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`

Gliederung

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

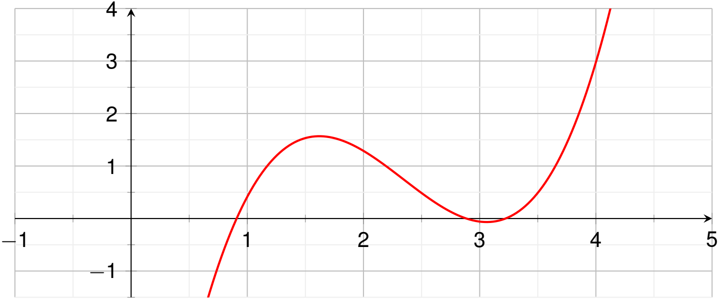
Domain Experts want to **Discover**

- 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

Explaining functions: Discussion of curves (binary classification)



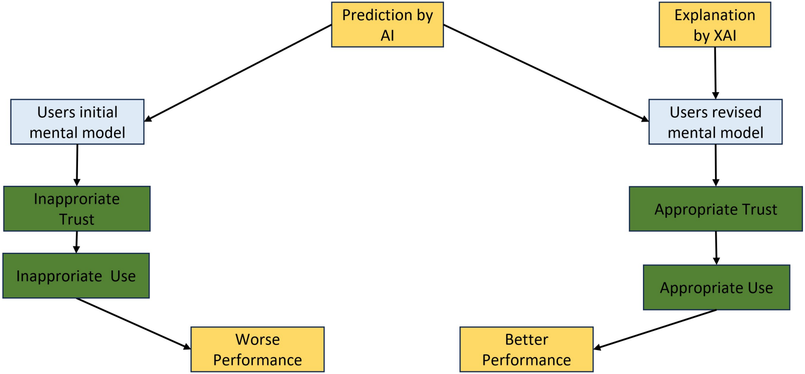
- **Extrema**: What are maxima / minima of the model?
- textbfZeros: Where does the model change labels?
- textbfMonotonous intervals (for functions in $\mathbb{R} \to \mathbb{R}$)
- textbfApproximate:
  - By a simpler function
  - By the same function on restricted input

Psychology of explanations [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
- 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

How explanations improve performance

Figure inspired by [9]



Problems by explaining AI to end users

- 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

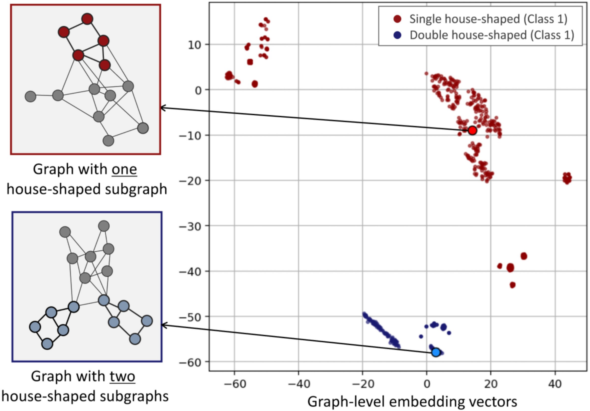
- Post-hoc vs. Intrinsic
  - the model output or the models' input as input
- Locality: Global vs. Instance explanation
  - whole predictions or just one prediction as input
- Portability: Model-specific vs. Model-agnostic
  - The model as input, or just the model output

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

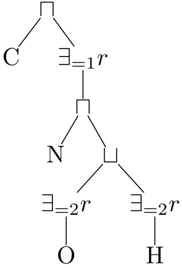
We train a GNN to classify graphs into the number of house-motifs they contain.



From Figure 3 in [14]

Logical Expressions

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



Class Expression for C with a NH_2 group or a NO_2 group.

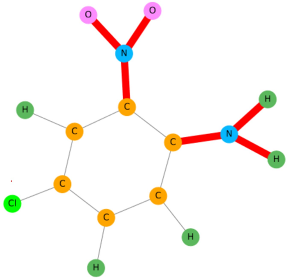


Figure from Figure 5 in [17]

Finding the best explanation

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

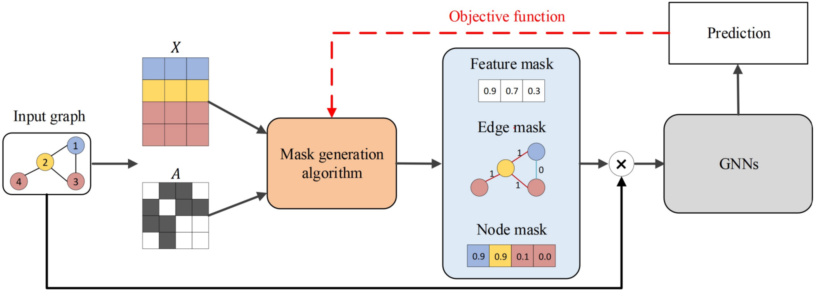
Explaining a GNN

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 a label
  - Select a prototype instance explanation [14]
  - Create synthetic graphs [18]

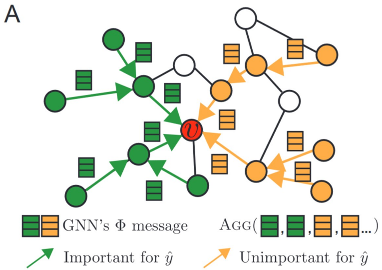
Masking the input data

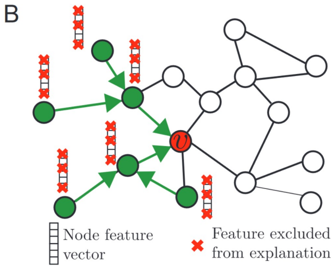
From Figure 2 in [19]:



Node masks: GNNExplainer [16]

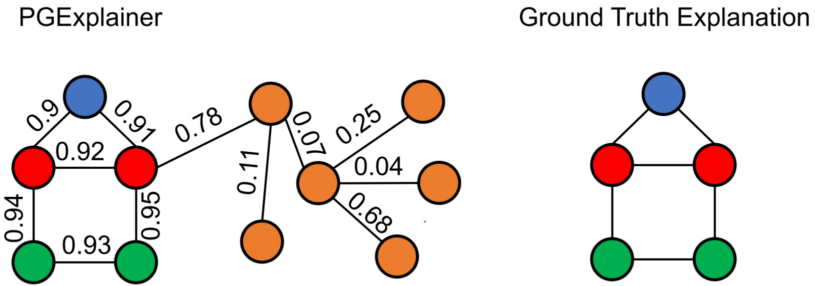
From Figure 2 in [16]:





Edge masks: PGExplainer [15]

From Figure 2 in [16]:



Obtaining an explanation by removing nodes: SubgraphX [20]

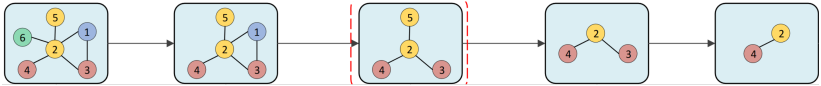
Notation

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)

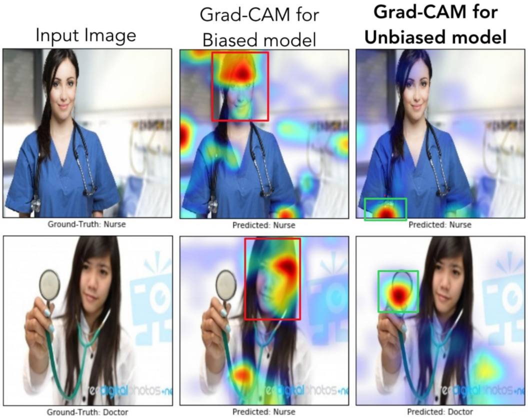
$$\phi(G_i) = \sum_{S \subset N} \frac{|S|!\,(|N| - |S|)\,!}{|N|!} \left(f(S \cup G_i) - f(S)\right)$$

This is how the subgraph contributing the most to the GNN prediction can be found.
From Figure 1 in [20]:



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

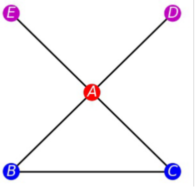


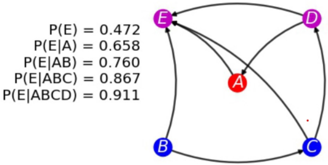
From Figure 8 in [21]

Probabilistic graph model (PGM): [24]

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

From Figure 1 in [24]:





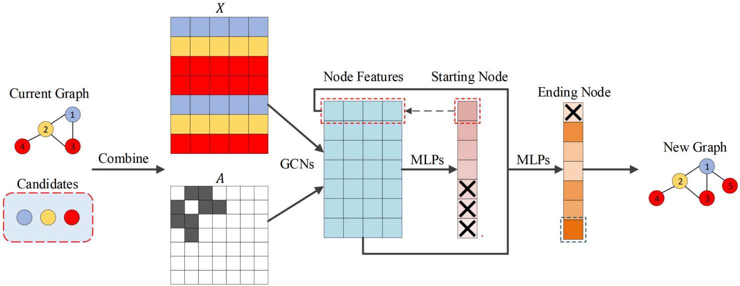
to-be-explained motif

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`
- You can install it yourself or use an available VM

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:

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

One can identify:

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

Definition

Mutual Information (MI) is measured as:

$$I(x, y) = H(x) - H(x \mid y)$$

MI in XAI

Reminder

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

$$I(x, y) = H(x) - H(x \mid y)$$

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

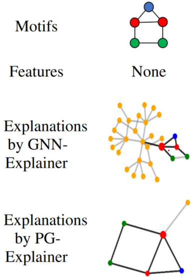
Regularization [25] [18] [15]

- 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]



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

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]

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

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

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*

Fidelity can be interpreted as follows:

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

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

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

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

This evaluation can be used for global and local explainers.

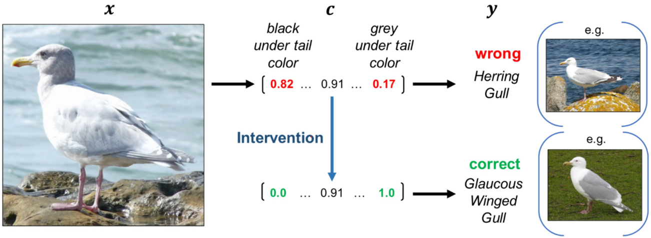
Conclusion

- XAI on graphs is helpful for many stackholders
- 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:

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- You can install it yourself or use an available VM

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`
- You can install it yourself or use an available VM

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