# Prototype-Based Explanations for Graph Neural Networks

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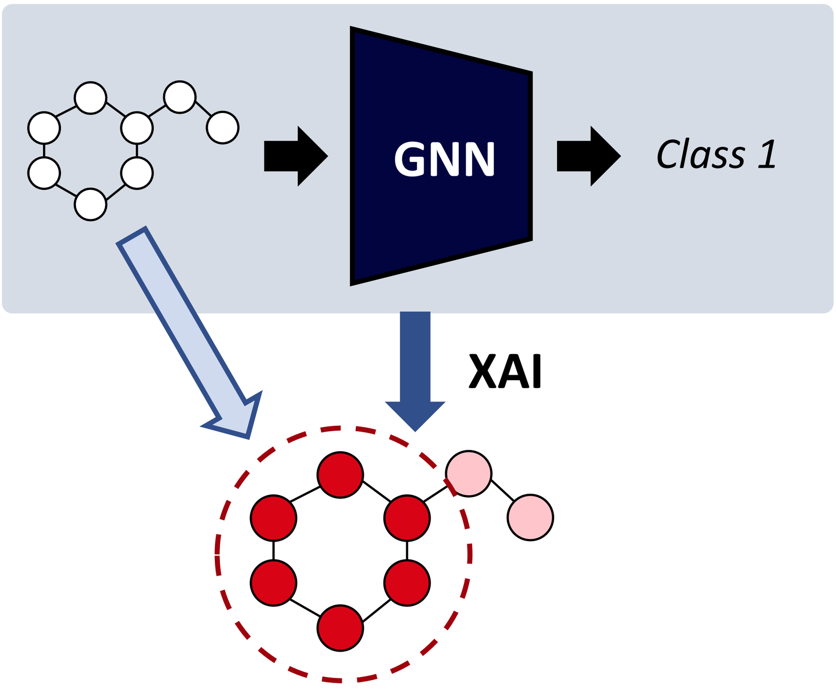
## Research Problem

### Explainable AI for graph neural networks (GNNs)

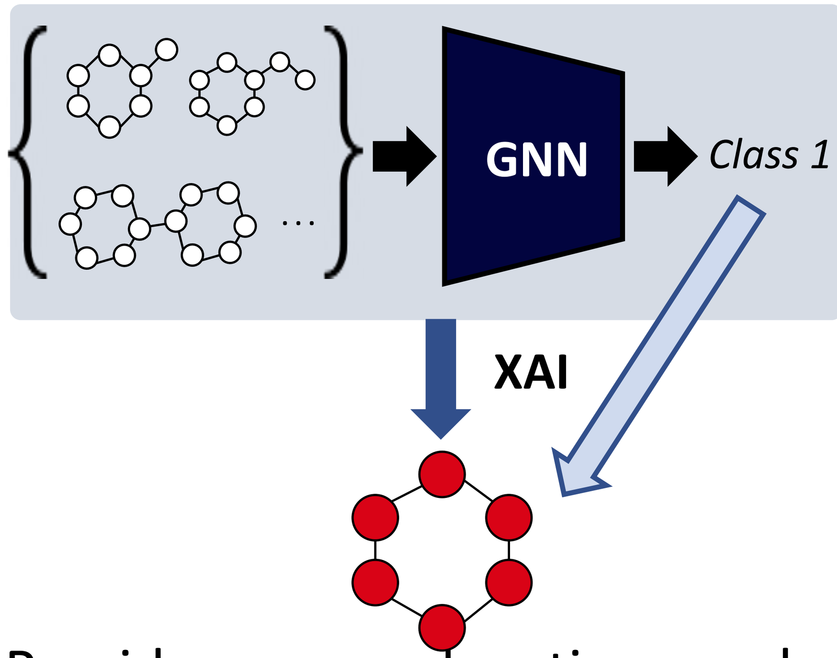
**Explainable AI (XAI)** is interested in explaining deep neural network models, which can provide model-user trust and avoid 'clever Hans' predictions [1].

#### Instance-level explanation



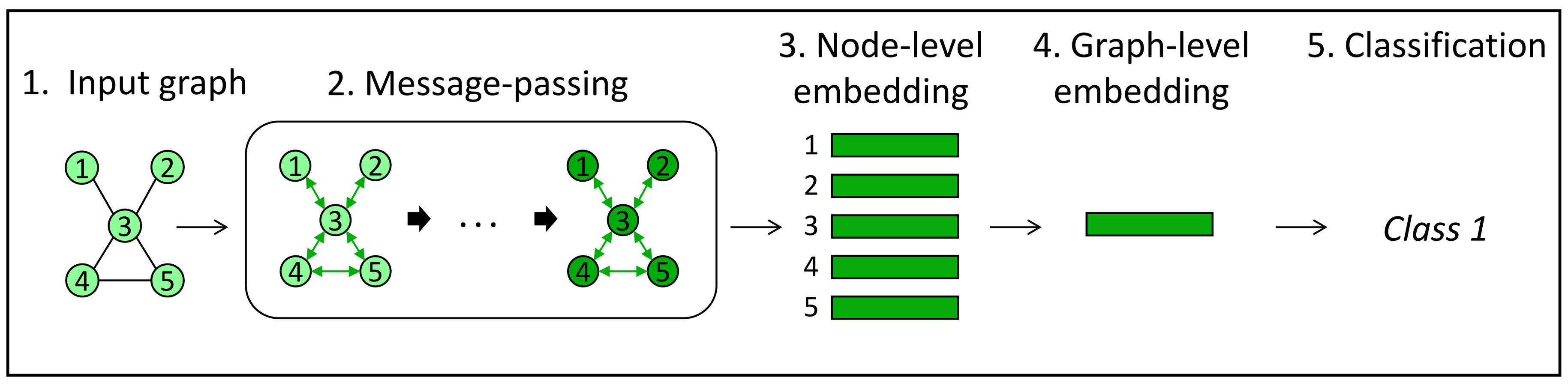

Provides explanation for **each instance**. Usually highlights important subgraph or features of the given instance.
Most XAI methods for GNN models consider this approach.

#### Model-level explanation




Provides explanation by describing the **general behavior** of a model without referring to a specific example.
Our work aims to design a XAI method for GNNs by adopting this approach.

### GNNs for graph classification

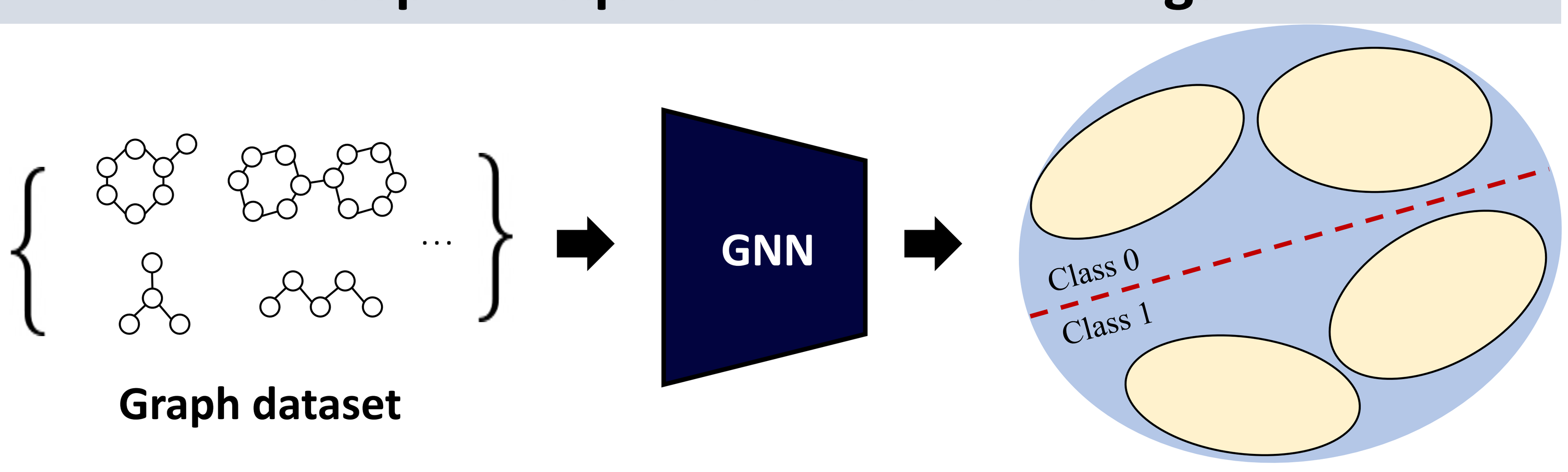



### Problem formulation

In our study, we aim at designing a **model-level explanation method** of GNNs for graph classification, which provides an abstract and concise explanation by capturing what the model has learned from the training data.

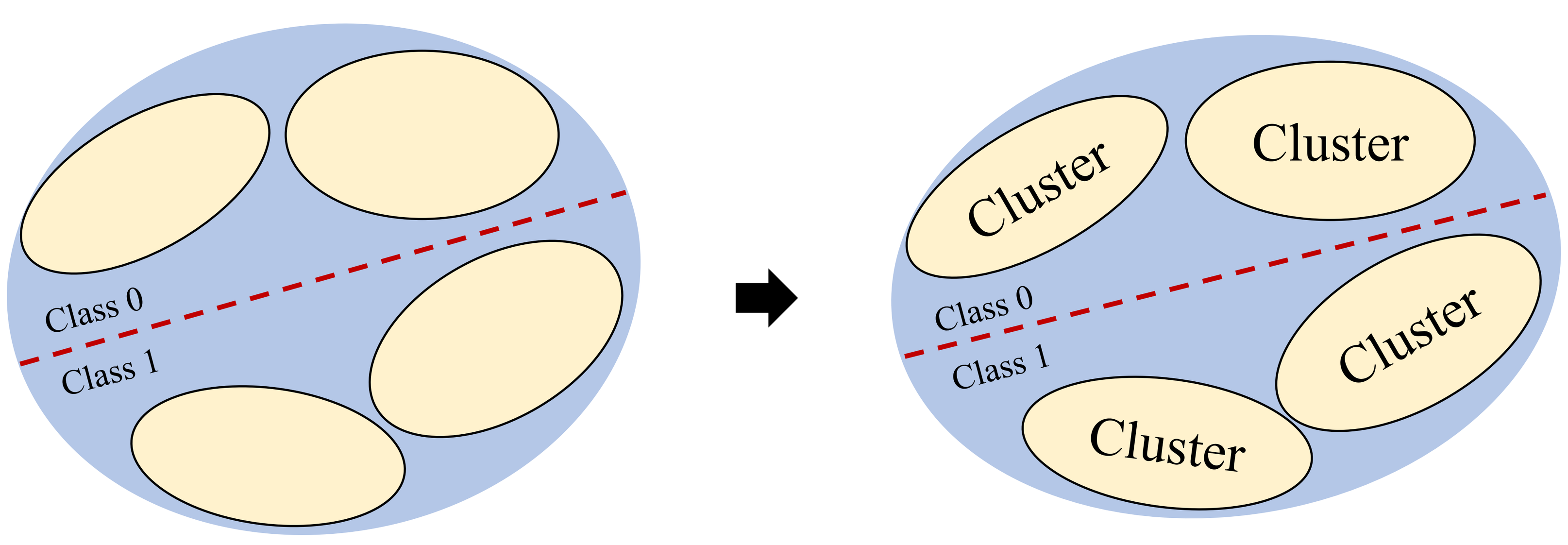
## Proposed methodology: PAGE

### Step 1: Acquisition of embeddings



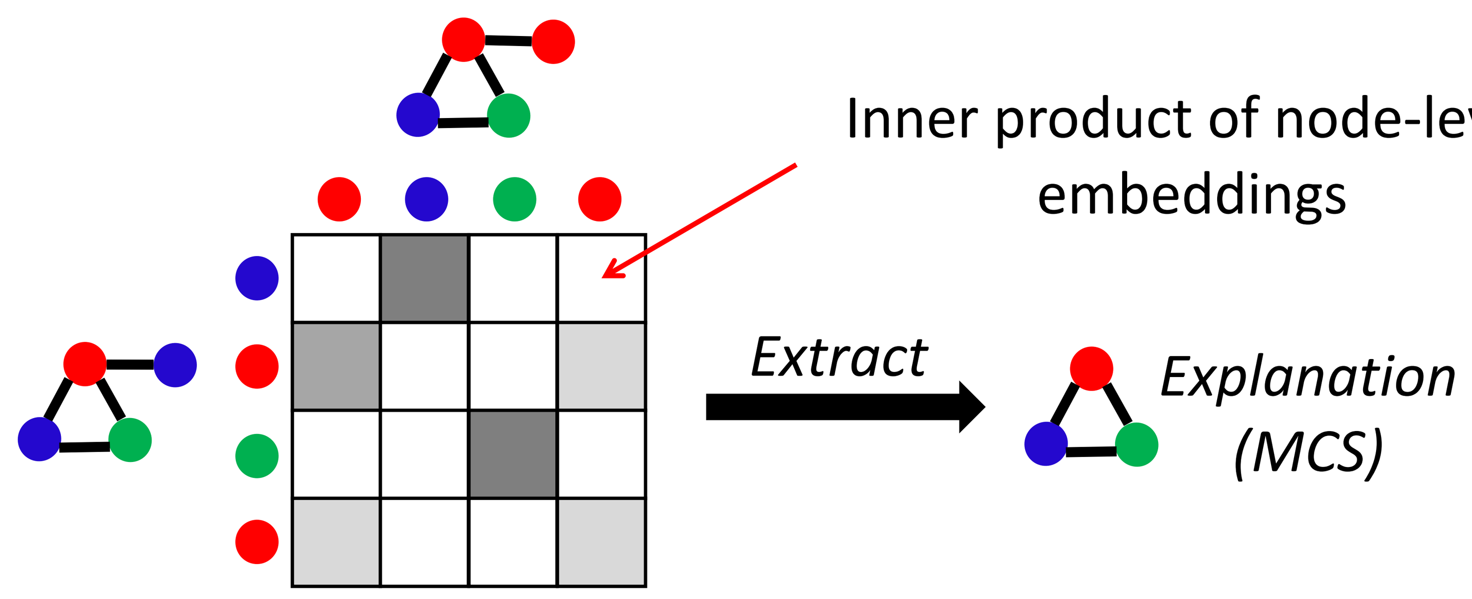

First, we **acquire graph-level embeddings** that are generated during the feed-forward process of GNN.

### Step 2: Clustering on the embedding space




Second, we fit a **Gaussian Mixture Model** to find clusters on the embedding space. The graph-level embedding vectors closest to each centroid is then **selected**.

### Step 3: Prototype discovery by calculating the MCS

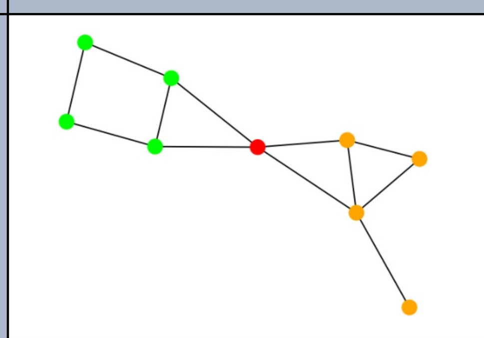
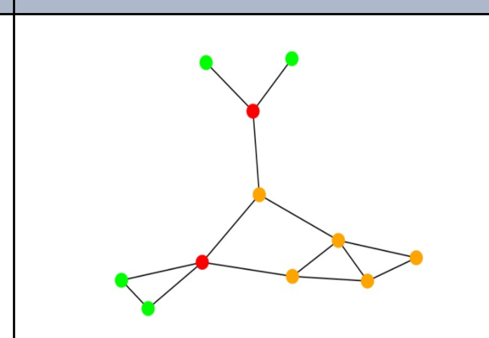
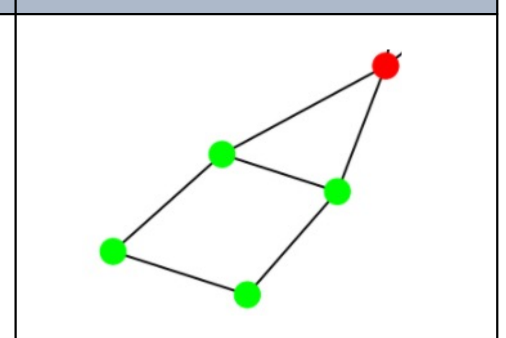
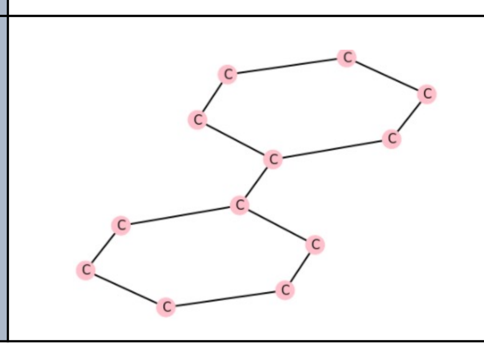
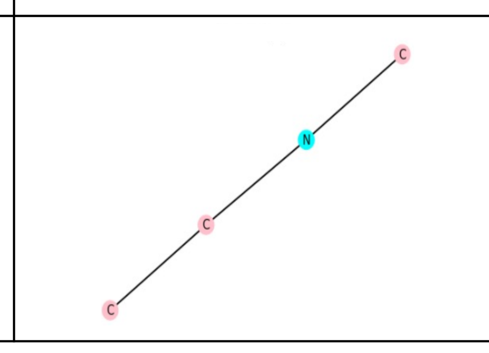
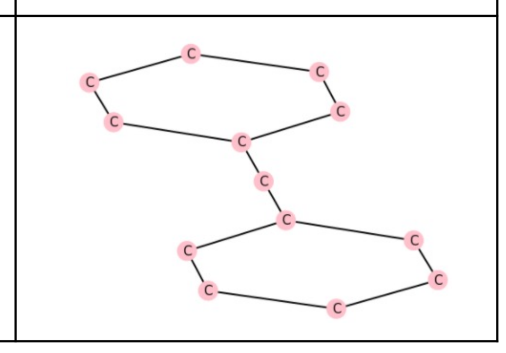



As the final step, we extract the **maximum common subgraph (MCS)** from the selected input graphs to acquire the **most important subgraph pattern** based on NeuralMCS [2].

## Experimental evaluation

We employ GCN [3] as the benchmark GNN model for our experiments.

### Qualitative evaluation

| | PAGE (Ours) | XGNN [4] | Ground-truth explanation |
|---|---|---|---|
| BA-house |  |  |  |
| Solubility |  |  |  |

### Quantitative evaluation

| | Consistency | | Faithfulness | |
|---|---|---|---|---|
| Dataset | **PAGE (Ours)** | XGNN [4] | **PAGE (Ours)** | XGNN [4] |
| BA-house | 0.048 | 0.312 | 0.733 | 0.328 |
| Solubility | 0.109 | 0.348 | 0.591 | 0.085 |

- **Consistency** measures the robustness of explanations across different GNN hyperparameters (the lower the better).
- **Faithfulness** measures the Kendall's tau coefficient between the performance of the GNN model and its explanation accuracy (the higher the better).

## Discussion & Conclusion

- In our work, we propose PAGE, a novel **model-level explanation of a GNN model** that performs graph classification.
- In contrast to XGNN, which relies on reinforcement learning that requires carefully designed reward functions along with domain knowledge, our method **discovers explanations within the dataset**.

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## Reference

[1] Wojciech Samek and Klaus-Robert Muller. Towards explainable artificial intelligence. In ¨ Explainable AI: Interpreting, Explaining and Visualizing Deep Learning, pages 5–22. Springer, Cham, Switzerland, 2019. doi: 10.1007/978-3-030-28954-6\ 1.
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