DOTGREEDX: EXPLAINING GNNS APPLIED TO CHEMOINFORMATICS

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1. Background and motivation

Context: development of GNNs in various chemoinformatics applications

- Molecular property prediction
- Drug design
- Biological activity prediction

Problem: GNNs often operate as black boxes, making their decision-making process difficult to understand

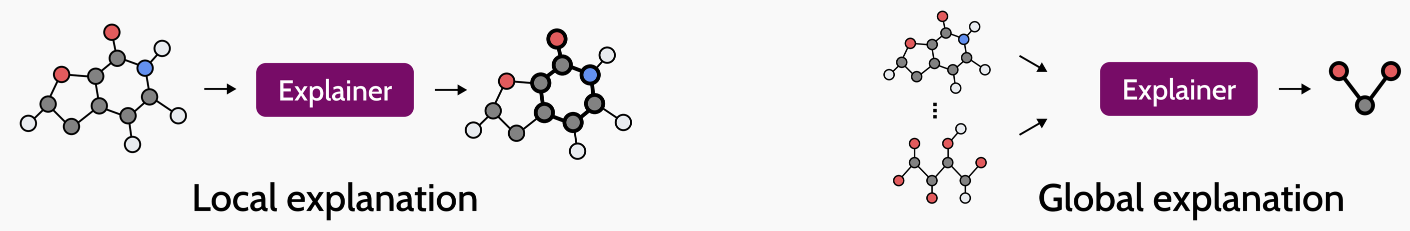
Why this prediction? **How** was it made? Can we **trust** it?

Solution: development of XAI techniques for GNN explainability

- Transparency & Reliability
- Error detection & Improvement
- Decision Support & Pattern Discovery

2. Taxonomy of GNN Explanations[1]

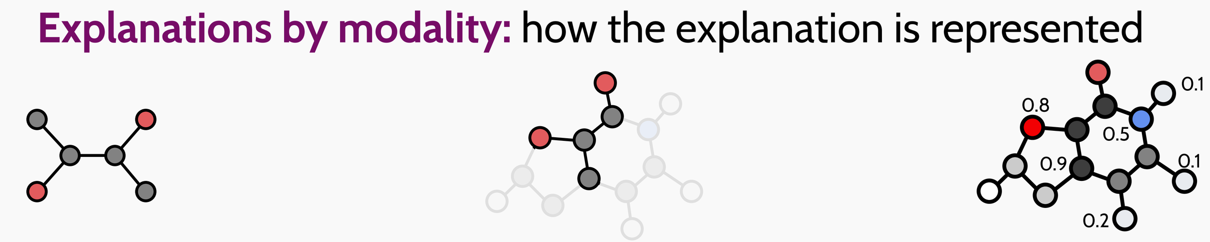
Explanations by level: the scope of the graph information



Local explanation

Global explanation

Explanations by modality: how the explanation is represented



Generation — Extraction — Scoring

Disadvantages of existing methods

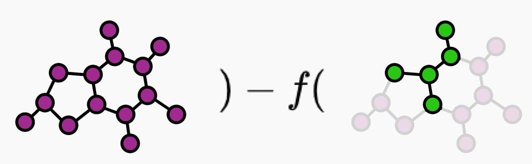
- Fidex-size explanation and need for hyperparameters
- Usually unclear how to identity important elements
- May not reflect a rankable importance score

→ DotGreedX

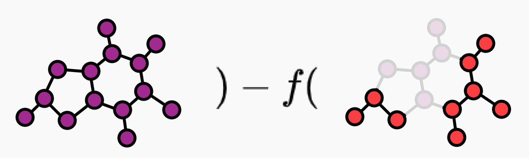
3. DotGreedX : combining scoring-based method and greedy search algorithm

Evaluation metrics[2]

$Fidelity^{-} = f(\;) - f(\;)$

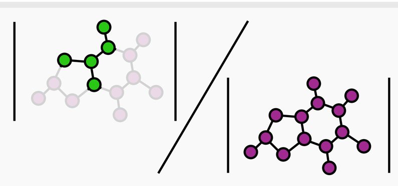


$Fidelity^{+} = f(\;) - f(\;)$



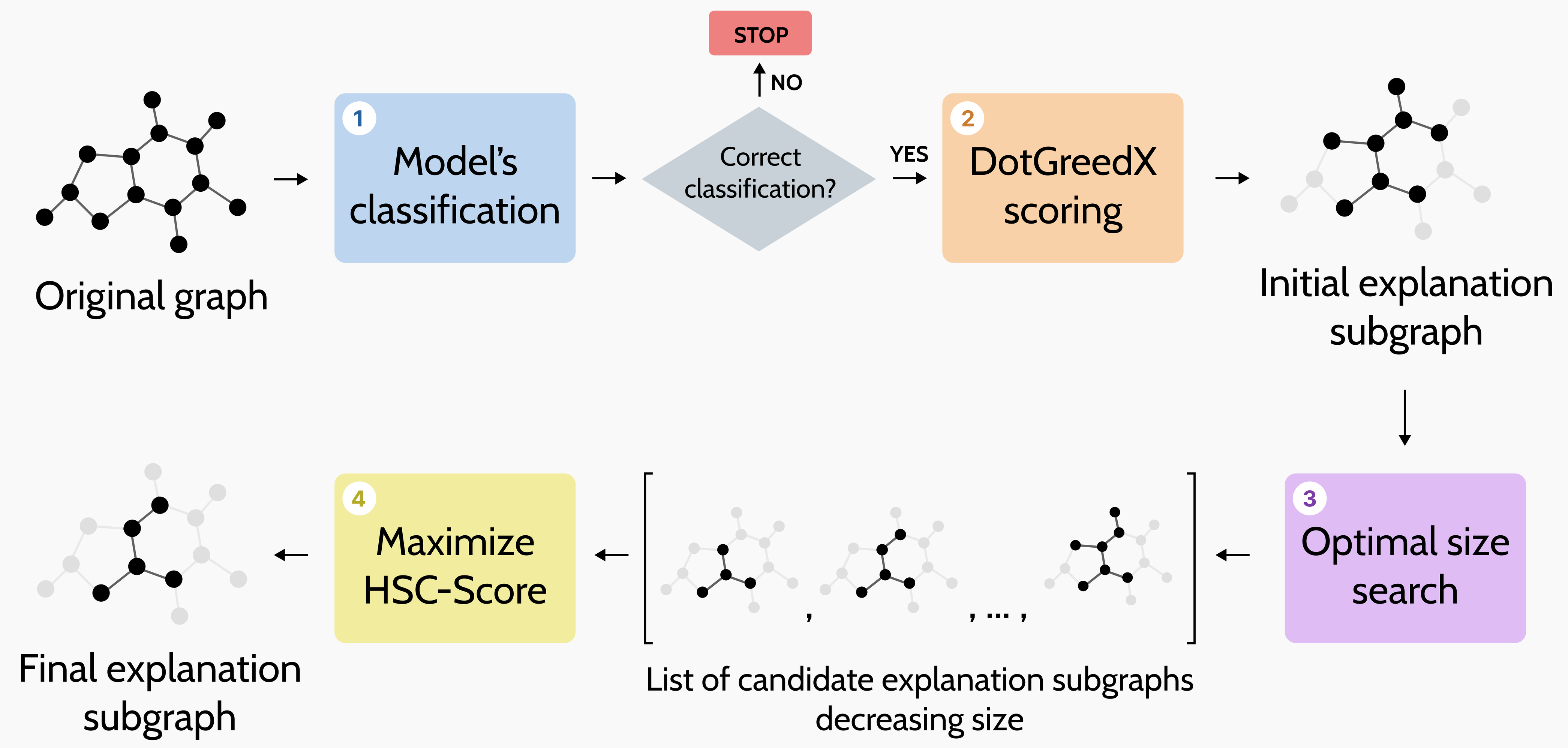
$$Characterization_{score} = \frac{2 \cdot Fidelity^{+} \cdot (1 - Fidelity^{-})}{Fidelity^{+} + (1 - Fidelity^{-})}$$

$Sparsity = 1 - | \; | / | \; |$



$$HSC_{score} = \frac{2 \cdot Characterization_{score} \cdot Sparsity}{Characterization_{score} + Sparsity}$$

Methodology[3]



4. Experimental results

Dataset	Explainer	Exp_{acc}	$Charac_{score}$	$Sparsity$	HSC_{score}	$Time(s)$
Mutagenicity	SA	0.517±0.171	0.570±0.073	0.573±0.025	0.569±0.039	0.65±0.06
	IG	0.379±0.196	0.528±0.102	0.605±0.048	0.559±0.067	20.55±1.16
	CAM	0.555±0.162	0.614±0.076	0.664±0.016	0.636±0.047	**0.64±0.04**
	GNNExp.	0.481±0.296	0.529±0.143	0.490±0.039	0.498±0.071	62.35±2.25
	EiG-Search	0.863±0.141	0.712±0.037	**0.677±0.017**	0.694±0.021	10.58±0.68
	DotGreedX	**0.928±0.068**	**0.794±0.044**	0.651±0.077	**0.714±0.060**	85.28±21.60
Mutagenicity with DotGreedX	SA	**0.783±0.159**	**0.707±0.069**	**0.606±0.090**	**0.651±0.079**	-
	IG	**0.602±0.212**	**0.671±0.087**	0.535±0.085	**0.593±0.082**	-
	CAM	**0.871±0.114**	**0.771±0.061**	0.646±0.070	**0.702±0.064**	-
	GNNExp.	**0.928±0.068**	**0.733±0.062**	**0.607±0.048**	**0.663±0.046**	-
	EiG-Search	**0.999±0.002**	**0.785±0.049**	0.632±0.041	**0.699±0.032**	-

5. Perspectives

- Optimizing the runtime of the greedy search algorithm
- Extending DotGreedX to other tasks
  - Node classification
  - Multi-class classification
  - Regression tasks
- Extending DotGreedX to other types of graphs

GNN Global Explanations

- A coherent vision of the model's behavior
- Improved results analysis
- Pattern recognition and definition of general rules

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