Global Counterfactual Explainer for Graph Neural Networks

WSDM’23

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Explainability in Deep Learning

Explainability in Deep Learning

- **Why Explainability Should Be The Core Of Your AI Application**

  Vikas Gupta Forbes Councils Member Jan 23, 2023, 08:30am EST

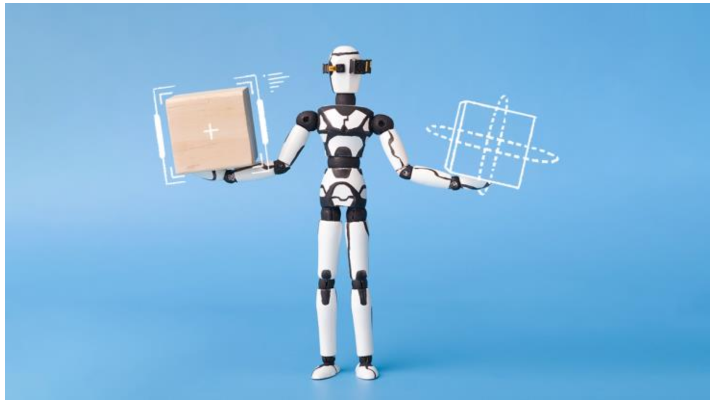
  "When something goes wrong, what do you tell your customer?"

- **Tools such as ChatGPT threaten transparent science** *Nature* **613**, 612 (2023) | 24 January 2023

  "Some scientists were already using chatbots as research assistant…"

- **Chatbots are creating thorny ethical questions about transparency in mental health care**  By Mohana Ravindranath Jan. 23, 2023 STAT

GETTY



HBR Staff/Milkos/Getty Images

AI Decisions and Explanations

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- AI Decision System

{Credit Score: Medium, Stable Job Year: 2, Debts: Medium} → Denied

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  - Feature importance [1, 2]

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  - Global counterfactual [5]

  if Credit Score = Medium and Stable Job Year = 2, then Debts <= Low → Approved

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Graph Explanations

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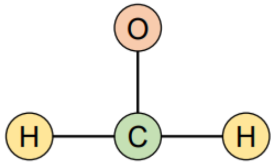
- GNN decisions



Formaldehyde

Mutagen

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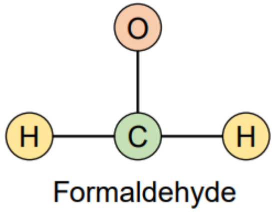

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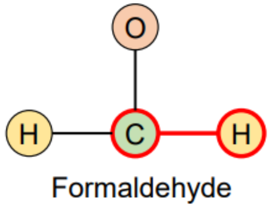
  - Subgraph importance [6, 7]



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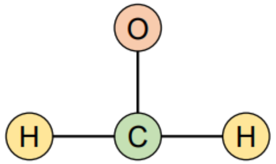

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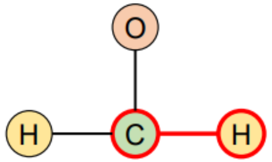

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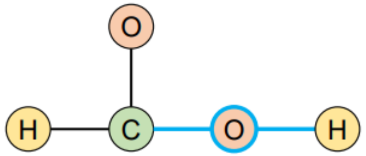
- Local counterfactual [8, 9, 10]



Formic acid

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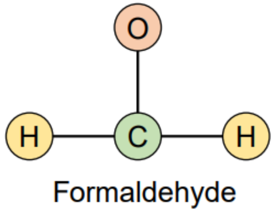

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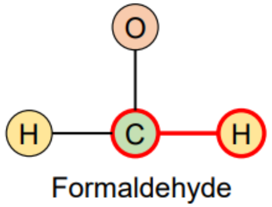

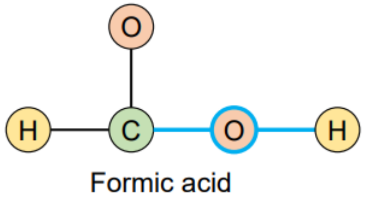

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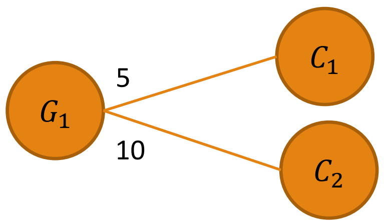

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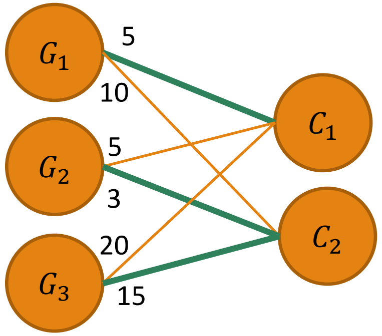

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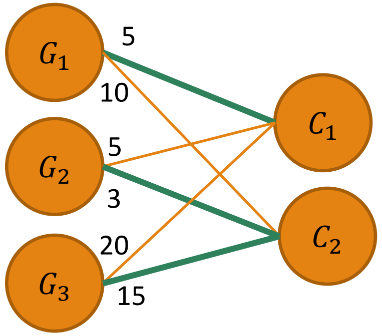

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- Coverage: maximize the number of undesired graphs having counterfactual within distance θ.

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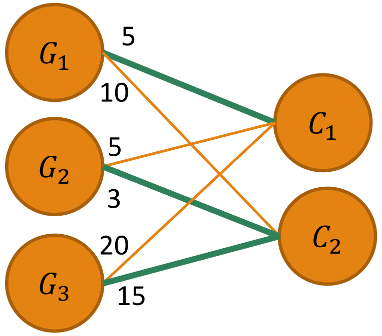

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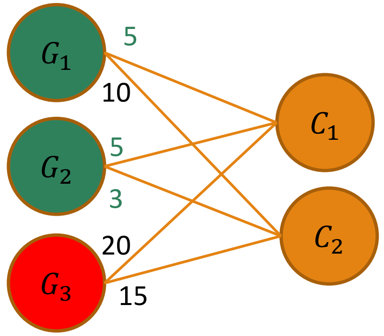

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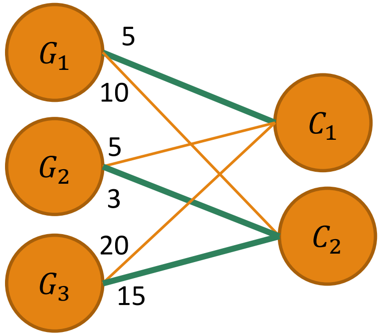

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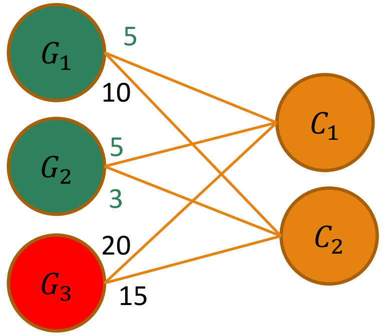

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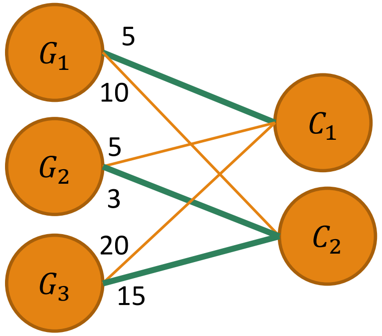

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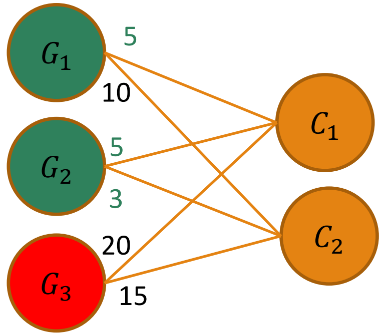

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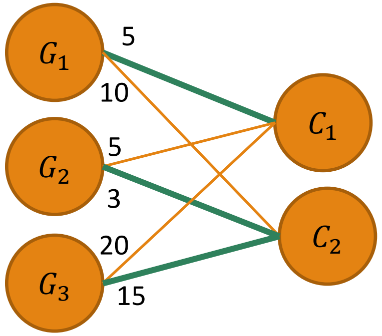

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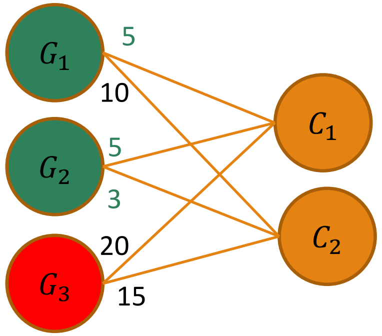

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  - NP-hard problem (reduction from Maximum Coverage problem)

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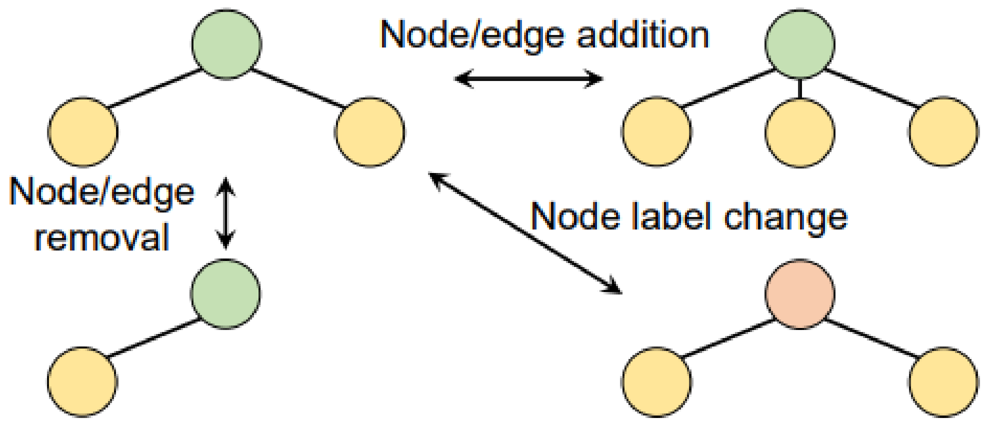

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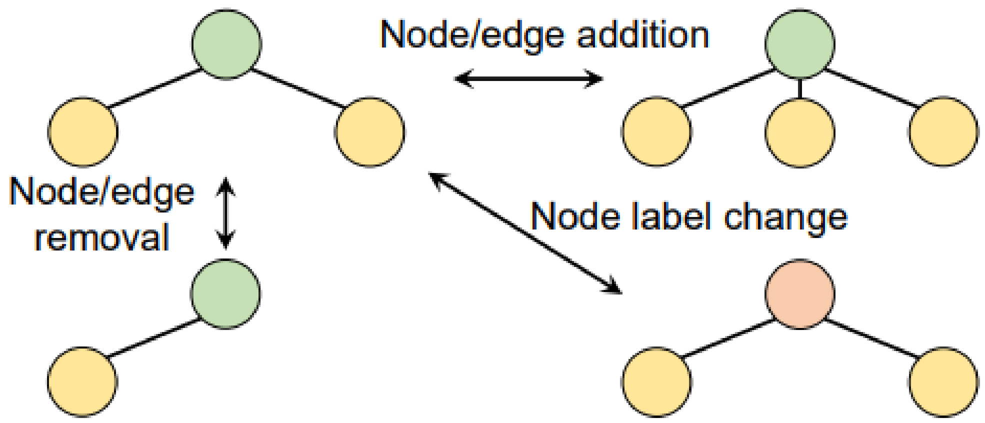

  - Vertex-reinforced random-walk [11]: $Prob(G \rightarrow G') \sim N(G')I(G')$.
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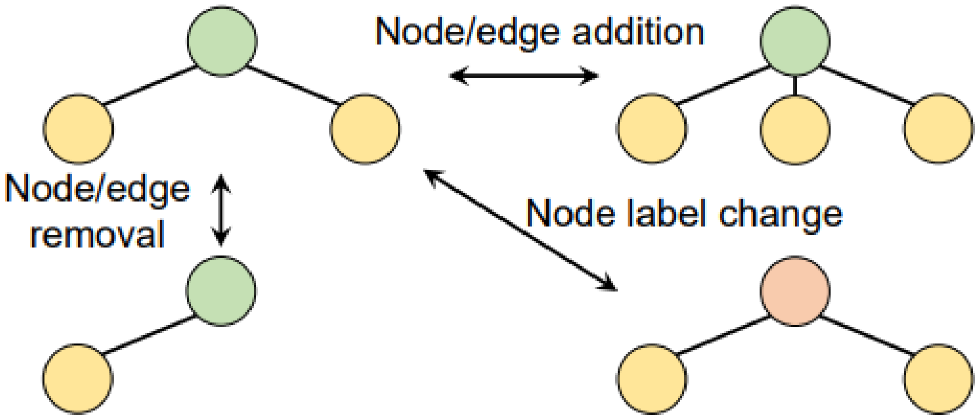

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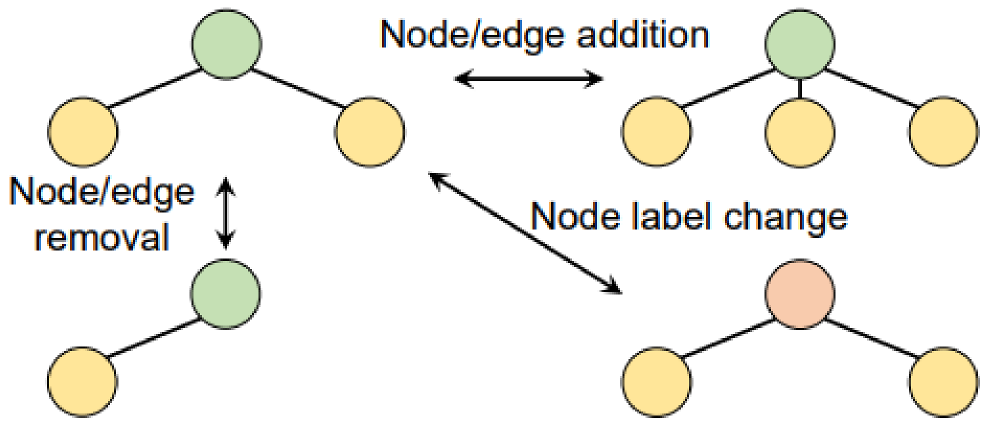

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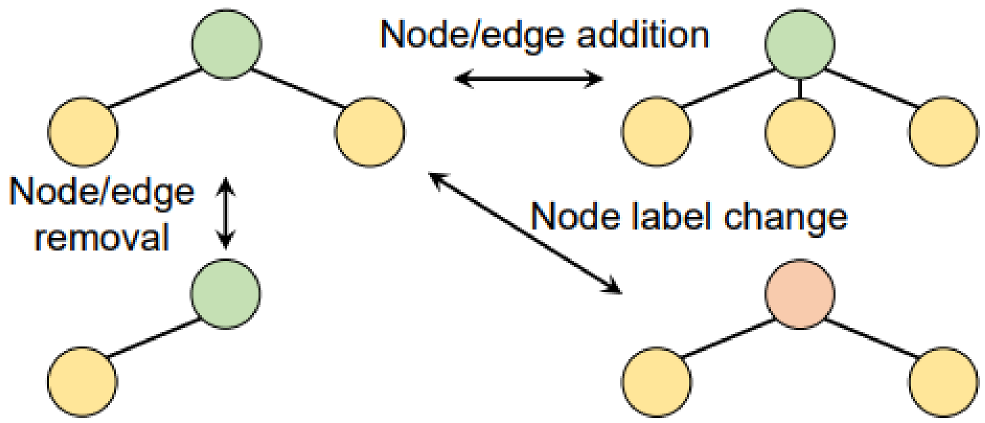

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$\mathbf{GNN}(G')$, $\mathbf{coverage}$, $\mathbf{gain}$

- Greedy summary
  - After finding $\mathbf{S}$, we apply greedy summary based on $\max \mathbf{gain}(C)$ where $C \in \mathbf{S}$ with k iterations.

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Experiments

- GCFExplainer consistently outperforms the baselines with 9.5% reduction in recourse cost, 46.9% gain in recourse coverage, for top 10 counterfactuals.

	NCI1		Mutagenicity		AIDS		Proteins	
	Coverage	Cost	Coverage	Cost	Coverage	Cost	Coverage	Cost
Ground-Truth	16.54%	0.1326	28.96%	0.1275	0.41%	0.2012	8.47%	0.2155
RCExplainer	15.22%	0.1370	31.99%	0.1290	8.96%	0.1531	8.74%	0.2283
CFF	17.61%	0.1331	30.43%	0.1327	3.39%	0.1669	3.83%	0.2557
GCFExplainer	**27.85%**	**0.1281**	**37.08%**	**0.1135**	**14.66%**	**0.1516**	**10.93%**	**0.1856**

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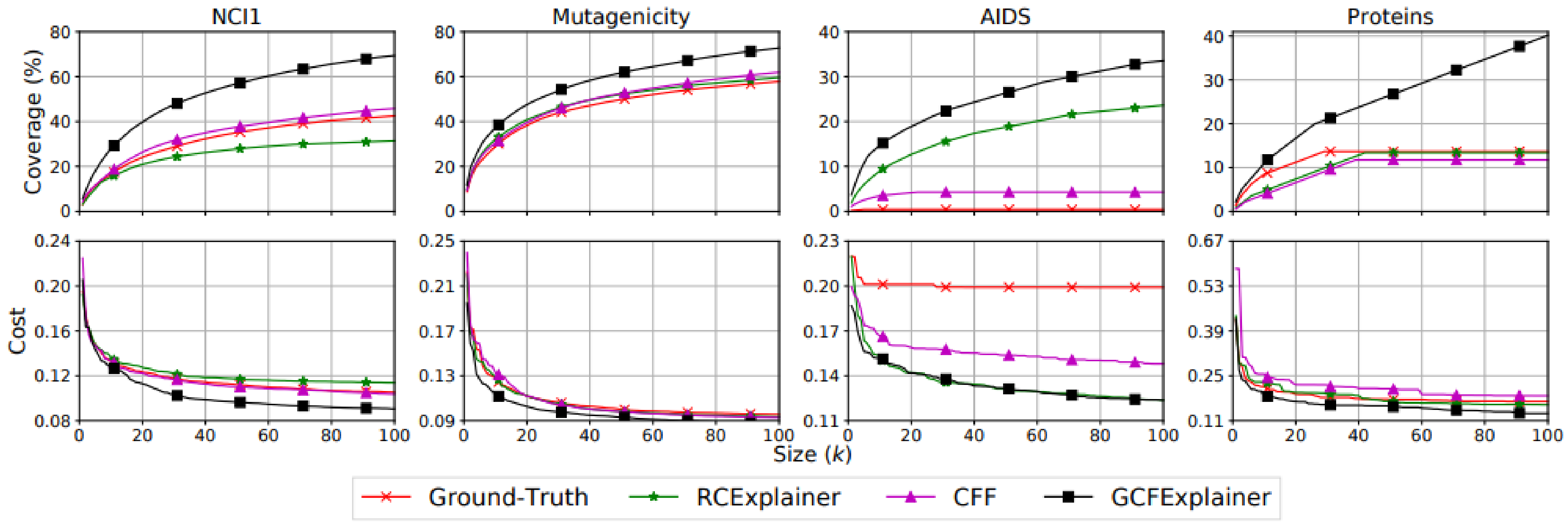
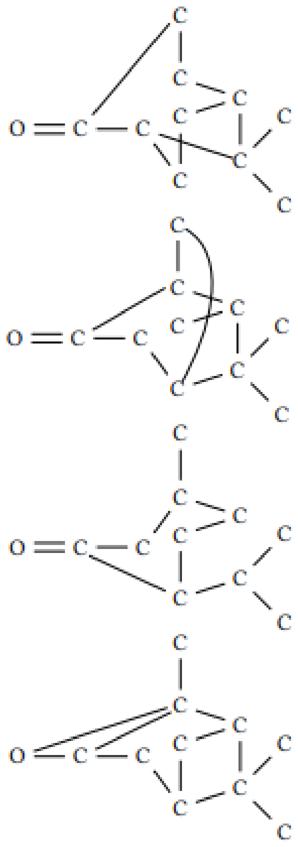
RCExplainer	15.22%	0.1370	31.99%	0.1290	8.96%	0.1531	8.74%	0.2283
CFF	17.61%	0.1331	30.43%	0.1327	3.39%	0.1669	3.83%	0.2557
GCFExplainer	**27.85%**	**0.1281**	**37.08%**	**0.1135**	**14.66%**	**0.1516**	**10.93%**	**0.1856**



Case Study

Case Study

- AIDS dataset [14]



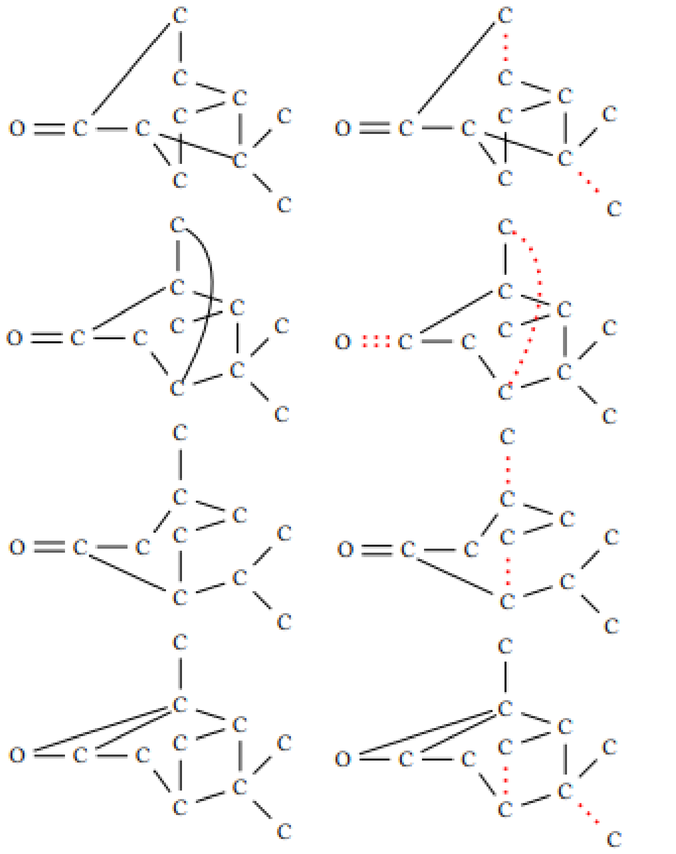
(a) Input graphs

[14] Kaspar Riesen and Horst Bunke. 2008. IAM graph database repository for graph based pattern recognition and machine learning. In Joint IAPR International Workshops on Statistical Techniques in Pattern Recognition (SPR) and Structural and Syntactic Pattern Recognition (SSPR).

Case Study

- AIDS dataset [14]

- Local counterfactuals
  - Hard to generalize



(a) Input graphs (b) Local counterfactuals

[14] Kaspar Riesen and Horst Bunke. 2008. IAM graph database repository for graph based pattern recognition and machine learning. In Joint IAPR International Workshops on Statistical Techniques in Pattern Recognition (SPR) and Structural and Syntactic Pattern Recognition (SSPR).

Case Study

- AIDS dataset [14]
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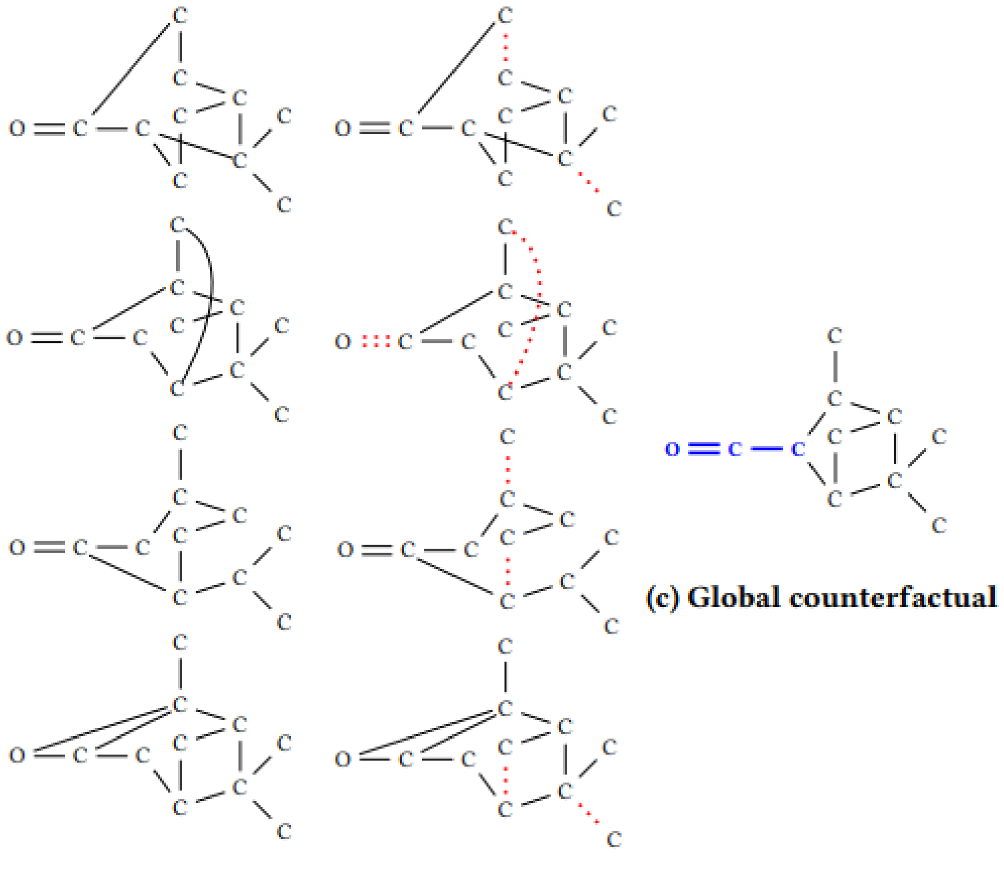
- Global counterfactual
  - High-level recourse rule

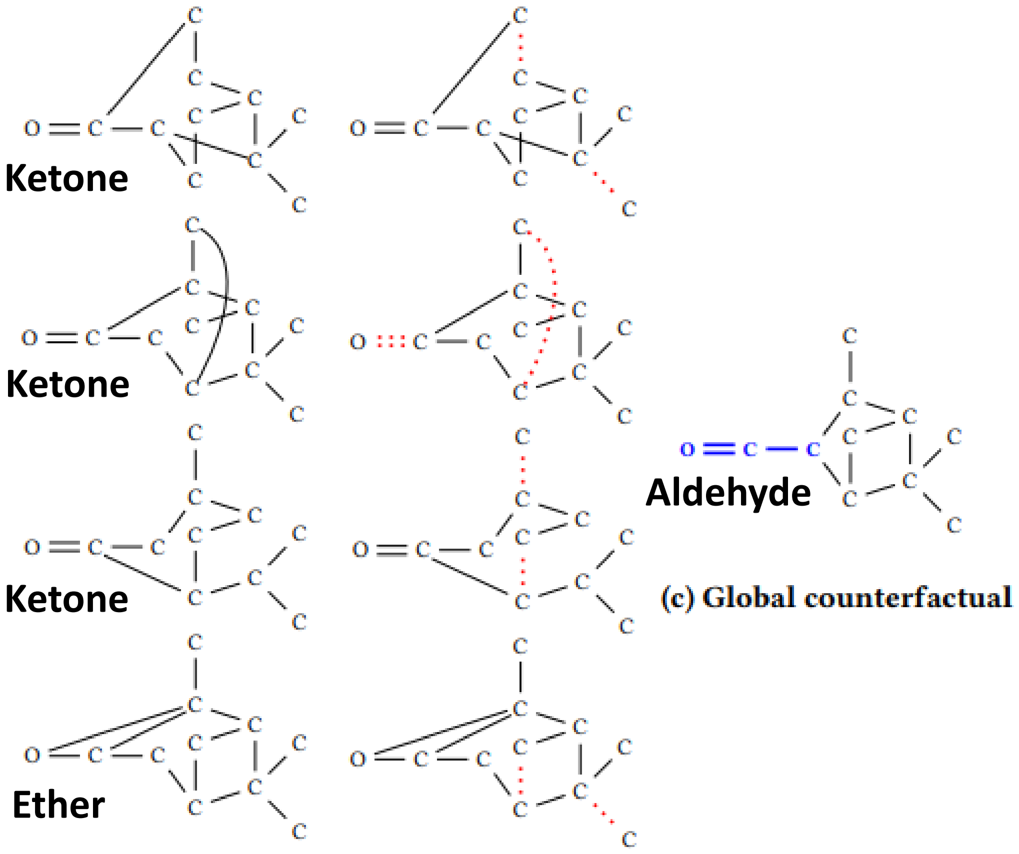


(a) Input graphs (b) Local counterfactuals (c) Global counterfactual

[14] Kaspar Riesen and Horst Bunke. 2008. IAM graph database repository for graph based pattern recognition and machine learning. In Joint IAPR International Workshops on Statistical Techniques in Pattern Recognition (SPR) and Structural and Syntactic Pattern Recognition (SSPR).

Case Study

- AIDS dataset [14]
- Local counterfactuals
  - Hard to generalize
- Global counterfactual
  - High-level recourse rule
  - Ketones and Ethers to Aldehydes

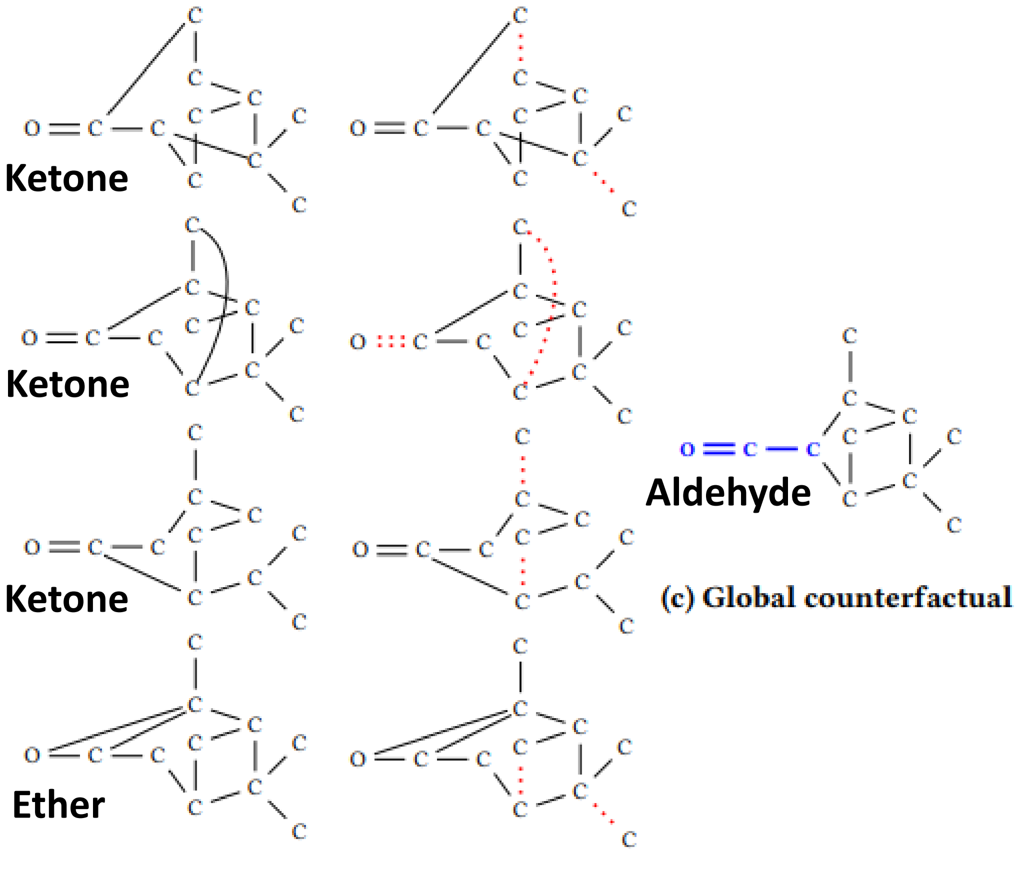


(a) Input graphs (b) Local counterfactuals (c) Global counterfactual

[14] Kaspar Riesen and Horst Bunke. 2008. IAM graph database repository for graph based pattern recognition and machine learning. In Joint IAPR International Workshops on Statistical Techniques in Pattern Recognition (SPR) and Structural and Syntactic Pattern Recognition (SSPR).

Case Study

- AIDS dataset [14]
- Local counterfactuals
  - Hard to generalize
- Global counterfactual
  - High-level recourse rule
  - Ketones and Ethers to Aldehydes
    - Combatting HIV [15]



(a) Input graphs (b) Local counterfactuals (c) Global counterfactual

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Global Counterfactual Explainer

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Global Counterfactual Explainer

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  - We formulate the novel problem of global counterfactual reasoning/explanation of GNNs for graph classification.
  - While the problem is NP-hard, we present the first global counterfactual explainer generating diverse and representative counterfactual candidates.
  - We demonstrate the effectiveness and usefulness of GCFExplainer in experiments.

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Global Counterfactual Explainer for Graph Neural Networks

WSDM'23

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