User Preferences in Graph Neural Network(GNN) Explanations

We welcome you to participate in our user study on Graph Neural Network(GNN) explanations, where we aim to understand user preferences regarding the different types of explanations offered by various explainer models for the predictions generated by machine learning model(s).

Machine learning's integration into human lives has become pervasive, influencing various facets of our daily experiences.

While the integration of machine learning brings numerous benefits, the need for explainable AI (XAI) becomes increasingly apparent. As machine learning models become more complex, they often function as "black boxes," making it challenging for users and even developers to understand how they arrive at specific decisions. In critical domains like healthcare, finance, and criminal justice, where accountability and transparency are paramount, the lack of explainability can lead to distrust and ethical concerns.

* Indicates required question

1. Have you ever encountered or worked with machine learning technologies in any capacity, either personally or professionally? *

   Mark only one oval.

   - Yes
   - No
   - Not Sure

2. Are you familiar or have any initial experinece with the concept of Explainable AI? *

   Mark only one oval.

   - Yes
   - No

The Explanation Scenario

As a scientist in a laboratory, your work now revolves around studying chemical compounds to determine their potential carcinogenic properties. This research is crucial for drug development and environmental safety, as identifying carcinogens helps in preventing cancer and ensuring the safety of chemicals used in various industries. The MUTAG dataset includes 340 chemical compounds that are potentially "Carcinogenic", represented using graph structure with nodes (atoms, bonds and Literal values) and edges (chemical bonds, structural properties, chemical test types etc). The selected moeclues or nodes in the dataset are to be classified as "Mutagenic" or "Non-Mutagenic".

Your task is to use machine learning models to predict whether a compound is mutagenic (can cause mutations) or not. However, it's not just about the prediction; you need to understand why the model made its decision. This is where XAI comes into play. You are presented with two types of explanations for each prediction:

1. **Logical Explanation:** A set of rules describing why a compound is classified as mutagenic or not.
2. **Sub-Graph Explanation:** A (sub-graph) excerpt from the graph dataset highlighting key features leading to its classification.

Your role is to assess these explanations not only for their correctness but also for how understandable and useful they are from a scientific perspective. This will help in developing more transparent and trustworthy AI models in your field.

Sub-Graph Explanation: This image is provided as an explanation to why a node was classified as mutagenic.

'd' (Atoms): Represents atoms in molecular structures, crucial for defining the compound's properties.

'bond': Indicates chemical bonds between atoms, fundamental for molecular connectivity.

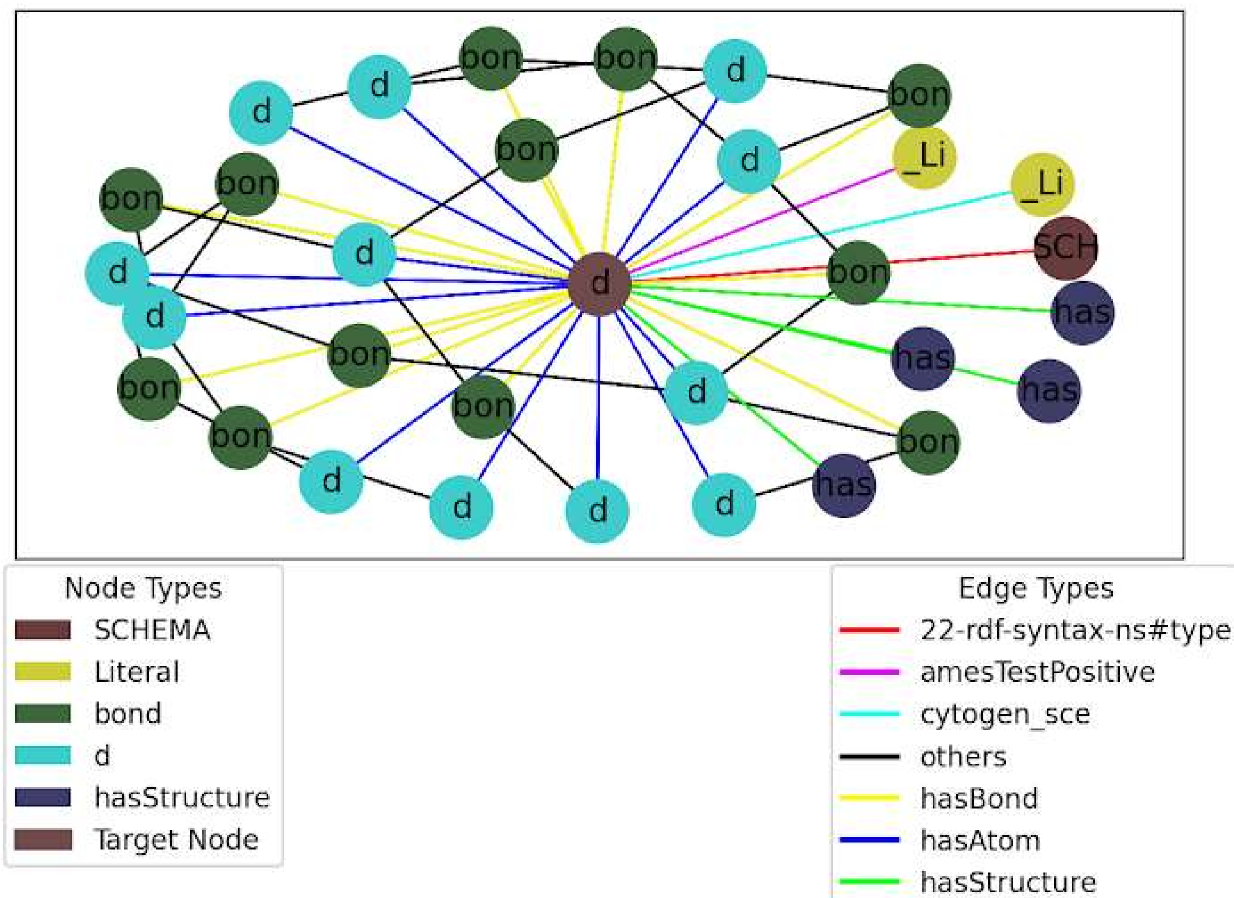
'SCHEMA': Defines the overall structure and organization of the graph's data model.

'_Literal': Contains specific values or properties of atoms, like charge of an atom or boolen value of some test results.

'hasStructure': Connects atoms to their respective molecular structures, delineating the compound's layout.

'Taget node' : It is the node being classified as Mutagenic

Similarly, the edge types contain relational information of the target node with other nodes.



3. On a scale of 1 to 5, how confident do you feel in your understanding of the **"SUB-GRAPH"** explanation provided? *

Mark only one oval.

1	2	3	4	5
⬭	⬭	⬭	⬭	⬭

4. On a scale of 1 to 5, how clear was the **"SUB-GRAPH"** explanation? *

Mark only one oval.

1	2	3	4	5
⬭	⬭	⬭	⬭	⬭

5. How did you find the length/size of the **"SUB-GRAPH"** explanation? *

Mark only one oval.

- ⬭ Sufficient
- ⬭ Excessive
- ⬭ Insufficient

Logical Explanation : This image below depicts a logical rule used as an explanation for any entity labelled as Mutagenic. All the entities in the dataset that are defined by this rules are considered Mutagenic.
In the explanation :
hasAtom.Carbon-10: This specifies a relationship indicating the presence of a Carbon-10 atom.

hasStructure: This denotes a relation to a certain structural characteristic or configuration.

¬Non_ar_6c_ring: This represents the negation of a non-aromatic six-carbon ring, implying that the structure is not a non-aromatic six-carbon ring.

$$(\exists\ \text{hasAtom.Carbon-10}) \wedge (\geq 10\ \text{hasStructure.}(\neg\text{Non\_ar\_6c\_ring}))$$

6. On a scale of 1 to 5, how confident do you feel in your understanding of the **"LOGICAL"** explanation provided? *

Mark only one oval.

1	2	3	4	5
◯	◯	◯	◯	◯

7. On a scale of 1 to 5, how clear was the **"LOGICAL"** explanation? *

Mark only one oval.

1	2	3	4	5
◯	◯	◯	◯	◯

8. How did you find the length/size of the **"LOGICAL"** explanation? *

Mark only one oval.

- Insufficient
- Sufficient
- Excessive

Preference

In this section, we would like to know about your preference regarding the explanations.

9. Among the types of explanations provided, which type of explanation would you prefer? *

Mark only one oval.

- Sub-graph Explanation
- Logical Explanation

10. Among the types of explanations provided, which type of explanation do you feel easier to understand? *

Mark only one oval.

- Sub-graph Explanation
- Logical Explanation

11. In the context of Explainable AI (XAI) *

Interpretability: Refers to the ease with which a human can understand the reasoning behind a model's prediction. In graph machine learning, this means how clearly a model can explain its decisions using the graph's structure, such as highlighting specific nodes or edges that influenced a prediction.

Fidelity: Indicates the accuracy with which the explanation reflects the model's actual decision-making process. High fidelity means the explanation closely mirrors how the model uses the graph's features to arrive at its conclusions, ensuring the explanation is not just understandable, but also truthful to the model's operation.
In your opinion, what is the most important aspect of an explanation among the options provided?

Mark only one oval.

- Fidelity
- Interpretability

General Remarks

Please provide any general remarks or feedback you have about this survey. Your comments are valuable and will help us improve the survey experience.

12. Do you have any remarks about the explanations provided in this Survey? If yes, please provide a short comment.

13. Do you have any remarks about the overall experience of this Survey? If yes, please provide a short comment.