-output

- MI:
  - Finds input, which very clearly explains one label (not necessary the to-be-explained label)
  - Assumption: Masking the input only purifies the label, instead of changing the prediction
- GNN-output
  - Finds input, which is most relevant for the to-be-explained label, but possible also for other labels

# Regularization [25] [18] [15]

- Length of the explanation
  - Number of Nodes
  - Upper sum on probabilities of selected nodes
  - Maximal distance of 2 nodes
- Connected subgraphs
  - Directly from optimization framework
  - Higher likelihood for adjacent edges of selected explanatory output
- Similarity
  - Similarity of node representations
  - Explanation graph being "realistic" compared to the input data, e.g. molecule data



## Different scopes of explanations [27]

- Functionally Grounded: Accuracy, Faithfulness, fidelity, ...
- Human Grounded: Degree of understanding
- Application Grounded: Performance increase

# Accuracy to ground-truth [1]

Motifs



Features

None

Explanations  
by GNN-  
Explainer



Explanations  
by PG-  
Explainer



$$acc = \frac{TP}{TP + FP + FN}$$

Here:

- TN is not counted, as the explanatory motif only gives positives as feedback
- positives and negatives can be counted on nodes or edges

# Fidelity: How well can the explanation approximate the model? [28]

$$\text{fid}_+(S) = \frac{1}{n} \sum_{i=1}^n |\mathbf{1}_{\hat{y}_{i,G}=\hat{y}_{i,G \setminus S}}|$$

$$\text{fid}_-(S) = \frac{1}{n} \sum_{i=1}^n |\mathbf{1}_{\hat{y}_{i,G}=\hat{y}_{i,S}}|$$

Fidelity can be interpreted as follows:

$\text{fid}_+(S)$

- Remove explanatory subgraph
- Measure, how much relevant input is found

This evaluation can be used for global and local explainers.

## Notation

- $\hat{y}_{ind}$  is the prediction of the GNN evaluated on the input  $ind$
- $G$  is the computation graph
- $S$  is the explanatory subgraph
- $n$  is the number of instances

$\text{fid}_-(S)$

- Only look at the output of the explanatory subgraph
- Measure, if sufficient input is found for this label

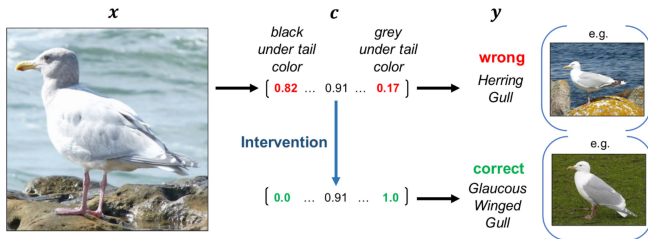
# Conclusion

- XAI on graphs is helpful for many stakeholders
- Finding the right explanation for the right audience stays challenging
- There exists an available framework for creating and evaluating local and global explanations
- Still a lot of research possible

## Outlook 1: Intrinsic Explainers [29] [30]

- Idea: Classify many intermediate concepts and base the prediction on these.
- Advantage: Intermediate predictions are changeable by humans, hence it is easier to find the errors of the model

Figure from Figure 3 in [29]



## Outlook 2: Further Research

- Identifying important concepts in graphs
- Global Explanations
  - Generating synthetic graphs
  - Extracting meaningful explanations
- Explainers for tasks beyond node and graph classification
- Explaining heterogeneous graph data (graphs with different node types)
- Using methods from knowledge graphs for XAI of GNNs
- Finding the optimal way for introducing XAI to end-users

# Questions

Any questions??

# HoT2

- Task: Find the optimal graph with features in 0, 1, 2, 3, which has the highest summed up prediction for all nodes
- Maximal 6 nodes
- input:
  - List of edges [(0,1), (1,2)] between node types
  - List of features [0,1,2], i-th space for the i-th node

Setup:

- Link: [https://github.com/mathematiger/Hands\\_on\\_GraphXAI](https://github.com/mathematiger/Hands_on_GraphXAI)
- You can install it yourself or use an available VM



- Time: until 12.00
- No cheating! If any questions arise, ask me.



# HoT3

- Task: Explore Class Expressions as explanations: Find the Class Expression with the highest fidelity.
- Input: A tree as list-form: [class, [subtree 1], [subtree 2]]. The subtrees will be added with an intersection.
- Allowed Classes are '0','1', '2','3'. Please don't forget to write the numbers as strings.

Setup:

- Link: [https://github.com/mathematiger/Hands\\_on\\_GraphXAI](https://github.com/mathematiger/Hands_on_GraphXAI)
- You can install it yourself or use an available VM



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