

Graphs' Counterfactual Explainability Landscape: current state and frontiers

giovanni stilo

(mario prado-romero, bardh prenkaj)

giovanni.stilo@univaq.it



Part One

Background

Explainability and its importance

- Explainability is **crucial** in **sensitive** domains
 - It helps users and service providers make informed and reliable decisions [1]
- DNNs suffer from the **black-box** problem [2]
 - Can **not** be **used** in **finance** nor **healthcare** domains (critical domains)
 - White-boxes are preferred for decision-making purposes [3]
- Black-boxes are **more performant** than white-boxes [4-7]

[1] Guidotti, R., Monreale, A., Ruggieri, S., Turini, F., Giannotti, F., Pedreschi, D.: A survey of methods for explaining black box models. ACM computing surveys (CSUR) 51(5), 1–42 (2018)

[2] Petch, J., Di, S., Nelson, W.: Opening the black box: the promise and limitations of explainable machine learning in cardiology. Canadian Journal of Cardiology (2021)

[3] Verenich, I., Dumas, M., La Rosa, M., Nguyen, H.: Predicting process performance: A white-box approach based on process models. Journal of Software: Evolution and Process 31(6), e2170 (2019)

[4] Aragona, D., Podo, L., Prenkaj, B., Velardi, P.: Corona: a deep sequential framework to predict epidemic spread. In: Proceedings of the 36th Annual ACM Symposium on Applied Computing. pp. 10–17 (2021)

[5] Feng, W., Tang, J., Liu, T.X.: Understanding dropouts in moocs. In: Proceedings of the AAAI Conference on Artificial Intelligence. vol. 33, pp. 517–524 (2019)

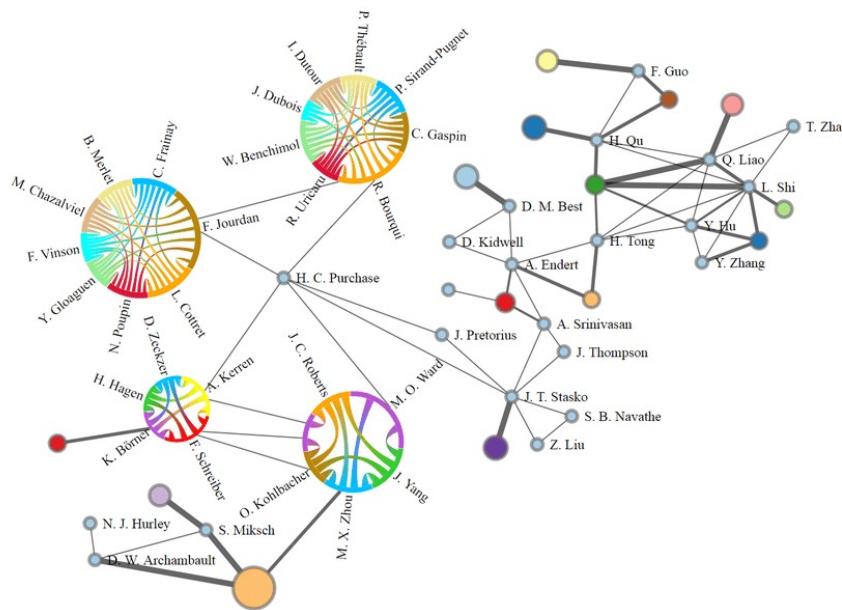
[6] Verma, H., Mandal, S., Gupta, A.: Temporal deep learning architecture for prediction of covid-19 cases in india. Expert Systems with Applications 195, 116611 (2022)

[7] Prenkaj, B., Distante, D., Faralli, S., Velardi, P.: Hidden space deep sequential risk prediction on student trajectories. Future Generation Computer Systems 125, 532–543 (2021)

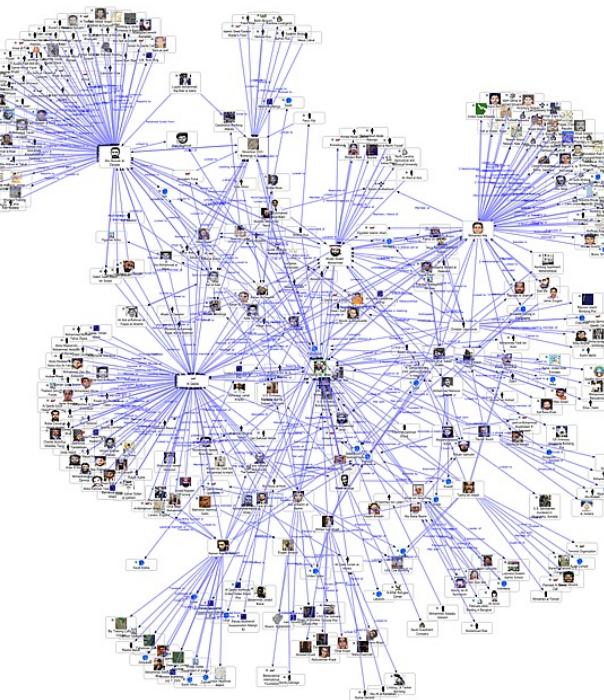
What's a graph?

A **graph** $G = (V, E)$ consists of:

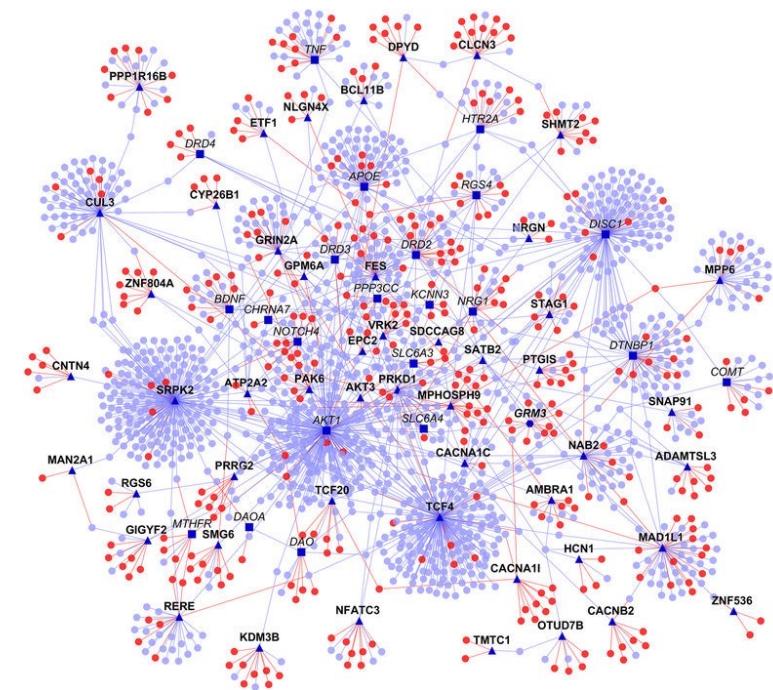
a **nodes set** $V = \{v_1, \dots, v_n\}$ and an **edges set** $E = \{(v_i, v_j) | v_i, v_j \in V\}$



DBLP co-authorship



Social network



Schizophrenia PPI

Challenges

There are **three main challenges** associated with processing graphs:

1. their **topology is variable**:

Thus it is hard to design a Neural Network that both **sufficiently expressive** and can cope with this **variation**;

2. graphs may be **enormous**:

a graph representing connections between users of a social network might have a **millions nodes** and **billion of edges**;

3. there may only be a **single monolithic graph** available:

so the **usual protocol** of training with many data examples and testing with new data is **not always appropriate or possible**.

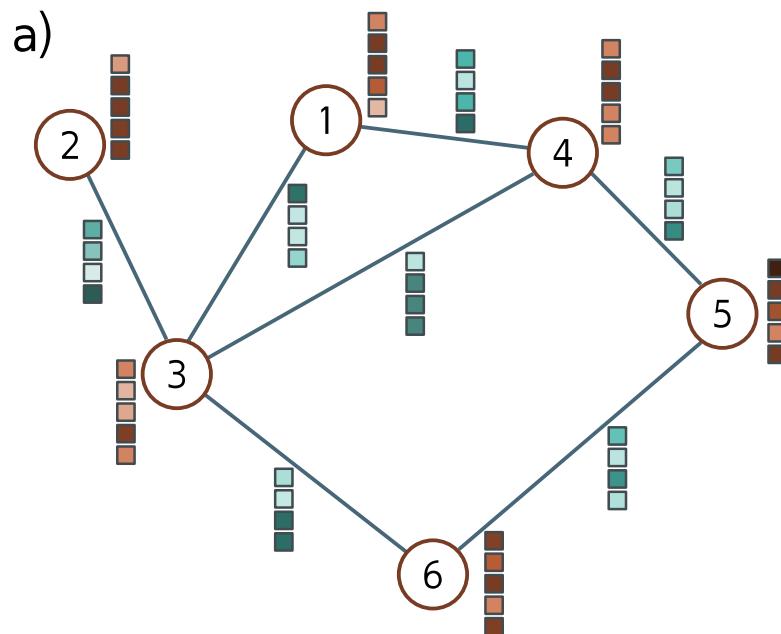
Graph Representation (learning)

More formally, a graph consists of **a set of N nodes** connected by **a set of E edges**.

The graph can be **encoded** by **three matrices**:

- **adjacency matrix**, A is an $N \times N$ matrix where entry (m, n) is set to one if there is an edge between nodes m and n and zero otherwise (symmetric for undirected graphs).
- **nodes embeddings** X is an $D \times N$ matrix where n^{th} node has an associated node embedding X^n of length D .
- **edges embeddings** E is an $D_E \times N$ matrix where e^{th} edge has an associated edge embedding E^e of length D_E .

We want to learn a (dense) representation H of the Graph usable
for different downstream tasks



b)

Adjacency
matrix, A
 $N \times N$

	1	2	3	4	5	6
1	0	1	1	1	1	0
2	1	0	1	1	1	0
3	1	1	0	1	1	0
4	1	1	1	0	1	0
5	1	1	1	1	0	0
6	0	0	0	0	0	0

c)

Node
data, X
 $D \times N$

	1	2	3	4	5	6
1	brown	light brown	brown	dark brown	brown	dark brown
2	light brown	brown	dark brown	brown	dark brown	brown
3	brown	light brown	brown	dark brown	brown	dark brown
4	dark brown	brown	light brown	brown	dark brown	brown
5	brown	dark brown	brown	light brown	brown	dark brown
6	dark brown	brown	light brown	brown	dark brown	brown

d)

Edge
data, E
 $D_E \times E$

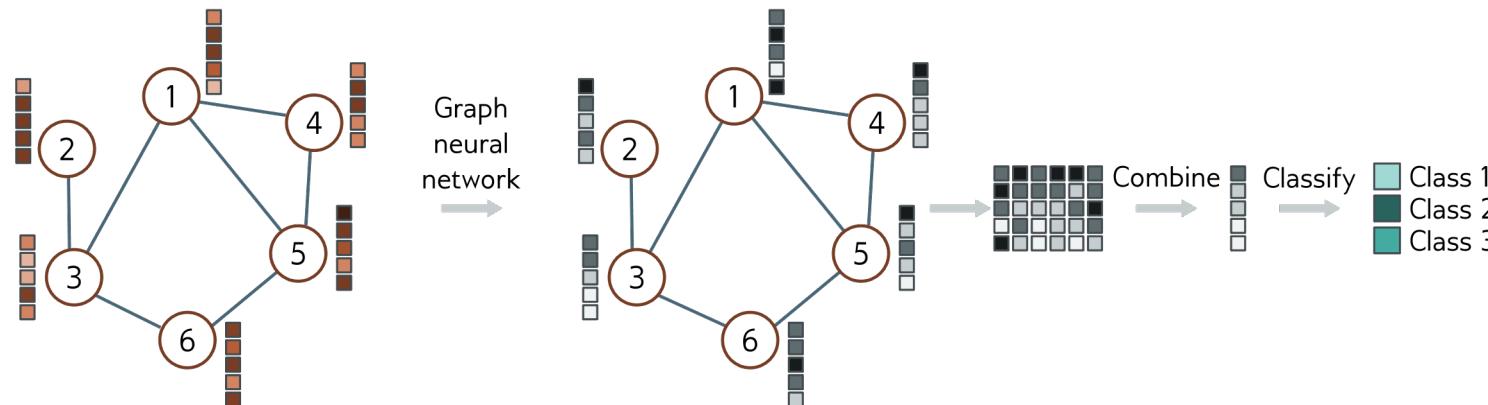
	1	2	3	4	5	6
1	dark teal	teal	light teal	teal	dark teal	teal
2	teal	dark teal	teal	light teal	teal	dark teal
3	light teal	teal	dark teal	teal	light teal	teal
4	teal	dark teal	teal	light teal	teal	dark teal
5	dark teal	teal	light teal	teal	dark teal	teal
6	teal	dark teal	teal	light teal	teal	dark teal

Graph-level Tasks

For example, we might want to **predict**:

- the **temperature** at which a **molecule** becomes **liquid** (a regression task);
- whether a **molecule** is **poisonous** to human beings or not (a classification task).

For graph-level tasks, the output **node embeddings are combined** (e.g., by averaging), and the resulting vector is **mapped** via a linear transformation or neural network to a **fixed-size vector**.



- for regression, the mismatch is computed using the **least squares loss**.
- for **binary classification**, the output is passed through a sigmoid function, and the mismatch is calculated using the **binary cross-entropy loss**.

$$Pr(y = 1 | \mathbf{X}, \mathbf{A}) = \text{sig} \left(\beta_k + \boldsymbol{\omega}_k \mathbf{H}_k \frac{\mathbf{1}}{N} \right)$$

where the scalar β_k and $1 \times D$ vector $\boldsymbol{\omega}_k$ are **learned parameters**.

$\mathbf{H}_k \frac{1}{N}$ has the effect of summing together all the embeddings and subsequently dividing by N .

A **graph neural network** is a model that takes the node embeddings X and the adjacency matrix A as inputs and passes them through a series of K layers. The node embeddings are updated at each layer to create intermediate “hidden” representations $\mathbf{h}_{k \neq K}$ before finally computing output embeddings \mathbf{h}_K .

- At the beginning each column of the input node embeddings X just contains information about the **node itself**.
- At the end, each column of the model output \mathbf{h}_K includes information about the **node and its context within the graph**.
- Typical GNN mechanisms are:
 - (random) walk based;
 - Message passing;
 - GCN;

Graph Classification e.g.

We want a **neural network** $f[X, A, \Phi]$ that **classifies** (predicts) **molecules** as toxic.

The **adjacency matrix** $A \in \mathbb{R}^{N \times N}$ derives from the molecular structure. The columns of the **node embedding** matrix $X \in \mathbb{R}^{118 \times N}$ are **one-hot vectors** indicating which of the 118 **elements of the periodic table** are present.

Note that the input **node embeddings** can be **transformed** to an **arbitrary** size D by the **first weight matrix** $\Omega_k \in \mathbb{R}^{D \times 118}$.

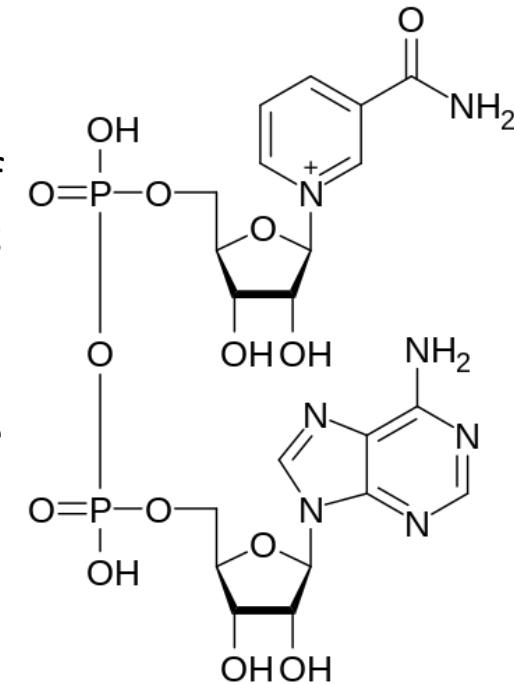
$$H_1 = a[\beta_0 \mathbf{1}^T + \Omega_0 X (A + I)]$$

$$H_2 = a[\beta_1 \mathbf{1}^T + \Omega_1 H_1 (A + I)]$$

$$\vdots = \vdots$$

$$H_k = a[\beta_{k-1} \mathbf{1}^T + \Omega_{k-1} H_{k-1} (A + I)]$$

$$f[X, A, \Phi] = \text{sig} \left[\beta_k + \omega_k H_k \frac{\mathbf{1}}{N} \right]$$



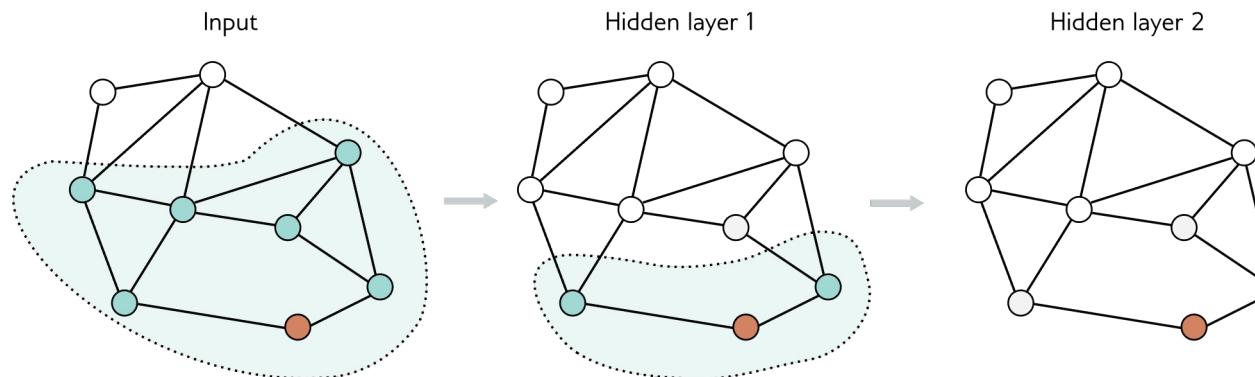
As intuition: H_k depends by $X(A + I)^k$, e.g $H_3: X(A + I)^3 = X(A^3 + 3A^2 + 3A + I^3)$

Batches and Receptive Field

One way to form a batch is to **choose a random subset** of **labeled nodes** at each training step. Each node depends on its neighbors in the previous layer and so on. Do you remember:

$$\mathbf{H}_k \text{ depends by } \mathbf{X}(\mathbf{A} + \mathbf{I})^k$$

In a GCN the size of the **receptive field** is equivalent to the *k-hop neighborhood*.

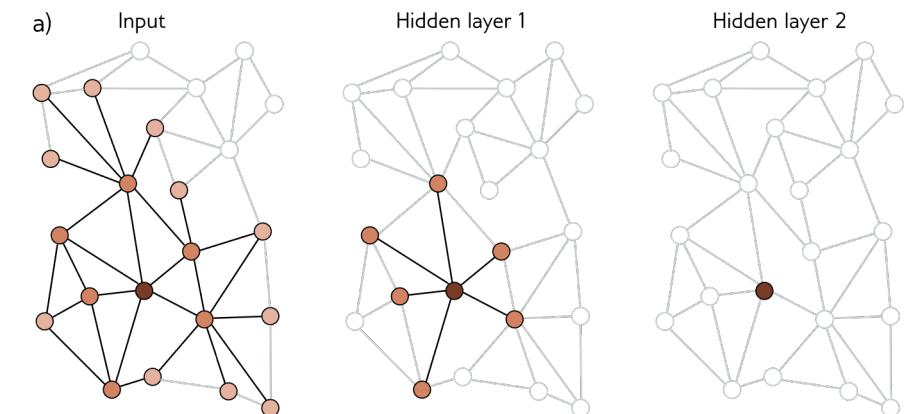


We can hence perform a gradient descent step using the **graph** that forms the **union of the k-hop neighborhoods** of the **batch nodes**; the remaining inputs do not contribute.

graph expansion problem

If there are **many layers** and the graph is **densely connected**: every input node may be in the receptive field of every output.

In general we want that $k \ll \text{diam}(G)$



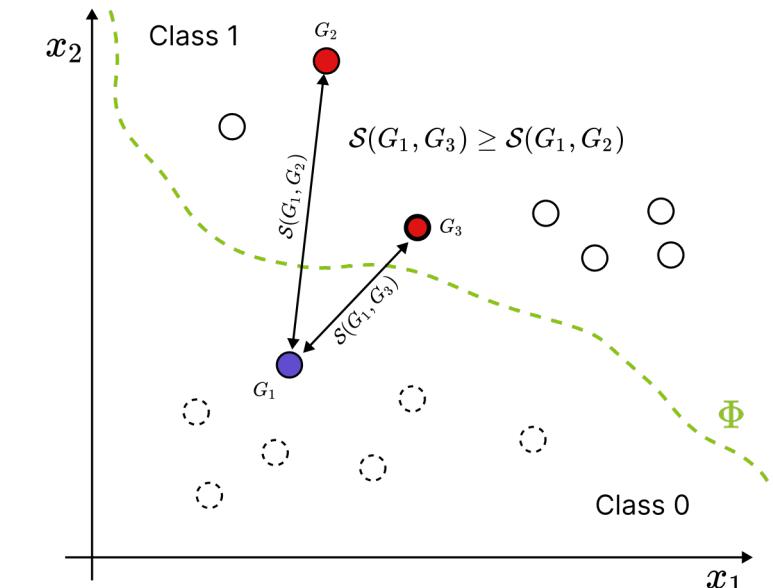
Counterfactual example

- We have a **social network** of different users
- User **U posts** an **illicit** advertisement that **violates** the **Terms of Services** (e.g., selling illegal goods online)
- A **counterfactual** explanation **of U's account suspension** would be:

*“If the user had **not violated** the **TOS**, their account would **not have been banned**.*

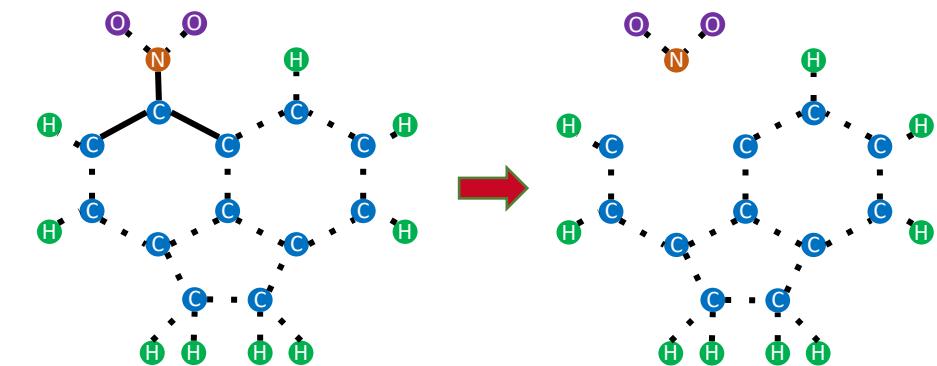
Graph Counterfactual Explainability (GCE)

- Given:
 - A **predictor** (oracle) $\Phi: \mathcal{G} \rightarrow \{0,1\}$ that we want to explain
 - A **graph** G or a set of graphs
$$\mathcal{G} = \{G_1, \dots, G_n\}$$
 - A **similarity function** $\mathcal{S}: \mathcal{G} \times \mathcal{G} \rightarrow \mathbb{R}$

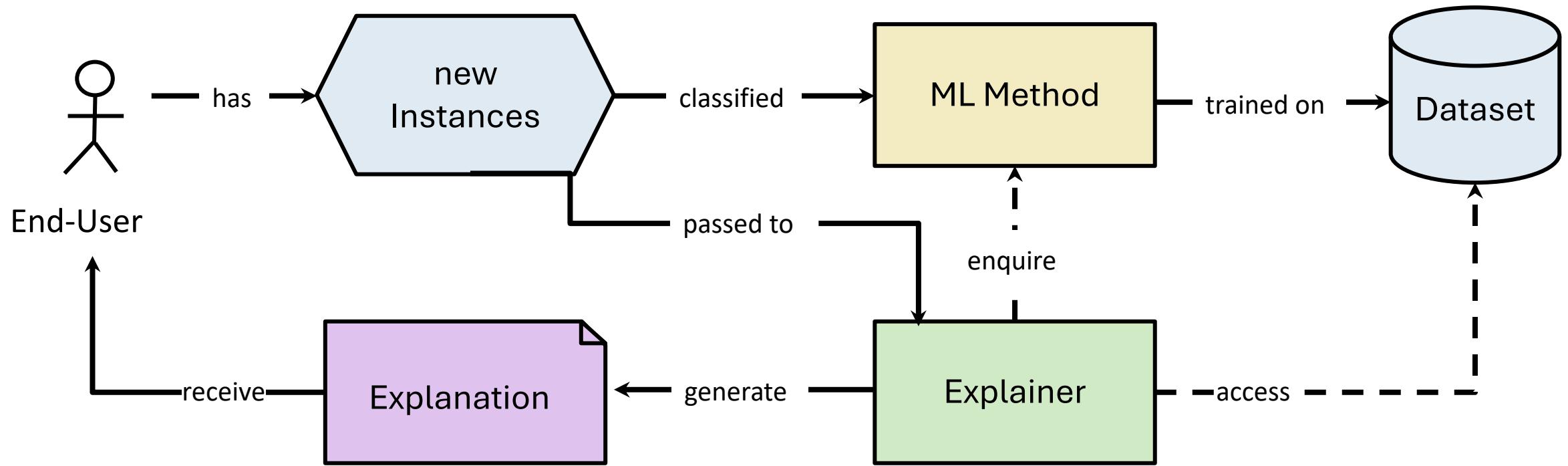


- We want to find a **counterfactual** G'

such that $\mathcal{E}_\Phi(G) = \arg \max_{G' \in \mathcal{G}, G \neq G', \Phi(G) \neq \Phi(G')} \mathcal{S}(G, G')$



Typical XAI Workflow



Part Two

SoTA

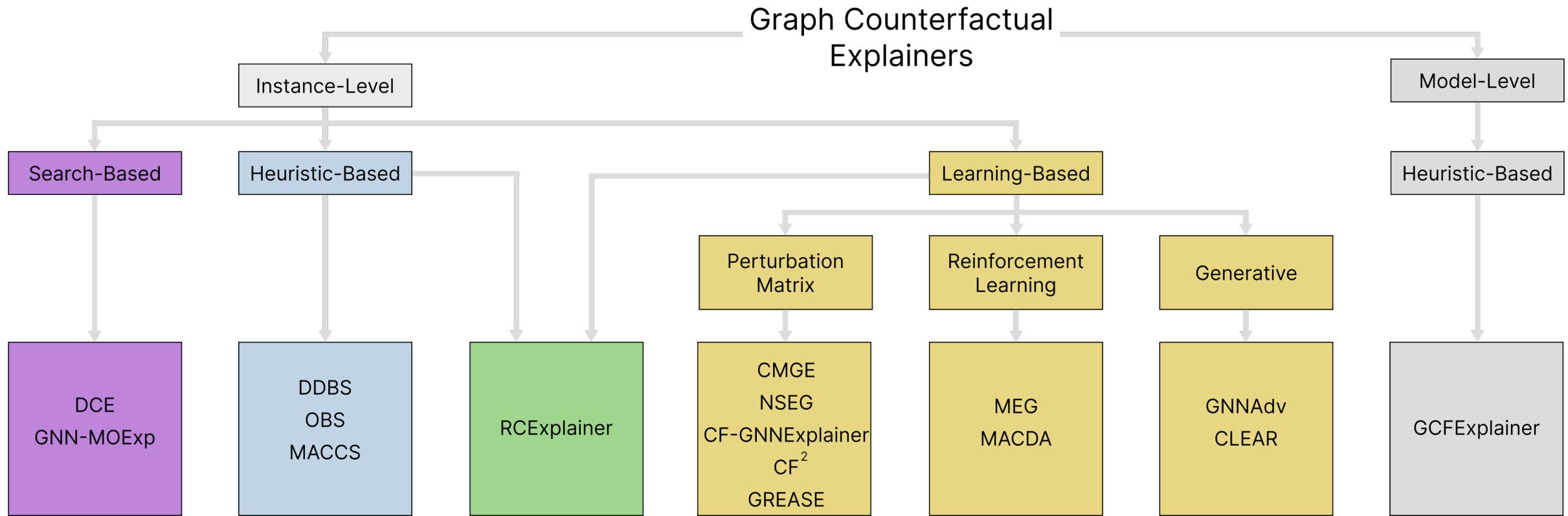
Based on

Mario Alfonso Prado-Romero, Bardh Prenkaj, Giovanni Stilo, and Fosca Giannotti. 2023.

A Survey on Graph Counterfactual Explanations: Definitions, Methods, Evaluation, and Research Challenges.

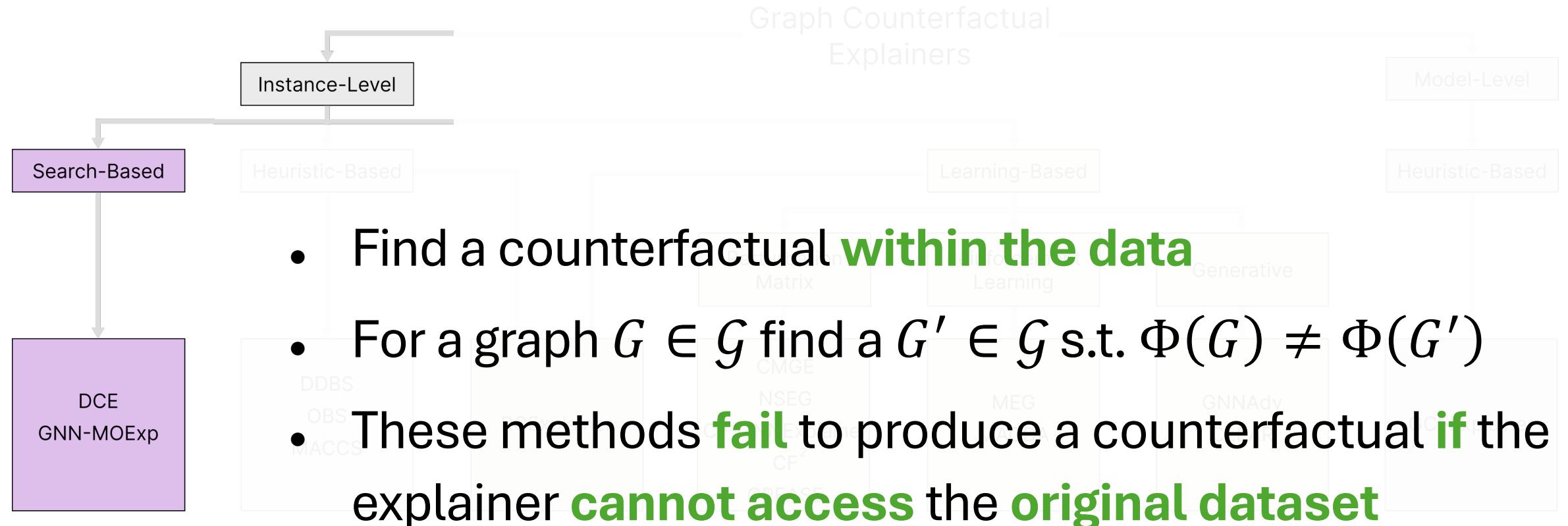
ACM Computer Survey (September 2023). <https://doi.org/10.1145/3618105>

GCE methods Taxonomy

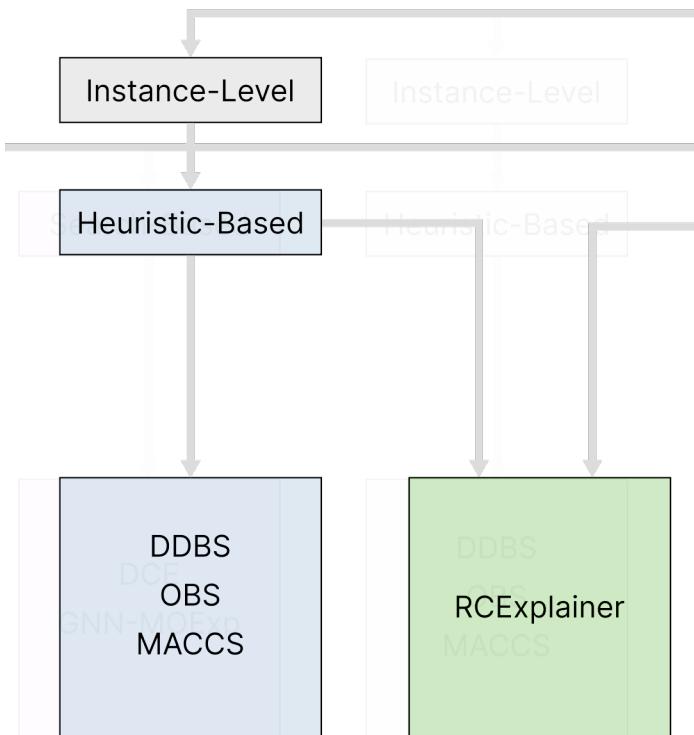


[8] Mario Alfonso Prado-Romero, Bardh Prenkaj, Giovanni Stilo, and Fosca Giannotti. 2023. A Survey on Graph Counterfactual Explanations: Definitions, Methods, Evaluation, and Research Challenges. ACM Comput. Surv. (September 2023). <https://doi.org/10.1145/3618105>

GCE Search-Based



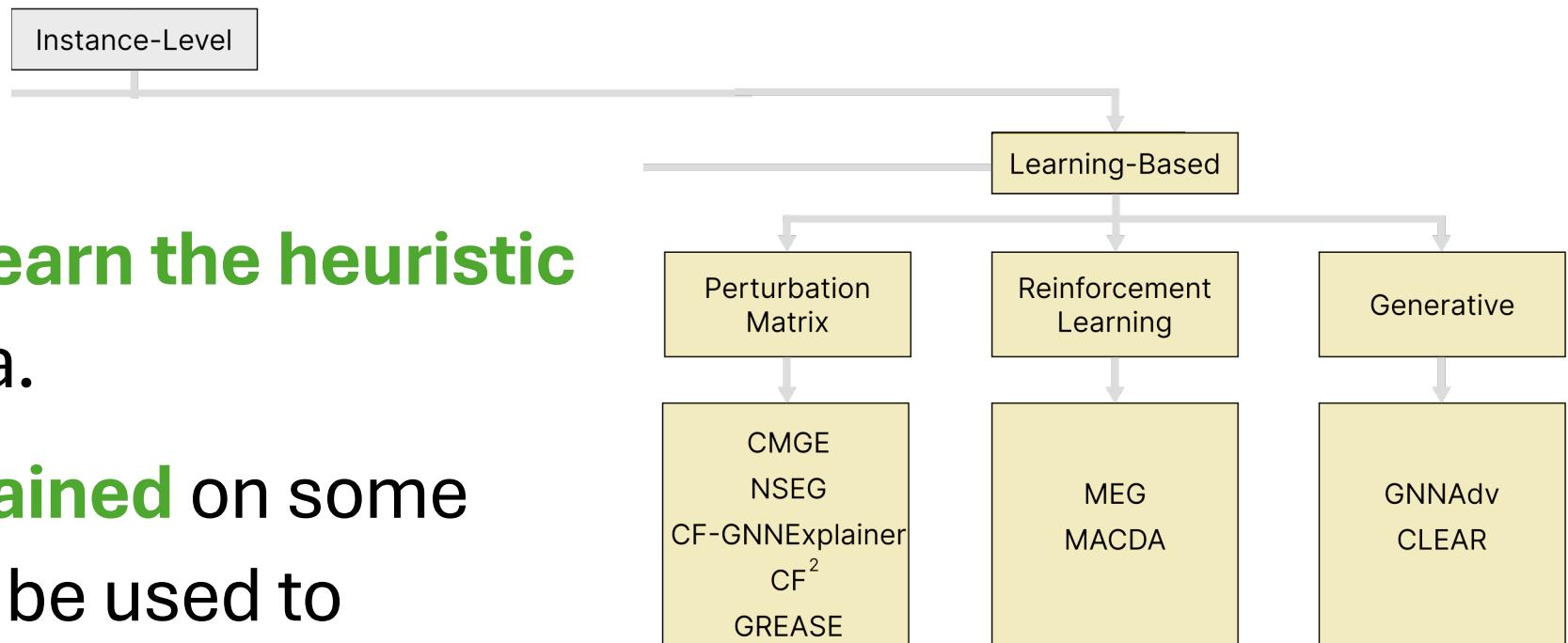
GCE Heuristic-Based



- **Perturb** the original graph such that $\Phi(G) \neq \Phi(G')$ **without** accessing the original **dataset**
- **Requires** to define the perturbation **rules** after a **careful examination** of the **data**

GCE Learning-Based

- Learning-based **learn the heuristic** based on the data.
- **Explainers** are **trained** on some samples and can be used to **produce counterfactuals** at inference



Comparison between GCE Methods

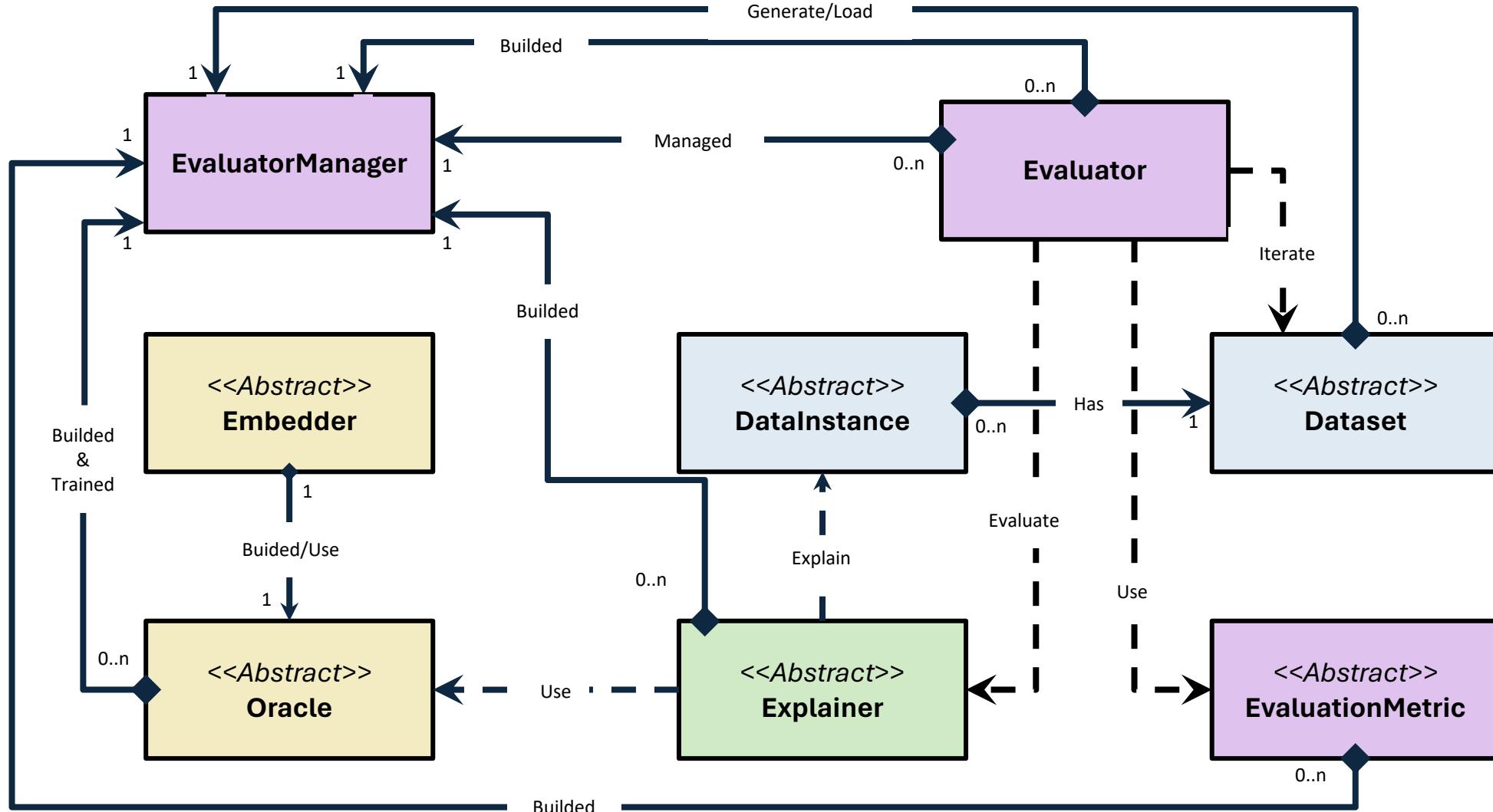
Method	Model Agnosticism	Model Access	Factual-Based Explanations	Minimal CE	Domain Agnosticism	Training Data Accessibility	Explanation Level	Classification Task	Generation Type	Approach
DDBS [1]	✓	·	·	✓	✓	✓	Instance	G	$E(+,-)$	Heuristic
OBS [1]	✓	·	·	✓	✓	·	Instance	G	$E(+,-)$	Heuristic
RCEExplainer [4]	✓	✓	✓	·	✓	✓	Instance	G, V	$E(-)$	Heuristic & Learning
GNN-MOExp [35]	✓	·	✓	·	✓	·	Instance	V	sub-graph	Search
MEG [52]	✓	✓	·	✓	·	~	Instance	G	$E(+,-), V(+,-)$	Learning
GNNAdv [67]	✓	✓	·	✓	✓	·	Instance	G	$E(+,-)$	Learning
CMGE [80]	·	✓	✓	·	·	✓	Instance	G	$E(+,-), V(-)$	Learning
NSEG [12]	✓	✓	✓	·	✓	·	Instance	G, V	$E(-), F(*)$	Learning
CF-GNNEExplainer [38]	✓	✓	·	✓	✓	·	Instance	V	$E(-)$	Learning
CLEAR [40]	✓	·	·	✓	✓	✓	Instance	G	$E(+,-), F(*)$	Learning
MACDA [49]	✓	·	·	✓	·	~	Instance	(G_1, G_2)	$E(+,-), V(+,-)$	Learning
CF ² [68]	✓	·	✓	·	✓	·	Instance	G, V	$E(-), V(-), F(-)$	Learning
MACCS [77]	✓	·	·	✓	·	·	Instance	G	$E(+,-), V(+,-)$	Heuristic
GCFExplainer [27]	✓	·	·	·	✓	·	Model	G	$E(+,-), V(+,-)$	Heuristic



GRETEL

Framework

GRETEL modules interaction



Empirical Explainers comparison

Dataset	Method	Runtime ↓	GED ↓	Oracle Calls ↓	Correctness ↑	Sparsity ↓	Fidelity ↑	Oracle Accuracy ↑
Tree-Cycles	RAND@5	0.01 ± 0.003	92.18 ± 5.44	0.00 ± 0.00	0.55 ± 0.50	1.45 ± 0.09	0.55 ± 0.50	1.00 ± 0.00
	RAND@10	0.02 ± 0.006	123.74 ± 7.43	0.00 ± 0.00	0.51 ± 0.50	1.94 ± 0.12	0.51 ± 0.50	1.00 ± 0.00
	RAND@15	0.01 ± 0.004	147.93 ± 8.26	0.00 ± 0.00	0.58 ± 0.50	2.33 ± 0.13	0.58 ± 0.50	1.00 ± 0.00
	DCE	0.13 ± 0.00	50.36 ± 0.00	501.00 ± 0.00	1.00 ± 0.00	0.79 ± 0.00	1.00 ± 0.00	1.00 ± 0.00
	OBS	0.07 ± 0.01	57.31 ± 0.03	149.45 ± 21.13	0.96 ± 0.01	0.90 ± 0.00	0.96 ± 0.01	1.00 ± 0.00
	DBDS	8.87 ± 0.10	71.79 ± 0.24	1342.62 ± 11.95	0.59 ± 0.01	1.13 ± 0.00	0.59 ± 0.01	1.00 ± 0.00
	MACCS	—	—	—	—	—	—	—
	CLEAR	2.47 ± 0.08	79.76 ± 3.60	0.00 ± 0.00	0.53 ± 0.10	1.26 ± 0.06	0.53 ± 0.10	1.00 ± 0.00
	CF ²	0.41 ± 0.01	31.54 ± 0.12	0.00 ± 0.00	0.47 ± 0.10	0.50 ± 0.00	0.47 ± 0.10	1.00 ± 0.00
	MEG	272.11 ± 5.66	159.70 ± 1.34	0.00 ± 0.00	0.53 ± 0.00	2.51 ± 0.02	0.53 ± 0.00	1.00 ± 0.00
ASD	RAND@5	1.45 ± 0.46	618.06 ± 8.27	0.00 ± 0.00	0.00 ± 0.00	0.80 ± 0.01	0.00 ± 0.00	0.79 ± 0.08
	RAND@10	2.76 ± 1.25	1152.93 ± 20.19	0.00 ± 0.00	0.00 ± 0.00	1.49 ± 0.02	0.00 ± 0.00	0.79 ± 0.08
	RAND@15	1.33 ± 0.39	1600.78 ± 18.22	0.00 ± 0.00	0.00 ± 0.00	2.08 ± 0.03	0.00 ± 0.00	0.79 ± 0.08
	DCE	0.09 ± 0.02	1011.69 ± 0.00	102.00 ± 0.00	1.00 ± 0.00	1.31 ± 0.00	0.54 ± 0.00	0.79 ± 0.08
	OBS	3.24 ± 1.13	9.89 ± 0.11	347.73 ± 15.11	1.00 ± 0.00	0.01 ± 0.00	0.54 ± 0.00	0.79 ± 0.08
	DBDS	83.46 ± 34.04	11.79 ± 0.29	362.05 ± 14.56	1.00 ± 0.00	0.02 ± 0.00	0.54 ± 0.00	0.79 ± 0.08
	MACCS	—	—	—	—	—	—	—
	CLEAR	0.45 ± 0.04	1739.60 ± 131.16	0.00 ± 0.00	0.47 ± 0.13	2.25 ± 0.17	0.25 ± 0.18	0.79 ± 0.08
	CF ²	0.69 ± 0.01	655.49 ± 2.87	0.00 ± 0.00	0.46 ± 0.09	0.85 ± 0.00	0.37 ± 0.15	0.79 ± 0.08
	MEG	×	×	×	×	×	×	×
BBBP	RAND@5	0.01 ± 0.03	30.98 ± 33.27	0.00 ± 0.00	0.85 ± 0.35	0.52 ± 0.23	0.62 ± 0.69	0.86 ± 0.02
	RAND@10	0.01 ± 0.03	52.98 ± 58.96	0.00 ± 0.00	0.86 ± 0.35	0.93 ± 0.41	0.65 ± 0.66	0.86 ± 0.02
	RAND@15	0.02 ± 0.12	82.97 ± 137.37	0.00 ± 0.00	0.85 ± 0.36	1.32 ± 0.70	0.61 ± 0.69	0.86 ± 0.02
	DCE	37.51 ± 5.21	27.92 ± 0.12	2040.00 ± 0.00	1.00 ± 0.00	0.59 ± 0.00	0.72 ± 0.00	0.86 ± 0.02
	OBS	2.92 ± 0.07	0.00 ± 0.00	314.61 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.61 ± 0.00	0.86 ± 0.02
	DBDS	×	×	×	×	×	×	×
	MACCS	31.35 ± 0.97	11.23 ± 0.08	1221.33 ± 0.22	0.40 ± 0.00	0.19 ± 0.00	0.23 ± 0.00	0.86 ± 0.02
	CLEAR@1	213.21 ± 5.64	27056.29 ± 9.69	0.00 ± 0.00	0.87 ± 0.02	91.89 ± 0.18	0.64 ± 0.03	0.86 ± 0.02
	CLEAR@5	214.80 ± 6.97	26711.57 ± 112.67	0.00 ± 0.00	0.85 ± 0.02	90.71 ± 0.37	0.62 ± 0.03	0.86 ± 0.02
	CLEAR@15	251.93 ± 36.01	25986.66 ± 170.41	0.00 ± 0.00	0.85 ± 0.01	88.20 ± 0.66	0.62 ± 0.06	0.86 ± 0.02
	CF ²	84.41 ± 49.06	25.72 ± 0.63	0.00 ± 0.00	0.85 ± 0.02	0.09 ± 0.00	0.63 ± 0.03	0.86 ± 0.02
	MEG	90.66 ± 29.51	269.35 ± 0.39	0.00 ± 0.00	0.51 ± 0.04	0.91 ± 0.00	0.32 ± 0.04	0.86 ± 0.02

GRETEL v1



Demo

<https://github.com/MarioTheOne/GRETEL>

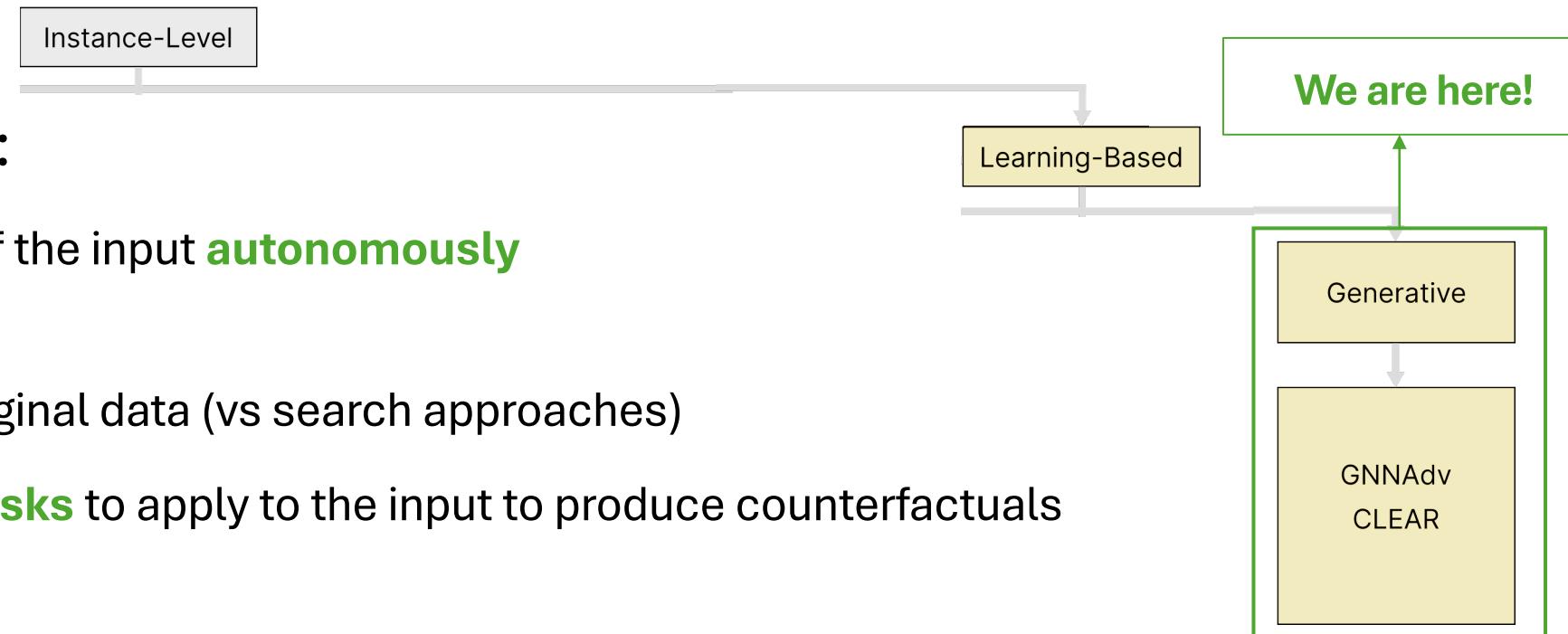
Part Three

G-CounterGAN

GCE Generative

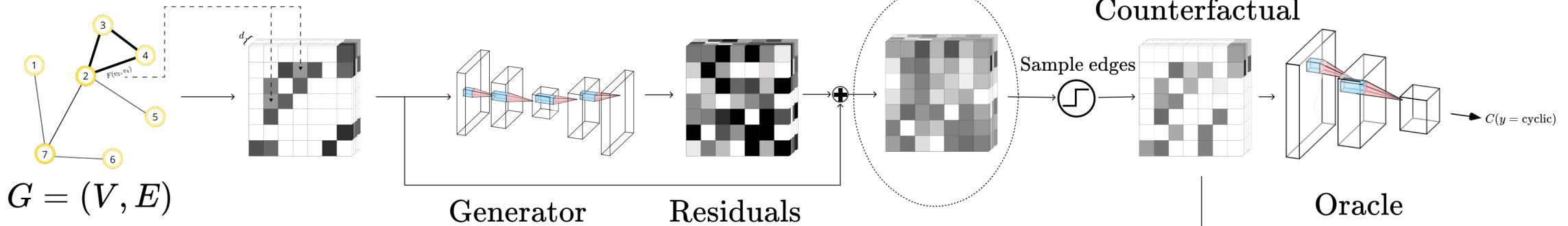
Generative approaches:

- Learn the perturbation of the input autonomously
(vs heuristic approaches)
- Aren't confined to the original data (vs search approaches)
- Don't rely on learned masks to apply to the input to produce counterfactuals
(vs learning approaches)
- Generative strategies allow to produce multiple counterfactuals from a learned latent space
- don't need to access the oracle at explanation time



Architecture overview

Training



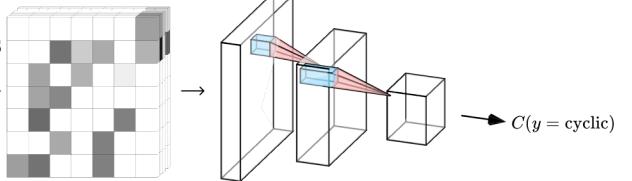
Generator

Residuals

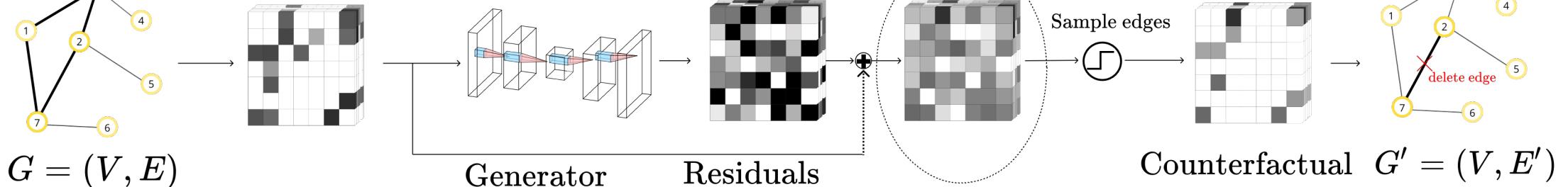
Counterfactual

Sample edges

Oracle



Inference

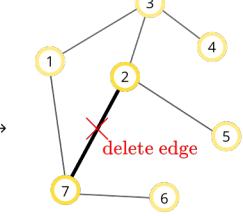


Generator

Residuals

Counterfactual $G' = (V, E')$

Sample edges



High Level Loss

$$\mathcal{L}_{\text{OUR}} = \mathcal{L}_1(G, D) + \mathcal{L}_\Phi(G, c) + \text{Reg}(G, A)$$

- c is the **class** to **explain**, and $\text{Reg}(G, A)$ is a **regularization** term that **controls** the sparsity of the residuals (i.e., feature perturbations)

Generator/Discriminator Loss

$$\mathcal{L}_{OUR} = \mathcal{L}_1(G, D) + \mathcal{L}_\Phi(G, c) + Reg(G, A)$$

$$\begin{aligned}\mathcal{L}_1(G, A) &= E_{A \sim p_{data}} \log D(A) \\ &+ E_{A \sim p_{data}} \log \left(1 - D(A + G(A)) \right)\end{aligned}$$

- We modify the **generator** to **take original** input data **instead of noise** sampled from a normal distribution to **directly** generates **Counterfactuals** of the input instance

Embedding the Oracle (1)

$$\mathcal{L}_{OUR} = \mathcal{L}_1(G, D) + \mathcal{L}_\Phi(G, c) + Reg(G, A)$$

$$\mathcal{L}_\Phi(G, c) = E_{A \sim p_{data}} \log(\mathbb{I}[\Phi(A + G(A)) \neq c])$$

- **Sampling instances** from the data distribution **could** make G **generate null residuals**
- Hence, **this loss** component **leverage** the **Oracle** to **steer** the **generator** away from this behavior, making it produce plausible counterfactuals

Embedding the Oracle (2)

$$\mathcal{L}_{OUR} = \mathcal{L}_1(G, D) + \mathcal{L}_\Phi(G, c) + Reg(G, A)$$

$$\mathcal{L}_\Phi(G, c) = E_{A \sim p_{\text{data}}} \cancel{\log(\mathbb{I}[\Phi(A + G(A)) \neq c])}$$

- **Problem:**
The oracle is a black-box and we cannot access its gradients to optimize this loss!

Final Loss

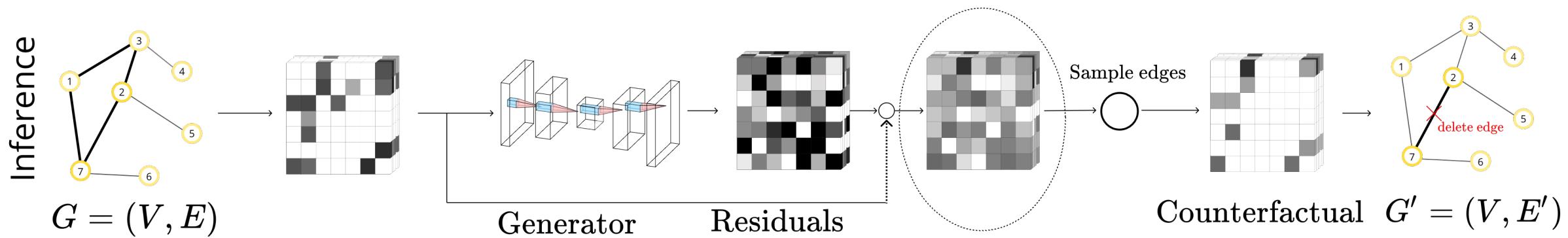
$$\mathcal{L}_{OUR} = \frac{\sum_{A \in \mathcal{A}} (1[\Phi(A) = c] \cdot \log D(A))}{\sum_{A \in \mathcal{A}} \mathbb{I}[\Phi(A) = c]}$$

$$+ \frac{1}{|\mathcal{A}|} \sum_{A \in \mathcal{A}} \log(1 - D(A + G(A))) + Reg(G, A)$$

- **Solution:**
- We **weight** the **first** term of the loss by the **prediction scores** of the oracle;
- $\mathbb{I}[\Phi(A) = c]$ is an **indicator function** that returns 1 if Φ classify the instance in the class c ; while \mathcal{A} is the set of all adjacency matrices corresponding to $G \in \mathcal{G}$

G-CounteRGAN Inference

- Counterfactuals **generation** are made by **sampling** edges by the edge probabilities **learned** in the **latent space**;
- We **keep** the **node order** to avoid CLEAR's graph matching problem (NP-hard)



[9] Ma, J., Guo, R., Mishra, S., Zhang, A., Li, J.: CLEAR: generative counterfactual explanations on graphs. In: NeurIPS (2022)

Performances on TreeCycles@n

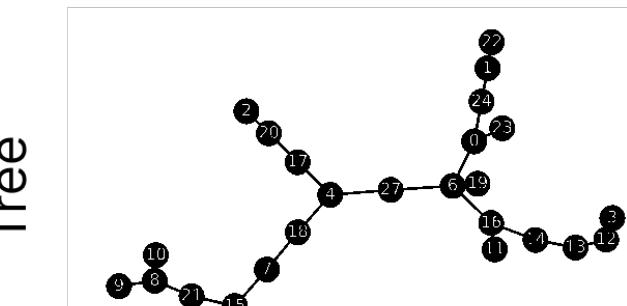
Dataset	Method	Runtime ↓	GED ↓	Oracle calls ↓	Correctness ↑	Sparsity ↓	Fidelity ↑	Oracle accuracy ↑
Tree-Cycles@28	DCE *	<u>0.125</u>	42.570	501.000	1.000	0.766	1.000	1.000
	OBS *	0.067	49.444	<u>139.545</u>	<u>0.965</u>	0.889	<u>0.965</u>	1.000
	iRand *	0.218	0.588	484.599	0.569	0.011	0.569	1.000
	CF ² †	0.581	<u>27.566</u>	0.000	0.496	<u>0.496</u>	0.496	1.000
	CLEAR ‡	22.121	64.006	0.000	0.504	1.152	0.504	1.000
	G-CounteRGAN ‡	4.120	271.822	0.000	0.524	4.893	0.524	1.000
Tree-Cycles@32	DCE *	0.143	50.112	501.000	1.000	0.788	1.000	1.000
	OBS *	0.143	57.542	<u>159.260</u>	<u>0.964</u>	0.905	<u>0.964</u>	1.000
	iRand *	0.339	0.590	627.342	0.575	0.009	0.575	1.000
	CF ² †	0.412	<u>31.542</u>	0.000	0.474	<u>0.496</u>	0.474	1.000
	CLEAR ‡	30.227	80.351	0.000	0.526	1.265	0.526	1.000
	G-CounteRGAN ‡	<u>0.298</u>	359.698	0.000	0.504	5.659	0.504	1.000
Tree-Cycles@48	DCE *	<u>0.214</u>	82.000	501.000	1.000	0.858	1.000	1.000
	OBS *	0.147	89.268	<u>237.678</u>	<u>0.935</u>	0.934	<u>0.935</u>	1.000
	iRand *	1.627	0.533	1594.374	0.527	0.006	0.527	1.000
	CF ² †	3.771	<u>47.568</u>	0.000	0.494	<u>0.498</u>	0.494	1.000
	CLEAR ‡	31.081	171.983	0.000	0.506	1.800	0.506	1.000
	G-CounteRGAN ‡	6.612	<u>1121.550</u>	0.000	0.506	117.737	0.506	1.000

† symbolizes learning-based approaches; ‡ indicates generative approaches; * depicts search (heuristic) methods.

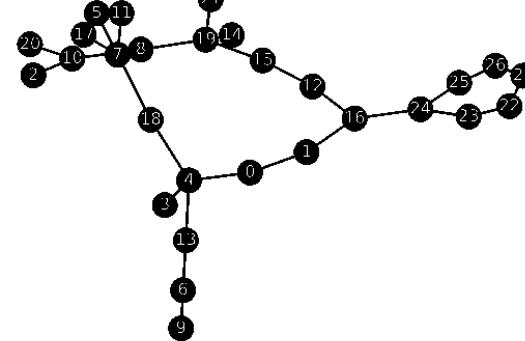
Bold values are the best overall; underlined are second-best on average per dataset

Anecdotal Counterfactual Visualization

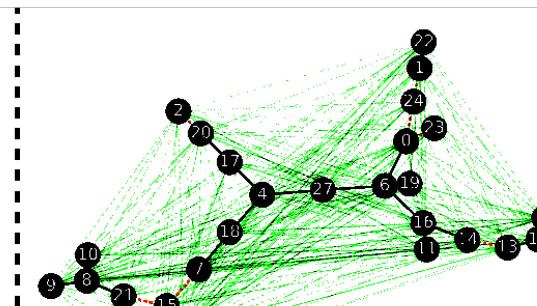
Original Graph



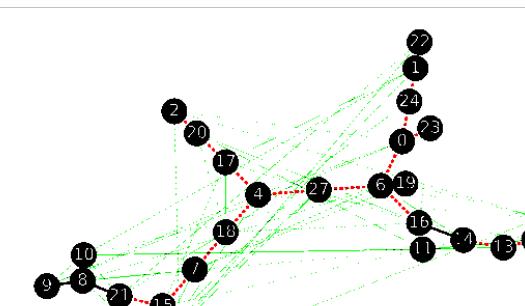
Cyclic Graph



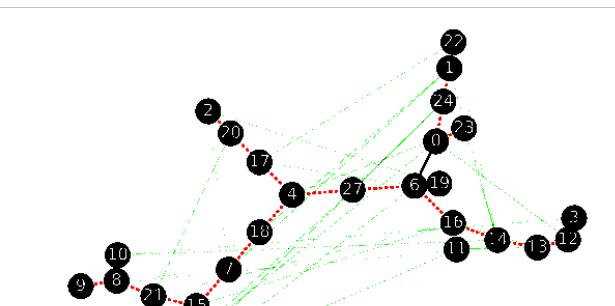
G-CounteRGAN



CLEAR

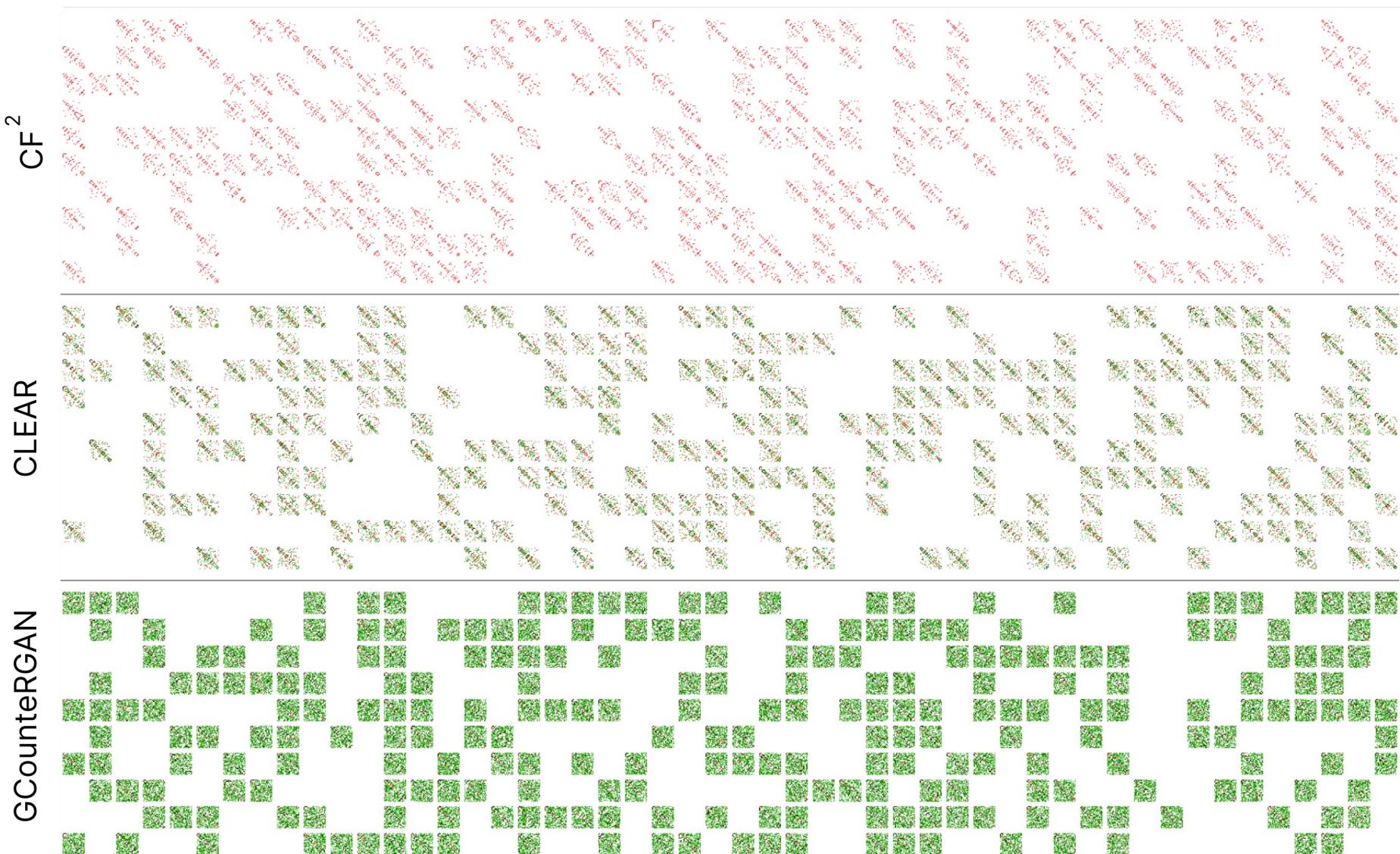


DCE



Counterfactual produced by G-CounteRGAN, CLEAR, and the optimistic baseline DCE on Tree-Cycles@28. As in the original graph, **green** edges are additions, **red** ones are removals, and **black** ones are maintained. An **X** denotes an invalid counterfactual, and a **✓** is valid.

Anecdotal Counterfactual Visualization



Counterfactual produced by CF^2 , CLEAR, and G-CounterGAN on Tree-Cycles@28.

Part Five

Conclusive Remarks

Conclusion

Q: “Can generative approaches compete with search/heuristic baselines in producing valid counterfactuals in synthetic datasets?” A: Not yet. But ...

- They are crucial to **produce multiple counterfactuals** by sampling their learned latent spaces
- **They can learn** the input perturbation strategy differently from heuristic-based approaches
- They have **the potential** to become akin to a **Swiss-knife in GCE**

Thanks for your attention!



Slides & More

Bibliography

- [1] Guidotti, R., Monreale, A., Ruggieri, S., Turini, F., Giannotti, F., Pedreschi, D.: A survey of methods for explaining black box models. *ACM computing surveys (CSUR)* 51(5), 1–42 (2018)
- [2] Petch, J., Di, S., Nelson, W.: Opening the black box: the promise and limitations of explainable machine learning in cardiology. *Canadian Journal of Cardiology* (2021)
- [3] Verenich, I., Dumas, M., La Rosa, M., Nguyen, H.: Predicting process performance: A white-box approach based on process models. *Journal of Software: Evolution and Process* 31(6), e2170 (2019)
- [4] Aragona, D., Podo, L., Prenkaj, B., Velardi, P.: Corona: a deep sequential framework to predict epidemic spread. In: *Proceedings of the 36th Annual ACM Symposium on Applied Computing*. pp. 10–17 (2021)
- [5] Feng, W., Tang, J., Liu, T.X.: Understanding dropouts in moocs. In: *Proceedings of the AAAI Conference on Artificial Intelligence*. vol. 33, pp. 517–524 (2019)
- [6] Verma, H., Mandal, S., Gupta, A.: Temporal deep learning architecture for prediction of covid-19 cases in india. *Expert Systems with Applications* 195, 116611 (2022)
- [7] Prenkaj, B., Distante, D., Faralli, S., Velardi, P.: Hidden space deep sequential risk prediction on student trajectories. *Future Generation Computer Systems* 125, 532–543 (2021)
- [8] Mario Alfonso Prado-Romero, Bardh Prenkaj, Giovanni Stilo, and Fosca Giannotti. 2023. A Survey on Graph Counterfactual Explanations: Definitions, Methods, Evaluation, and Research Challenges. *ACM Comput. Surv.* Just Accepted (September 2023). <https://doi.org/10.1145/3618105>
- [9] Ma, J., Guo, R., Mishra, S., Zhang, A., Li, J.: CLEAR: generative counterfactual explanations on graphs. In: *NeurIPS* (2022)