

# On Logic-Based Explanations for Graph Neural Networks: From Post-hoc Explanations to Self-Explainable Models

Alessio Ragno

# Who am I?

## Postdoc @ INSA Lyon:

- Jan 2025 (Nov 2024) - present
- Supervisors: Prof. Celine Robardet, Prof. Marc Plantevit
- WAIT4 Project:
  - *Caractérisation des activités animales et de leurs interactions sociales à l'aide de réseaux de neurones sur graphes interprétables.*

## PhD in Artificial Intelligence @ Sapienza University of Rome:

- Nov 2021 - Jan 2025
- Topology-based Explanations for Neural Networks

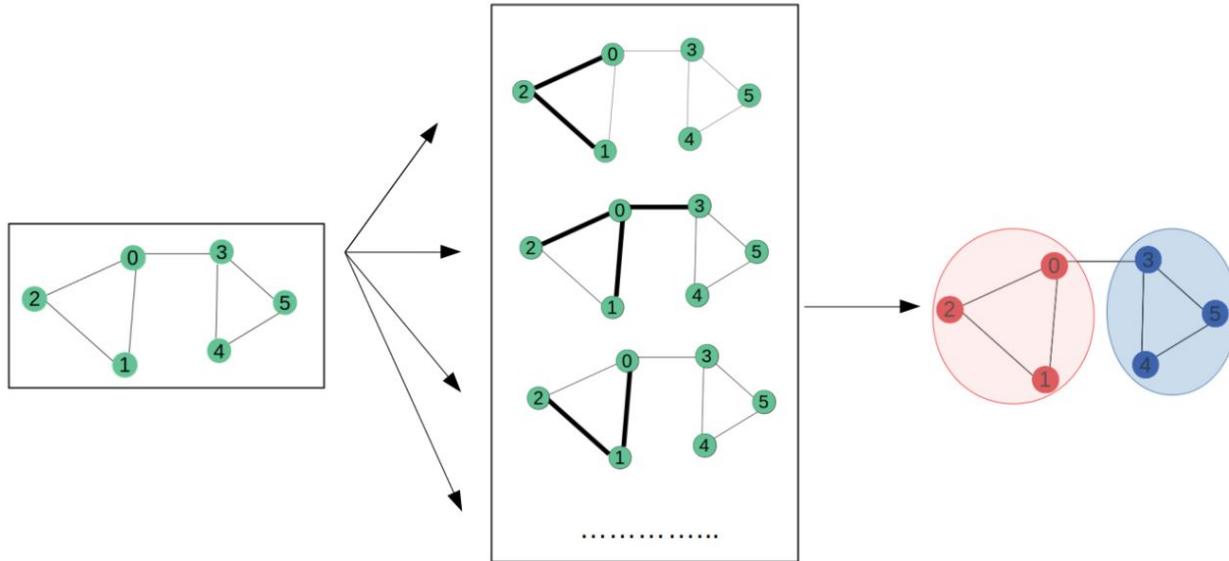
## Master's Degree in Artificial Intelligence and Robotics @ Sapienza University of Rome:

- Sep 2019 - May 2021

# Table of Contents

- **Graph Neural Networks & XAI**
- Logic-based Explanations with Transparent Explainable Logic Layer (TELL)
- Logic-based Post-hoc Explanations for GNNs
- Logic-based Self-Explainable GNNs
- Application of Logic-based Explanations to Drug Discovery

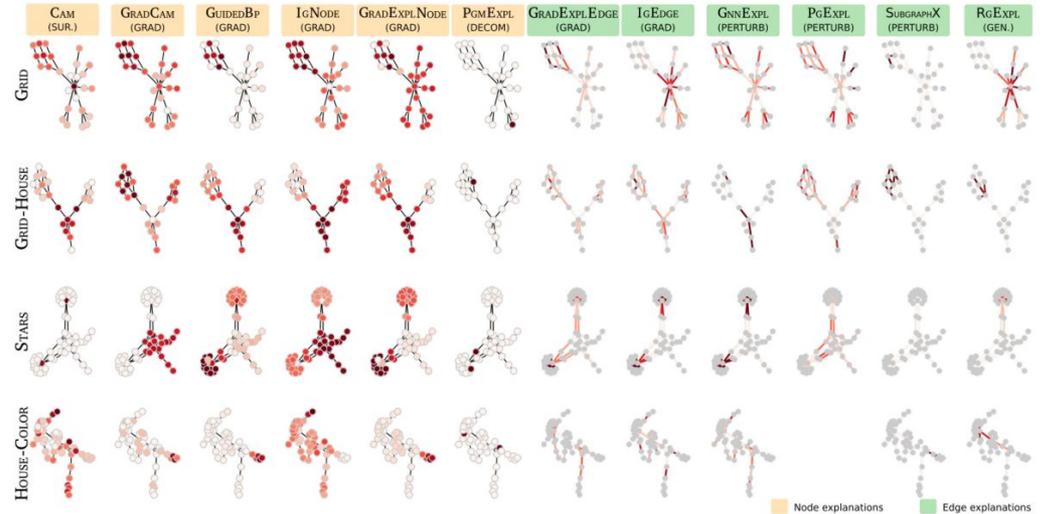
# Graph Neural Networks



# XAI for GNNs

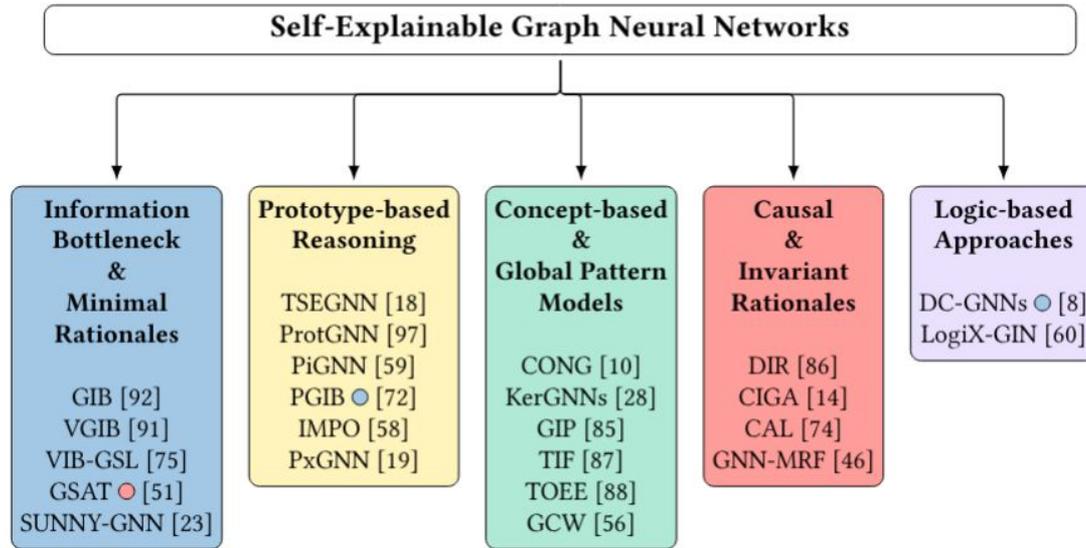
Post-hoc:

- gradient-based approaches  
(Li et al. 2021, Kasanishi 2021)
- perturbation-based approaches  
(Ying et al. 2019, Luo et al. 2020)
- optimization-based approaches  
(Yuan et al. 2021)
- pattern-based  
(Veyrin-Forrer et al. 2022, Kamal et al. 2023)



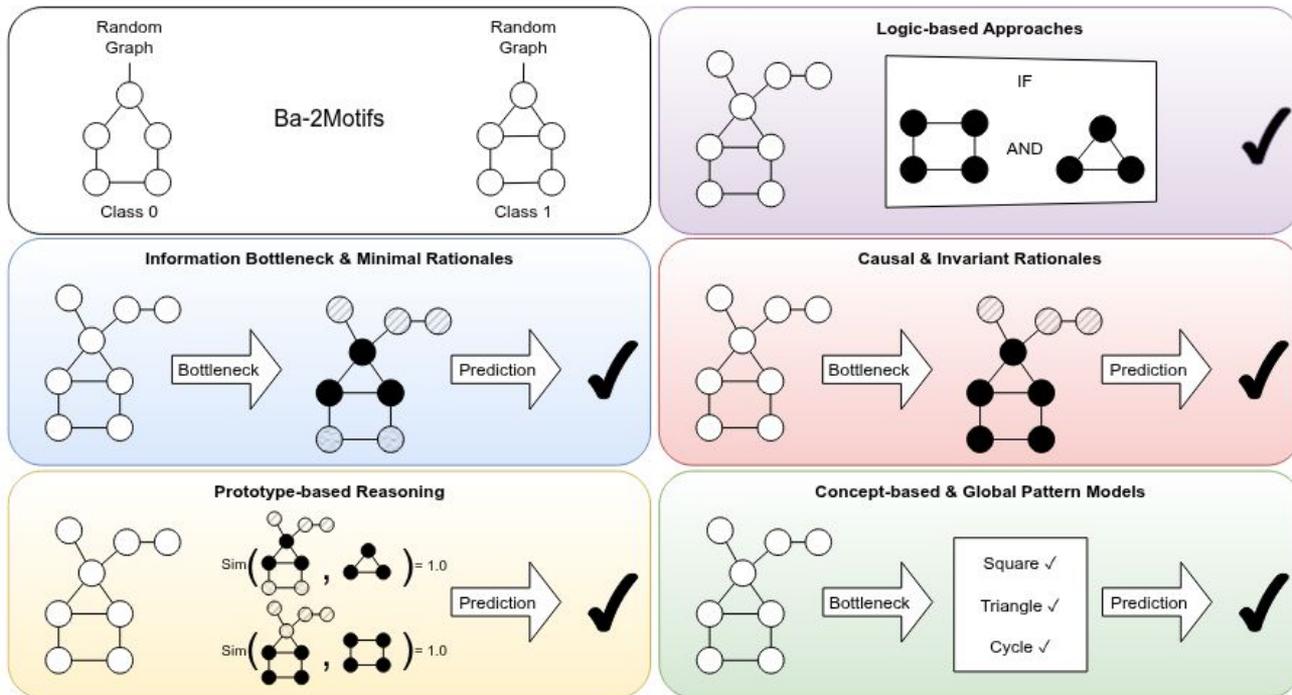
Explaining the Explainers in Graph Neural Networks: a Comparative Study (Longa et al., 2025, ACM Comp. Surv.)

# Self-Explainable GNNs



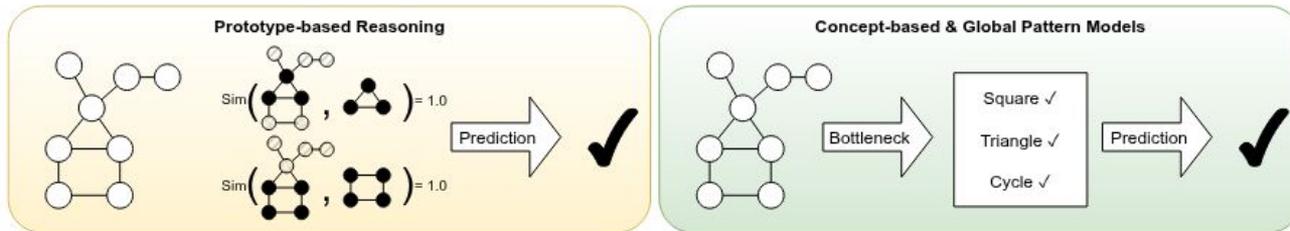
(Hopefully there will be a survey before too long xD)

# Self-Explainable GNNs



# Self-Explainable GNNs

In the beginning... there was nothing.

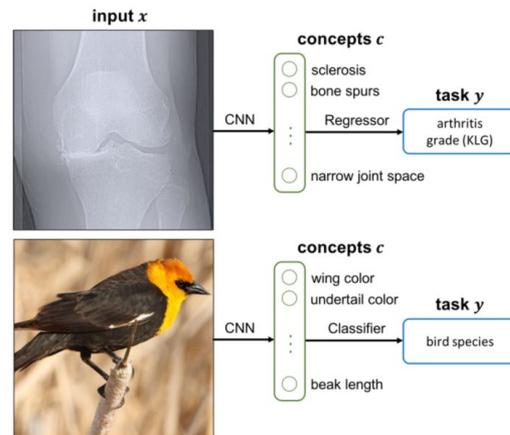
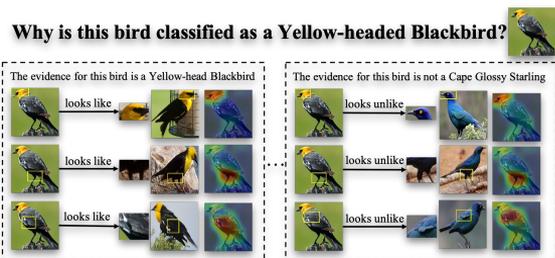


# Self-Explainable Neural Networks

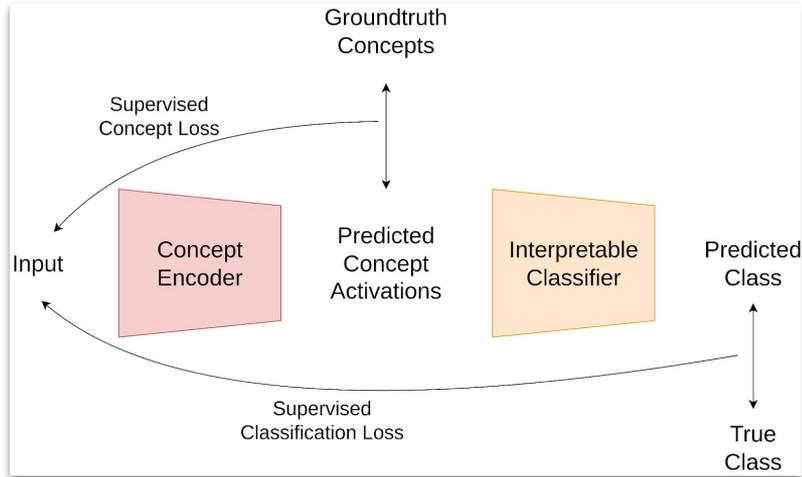
Explainable by-design models developed with interpretable reasoning process.

To achieve this result, researchers have developed:

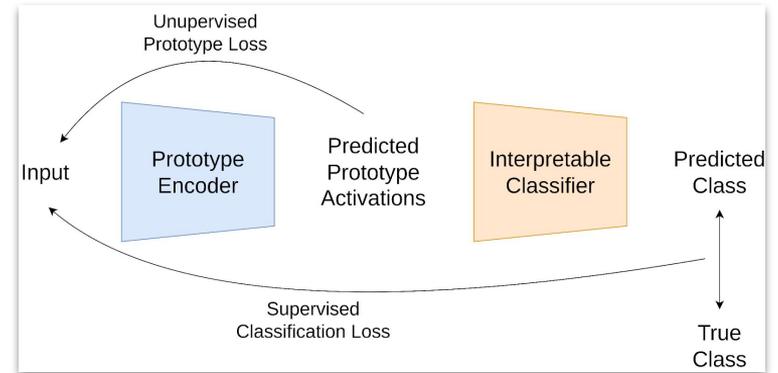
- Prototype-based Neural Networks (C. Chen, 2018; Wang, 2021; S.F. Stefenon, 2022)
- Concept-based Neural Networks (Z. Chen, 2020; P.W. Koh, 2020)



# Self-Explainable Neural Networks

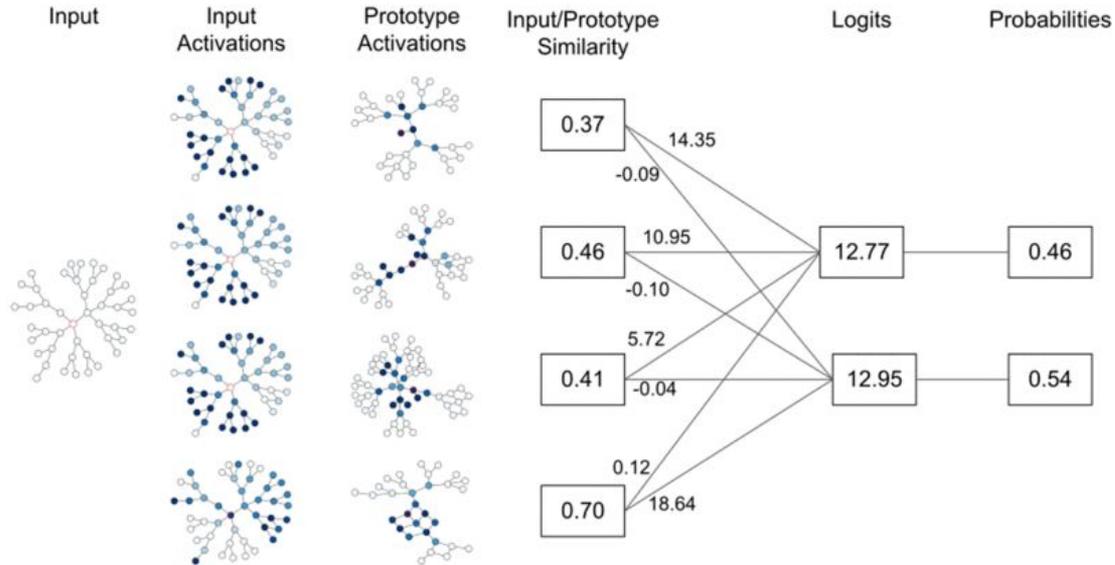


Concept-based



Prototype-based

# Self-Explainable GNNs

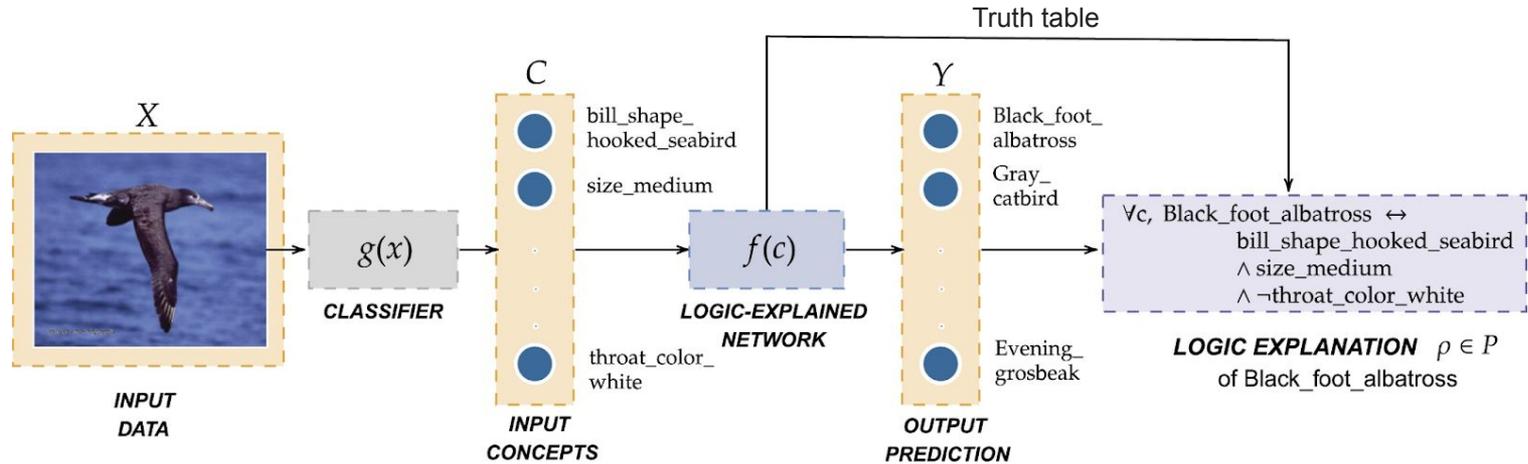


Prototype-based Interpretable Graph Neural Networks (Ragno et al., 2022, IEEE TAI)

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# Logic-Explained Networks



Logic Explained Networks (Ciravegna et al., 2023, Artificial Intelligence)

Entropy-based logic explanations of neural networks (Barbiero et al., 2022, AAAI)

# Motivating Experiment: Logic Induction

Ground Truth Rule:

$$y = 1 \iff (x_1 > 0.5 \wedge x_2 > 0.2) \vee (x_1 > 0.5 \wedge x_3 > 0.7)$$

Model	Accuracy (%)	Rules Accuracy (%)	Fidelity (%)	Complexity	Best Model's Rule
ENTROPY	94.68 ± 0.33	59.48 ± 0.56	74.62 ± 8.25	1.00 ± 0.00	$x_1 > 0.50$
$\psi$	89.98 ± 0.36	65.45 ± 0.60	64.74 ± 3.26	1.73 ± 0.13	$x_1 > 0.50$
RELU	<b>99.12 ± 1.00</b>	93.12 ± 0.14	92.92 ± 0.29	1.00 ± 0.00	$x_1 > 0.50$
$\mu$	<b>98.38 ± 0.41</b>	92.49 ± 0.23	92.11 ± 0.34	2.93 ± 0.48	$x_1 > 0.50$
DR-NET	96.72 ± 0.37	92.70 ± 0.35	90.85 ± 0.53	133.13 ± 2.07	Explanation too long

# Transparent Explainable Logic Layers

$$y = \sigma(w_1x_1 + w_2x_2 + w_3x_3 + b)$$

$$y_d = 1 \quad \Leftrightarrow \quad y > 0.5 \quad \Leftrightarrow \quad w_1x_1 + w_2x_2 + w_3x_3 + b > 0$$

# Transparent Explainable Logic Layers

$$y = \sigma(w_1x_1 + w_2x_2 + w_3x_3 + b)$$

$x_i$  is binary  
 $w_i \geq 0$

$$y_d = 1 \quad \Leftrightarrow \quad y > 0.5 \quad \Leftrightarrow \quad w_1x_1 + w_2x_2 + w_3x_3 + b > 0$$

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$$y = \sigma(5x_1 + 2x_2 + 2x_3 - 2.5)$$

# Transparent Explainable Logic Layers

$$y = \sigma(w_1x_1 + w_2x_2 + w_3x_3 + b)$$

$x_i$  is binary  
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$$y = \sigma(5x_1 + 2x_2 + 2x_3 - 2.5)$$

$$\text{es. } x = [1 \ 0 \ 1] \rightarrow y = \sigma(5 + 0 + 2 - 2.5) > 0.5 \rightarrow y_d = 1$$

# Transparent Explainable Logic Layers

$$y = s(w_1x_1 + w_2x_2 + w_3x_3 + b)$$

$x_i$  is binary  
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$$y = \sigma(5x_1 + 2x_2 + 2x_3 - 2.5)$$

$$\text{es. } x = [1 \ 0 \ 1] \rightarrow y = \sigma(5 + 0 + 2 - 2.5) > 0.5 \rightarrow y_d = 1$$

$$\text{es. } x = [0 \ 0 \ 1] \rightarrow y = \sigma(0 + 0 + 2 - 2.5) < 0.5 \rightarrow y_d = 0$$

# Transparent Explainable Logic Layers

$$y = \sigma(w_1x_1 + w_2x_2 + w_3x_3 + b)$$

$x_i$  is binary  
 $w_i \geq 0$

$$y_d = 1 \quad \Leftrightarrow \quad y > 0.5 \quad \Leftrightarrow \quad w_1x_1 + w_2x_2 + w_3x_3 + b > 0$$

$$y = \sigma(5x_1 + 2x_2 + 2x_3 - 2.5)$$

$$y_d = 1 \Leftrightarrow \sum_{i \in X} w_i > -b \quad X = \{i : x_i = 1\}$$

**we need to identify the subsets of features with corresponding weights that sum up to a value greater than -b**

# Transparent Explainable Logic Layers

$x_i$  is binary  
 $w_i \geq 0$

$$y = \sigma(w_1x_1 + w_2x_2 + w_3x_3 + b)$$

$$y_d = 1 \quad \Leftrightarrow \quad y > 0.5 \quad \Leftrightarrow \quad w_1x_1 + w_2x_2 + w_3x_3 + b > 0$$

$$y = \sigma(5x_1 + 2x_2 + 2x_3 - 2.5)$$

Logic Rule:  $x_1 \vee (x_2 \wedge x_3)$



# Working with continuous inputs

To work with continuous inputs:

- we add a preprocessing layer with sigmoid activation which thresholds the features
- we introduce a loss over thresholded features that pushes them towards 0 and 1

$$\hat{X} = \sigma(X \odot \exp(W_i) + b_i)$$

$$\text{s.t. } W_i \in \mathbb{R}^I, b_i \in \mathbb{R}^I$$

$$\hat{X} > 0.5 \iff X > -\frac{b_i}{\exp(W_i)}$$

$$\mathcal{L}_E = -\hat{X} \log(\hat{X}) - (1 - \hat{X}) \log(1 - \hat{X})$$

# Motivating Experiment: Logic Induction

Ground Truth Rule:

$$y = 1 \iff (x_1 > 0.5 \wedge x_2 > 0.2) \vee (x_1 > 0.5 \wedge x_3 > 0.7)$$

Model	Accuracy (%)	Rules Accuracy (%)	Fidelity (%)	Complexity	Best Model's Rule
TELL	96.84 ± 0.07	<b>95.70 ± 0.38</b>	<b>97.79 ± 0.39</b>	3.40 ± 0.17	$(x_1 > 0.48 \wedge x_2 > 0.20) \vee (x_1 > 0.48 \wedge x_3 > 0.70)$
ENTROPY	94.68 ± 0.33	59.48 ± 0.56	74.62 ± 8.25	1.00 ± 0.00	$x_1 > 0.50$
$\psi$	89.98 ± 0.36	65.45 ± 0.60	64.74 ± 3.26	1.73 ± 0.13	$x_1 > 0.50$
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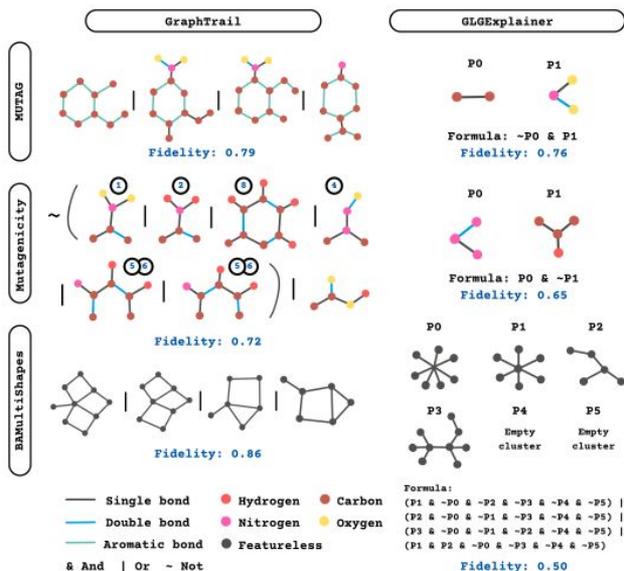
# Classification and Explanation

	Model	Binary Datasets				Concept-Bottleneck			
		MIMIC-II		V-DEM		MNIST E/O		CUB	
		Accuracy (%)	Fidelity (%)	Accuracy (%)	Fidelity (%)	Accuracy (%)	Fidelity (%)	Accuracy (%)	Fidelity
Explainable NN	TELL (ours)	<b>79.28 ± 0.80</b>	<b>96.15 ± 0.62</b>	<b>92.50 ± 0.43</b>	<b>97.56 ± 0.45</b>	99.85 ± 0.01	<b>99.98 ± 0.00</b>	92.39 ± 0.19	<b>97.99 ± 0.09</b>
	$\psi$	76.57 ± 0.69	58.38 ± 3.60	91.11 ± 0.29	60.30 ± 5.10	99.84 ± 0.01	69.62 ± 2.84	92.22 ± 0.19	75.35 ± 0.92
	RELU	<b>79.06 ± 0.87</b>	75.30 ± 2.57	<b>92.85 ± 0.42</b>	85.46 ± 3.77	99.85 ± 0.01	93.72 ± 3.88	92.43 ± 0.20	97.45 ± 0.07
	$\mu$	<b>79.16 ± 0.82</b>	91.15 ± 1.12	91.82 ± 0.42	<b>97.49 ± 0.48</b>	<b>99.90 ± 0.01</b>	99.90 ± 0.01	<b>92.65 ± 0.18</b>	94.80 ± 0.21
	ENTROPY	<b>78.89 ± 0.72</b>	71.47 ± 2.49	90.28 ± 0.60	87.44 ± 5.40	99.84 ± 0.01	41.03 ± 8.24	<b>92.57 ± 0.19</b>	97.56 ± 0.08
	DR-NET	74.16 ± 0.60	75.36 ± 1.72	N/A	N/A	85.69 ± 0.06	85.52 ± 0.07	N/A	N/A
ML	DT	76.52 ± 0.75	100.00 ± 0.00	84.91 ± 0.67	100.00 ± 0.00	99.89 ± 0.01	100.00 ± 0.00	80.59 ± 0.79	100.00 ± 0.00
	BRL	77.20 ± 1.10	100.00 ± 0.00	77.20 ± 1.10	100.00 ± 0.00	99.84 ± 0.01	100.00 ± 0.00	91.15 ± 0.45	100.00 ± 0.00

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# Logic-based Explanations for GNNs: SOTA



GRAPHTRAIL: Translating GNN Predictions into Human-Interpretable Logical Rules (Ranu et al., 2024, NeurIPS)

Global Explainability of GNNs via Logic Combination of Learned Concepts (Azzolin et al. 2023, ICLR)

# Applying TELL paradigm to GNNs

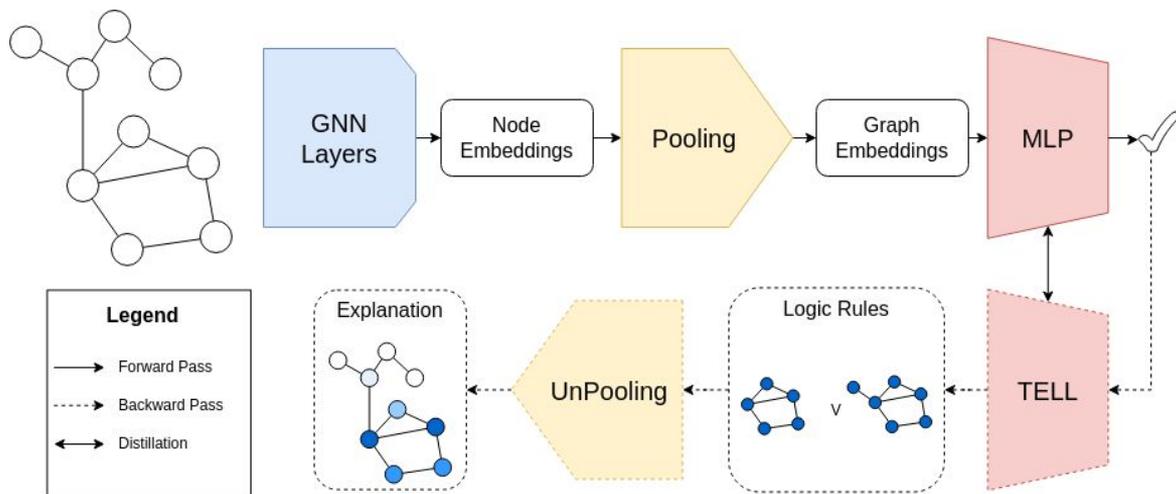
Post-hoc:

- We use TELL to approximate the GNN prediction and identify the most important nodes

Self-Explainable:

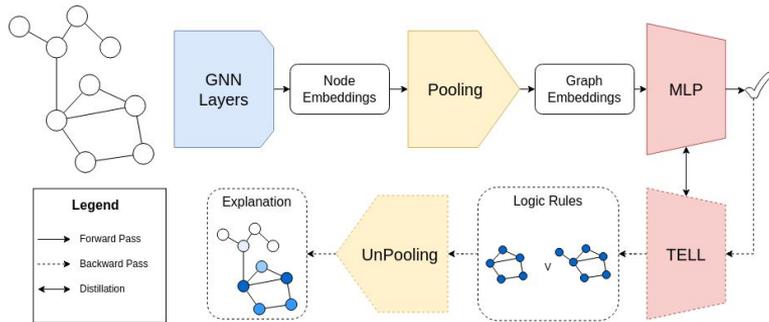
- We create a new GNN Layer upon TELL's paradigm to create a transparent GNN

# LogiX: Faithful Explanations for GNNs using Logic



Faithful Explanations for GNNs using TELL (Ragno et al., 2025, ECML-PKDD)

# LogiX: Rule Extraction



Node Embeddings

1	1	0
2	1	1
3	1	0
	$h_1$	$h_2$

Graph Embeddings

$h_1$	3	} sum
$h_2$	1	
$h_1$	1	} max
$h_2$	1	
$h_1$	1	} avg
$h_2$	.3	

TELL Rule  
 $\text{sum}(h_1) > 2 \wedge \text{max}(h_2) > 0.5$

Rule Contributions

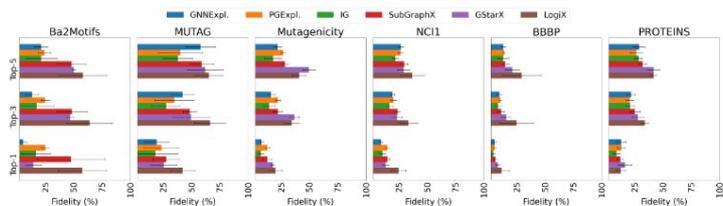
.3	0
.3	1
.3	0
$h_1$	$h_2$

Node Attributions

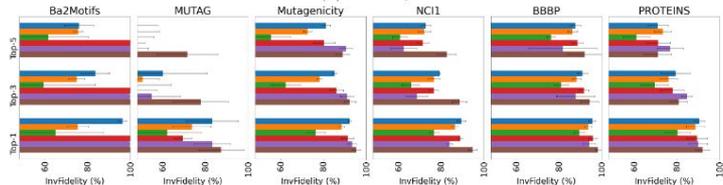
15%
70%
15%

Faithful Explanations for GNNs using Logic (Ragno et al., 2025, ECML-PKDD)

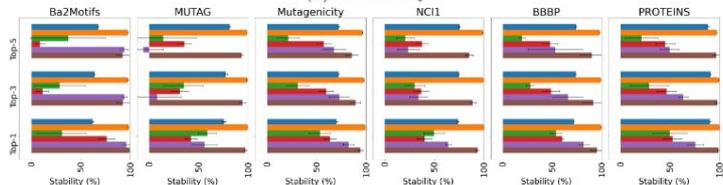
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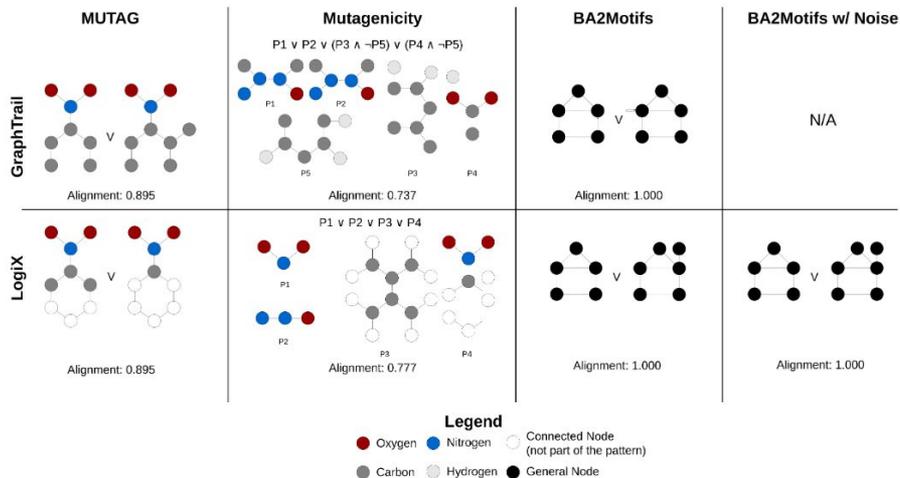
(a) Fidelity



(b) InFidelity



(c) Stability



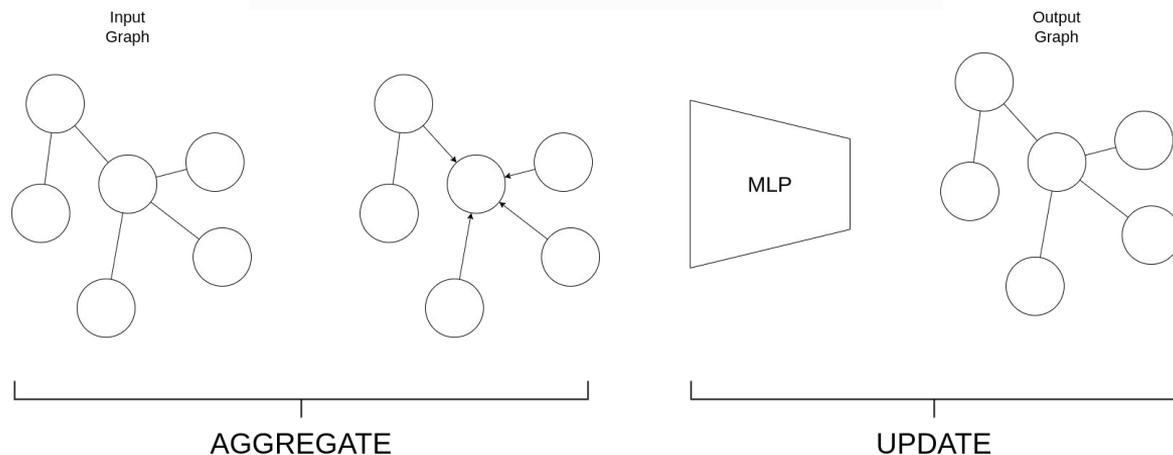
Faithful Explanations for GNNs using Logic (Ragno et al., 2025, ECML-PKDD)

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# Applying TELL to Graph Neural Networks: GIN

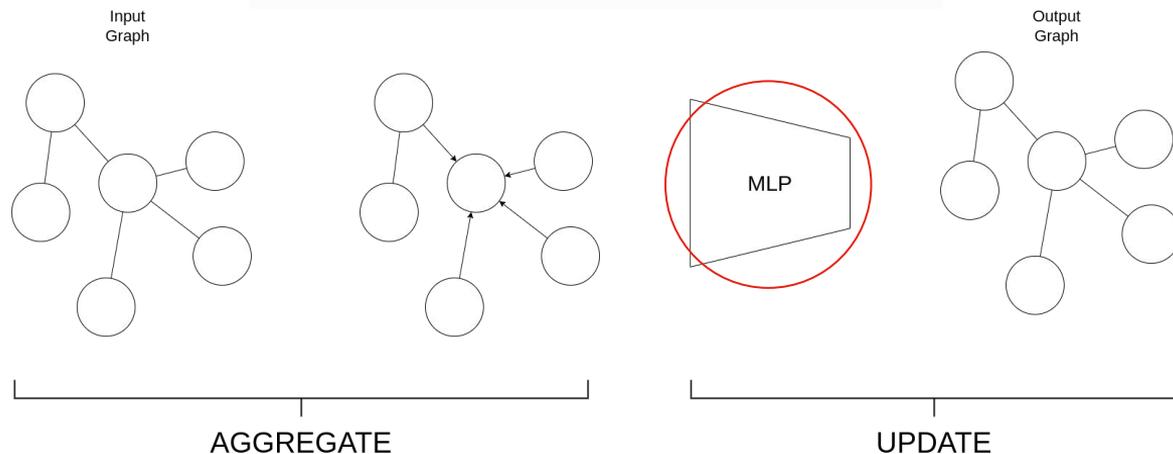
$$\mathbf{x}'_i = h_{\Theta} \left( (1 + \epsilon) \cdot \mathbf{x}_i + \sum_{j \in \mathcal{N}(i)} \mathbf{x}_j \right)$$



On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Applying TELL to Graph Neural Networks: GIN

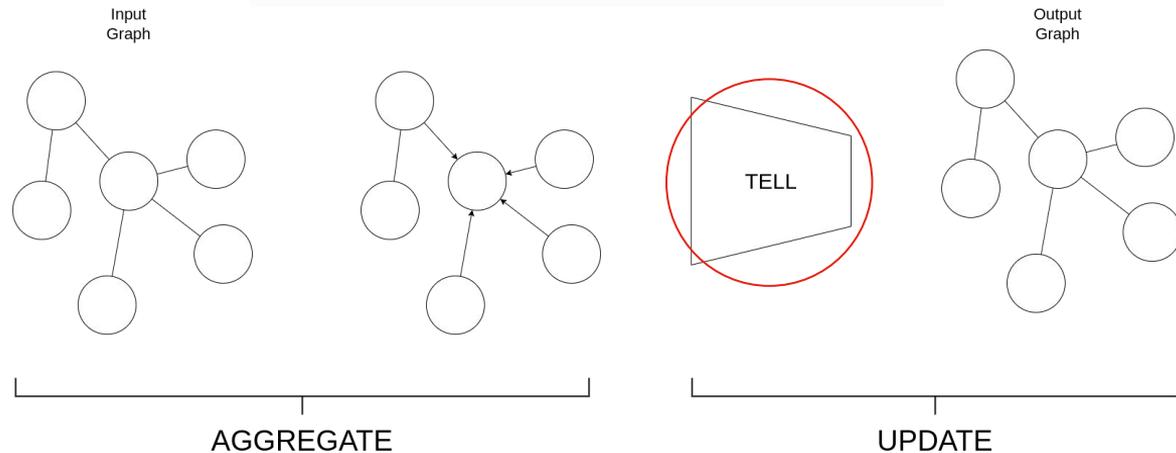
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On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Applying TELL to Graph Neural Networks: GIN

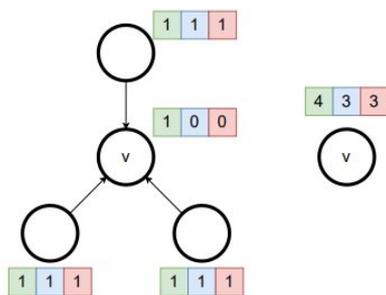
$$\mathbf{x}'_i = h_{\Theta} \left( (1 + \epsilon) \cdot \mathbf{x}_i + \sum_{j \in \mathcal{N}(i)} \mathbf{x}_j \right)$$



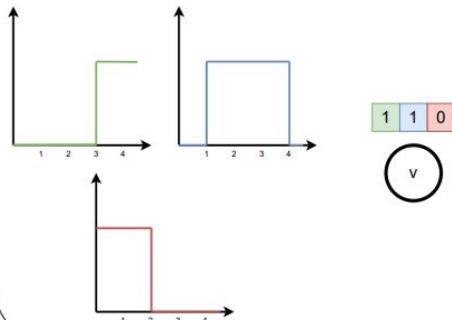
On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# LogiX-GIN

## Sum Aggregation



## Thresholding



## Symbolic Prediction

$$y = \sigma(2x_1 + x_2 + x_3 - 2.5)$$



$$x_1 \wedge (x_2 \vee x_3)$$

$$\sum_{v' \in \mathcal{N}(v) \cup \{v\}} \text{Green Circle} \geq 3 \wedge (1 \leq \sum_{v' \in \mathcal{N}(v) \cup \{v\}} \text{Blue Circle} \leq 4 \vee \sum_{v' \in \mathcal{N}(v) \cup \{v\}} \text{Red Circle} \leq 2)$$

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Main difficulties

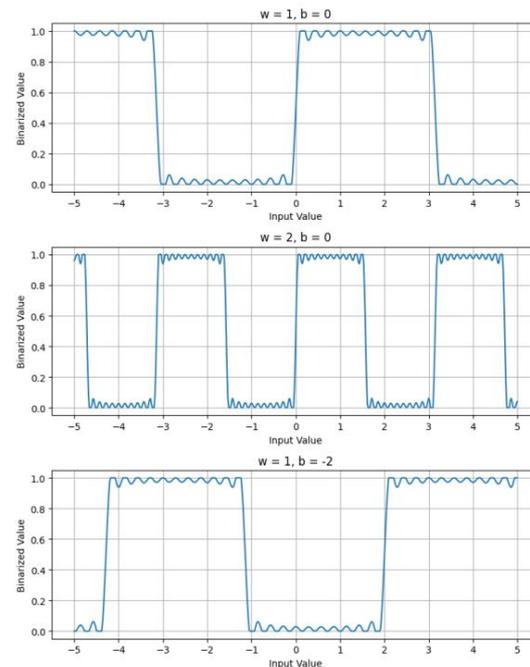
- When aggregating nodes, we apply rules on the number of neighbors which have a determinate pattern. Instead of using a simple threshold, can we learn ranges?

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Fourier Thresholding

We want a parametrizable function that learns step-shaped intervals

$$\tilde{a}_v^{(k)} = \beta^{(k)}(a_v^{(k)}) = \text{clamp} \left( \frac{1}{2} \left( \frac{\sum_{i=0}^{\tau} \frac{\sin((2i+1)(a_v^{(k)} \odot \tilde{W}^{(k)} + \tilde{b}^{(k)}))}{2i+1}}{\sum_{i=0}^{\tau} \frac{\sin((2i+1)\frac{\pi}{2})}{2i+1}} + 1 \right), 0, 1 \right)$$



On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Main difficulties

- ~~When aggregating nodes, we apply rules on the number of neighbors which have a determinate pattern. Instead of using a simple threshold, can we learn ranges?~~
- Sigmoid makes TELL hard to train in deep networks: vanishing gradient

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Training by distillation

- We train a model of 5 GIN layers with Gumbel-Sigmoid activation function

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Training by distillation

- We train a model of 5 GIN layers with Gumbel-Sigmoid activation function
- We then initialize a model of 5 Logic-GIN layers with the same characteristics

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Training by distillation

- We train a model of 5 GIN layers with Gumbel-Sigmoid activation function
- We then initialize a model of 5 Logic-GIN layers with the same characteristics
- We pretrain the logic model to replicate the first one layer-by-layer

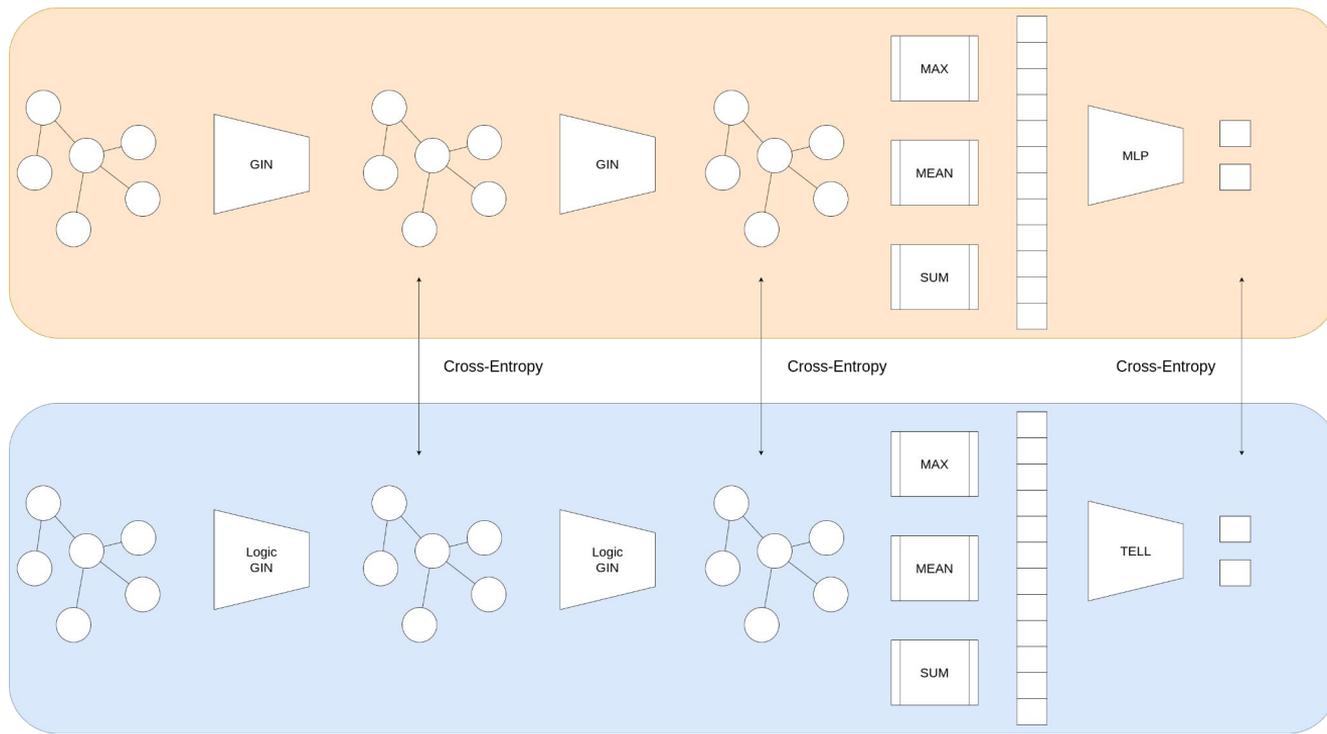
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# Training by distillation

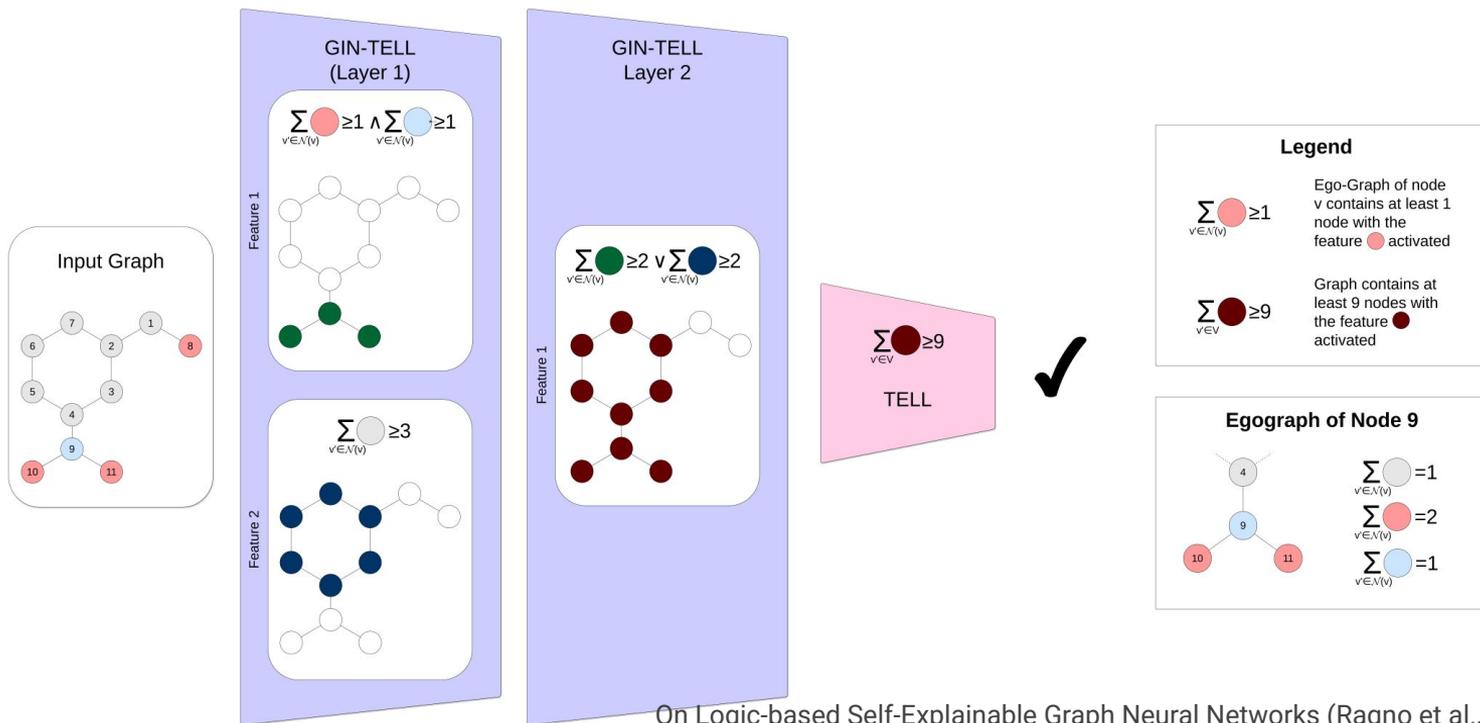
- We train a model of 5 GIN layers with Gumbel-Sigmoid activation function
- We then initialize a model of 5 Logic-GIN layers with the same characteristics
- We pretrain the logic model to replicate the first one layer-by-layer
- We terminate training with classic backpropagation on the classification task

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Pre-Training Procedure

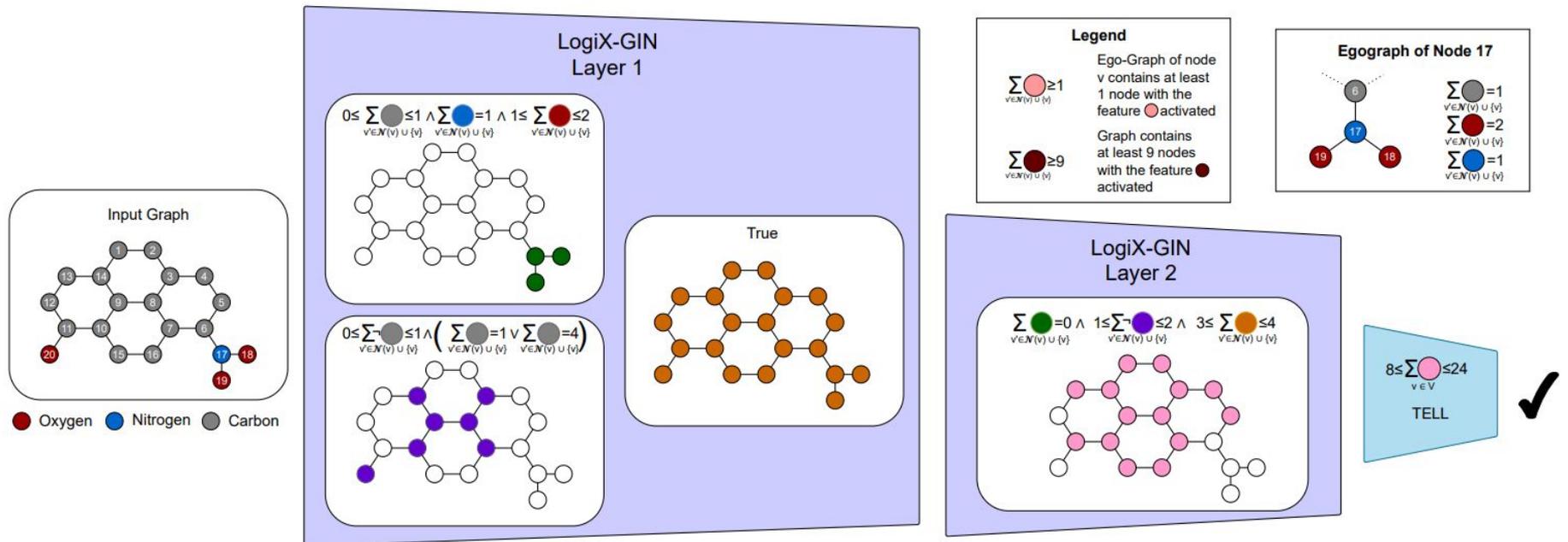


# How does Logic GIN work?



On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# An actual explanation...



On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Graded Modal Logic

Graph Structure :  $G = (V, E, \{P_i\}_{i \in I})$

- $V$  : finite set of nodes
- $E \subseteq V \times V$  : symmetric edge relation
- $P_i \subseteq V$  : unary relations interpreting predicates

Satisfaction Relation  $G, v \models \varphi(x)$  :

- $G, v \models P(x)$  : node  $v$  satisfies predicate  $P$
- $G, v \models \neg\psi(x)$  : node  $v$  does not satisfy  $\psi(x)$
- $G, v \models \psi_1(x) \wedge \psi_2(x)$  :  $v$  satisfies both formulas
- $G, v \models \psi_1(x) \vee \psi_2(x)$  :  $v$  satisfies at least one formula
- $G, v \models \exists^{\geq N} y (E(x, y) \wedge \psi_3(y))$  : at least  $N$  neighbors satisfy  $\psi_3$

Connection to GNNs : Barceló et al. show GML precisely characterizes node properties computable by certain GNN classes.

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Graded Modal Logic

**Unary Predicates:**  $Blue(x)$  and  $Red(x)$ , denote node colors

**Example 1: Atomic predicate**

$$\varphi(x) := Blue(x)$$

Formula holds if  $x$  is blue.

**Example 2: At least two red neighbors**

$$\varphi(x) := \exists \geq 2y (E(x, y) \wedge Red(y))$$

Node  $x$  has at least two neighbors that are red.

**Example 3: Blue node without red neighbors**

$$\varphi(x) := Blue(x) \wedge \neg \exists \geq 1y (E(x, y) \wedge Red(y))$$

Node  $x$  is blue and has no red neighbors.

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# The Circle of Logic

Barcelo et al. demonstrate that we can  
learn GML with GNNs



We demonstrate that we can learn a  
GNN that yields GML rules

# Results

Dataset	Black-box GIN	LogiX-GIN	Acc. Decay	Class. Obj.
BAMultiShapes	100.00 ± 0.00	100.00 ± 0.00	0.00	Graph
BA2Motifs	100.00 ± 0.00	100.00 ± 0.00	0.00	Graph
BBBP	87.95 ± 2.07	85.90 ± 0.99	2.05	Graph
MUTAG	84.74 ± 8.02	82.63 ± 5.58	2.11	Graph
NCI1	81.87 ± 1.39	78.93 ± 1.51	2.94	Graph
PROTEINS	72.59 ± 3.04	72.05 ± 5.77	0.54	Graph
Mutagenicity	82.21 ± 1.87	79.31 ± 1.25	2.90	Graph
BaShapes	97.14 ± 0.95	94.29 ± 2.52	2.85	Node
BaCommunity	81.00 ± 1.59	84.14 ± 4.55	-3.14	Node
TreeGrid	100.00 ± 0.00	98.71 ± 0.87	1.29	Node

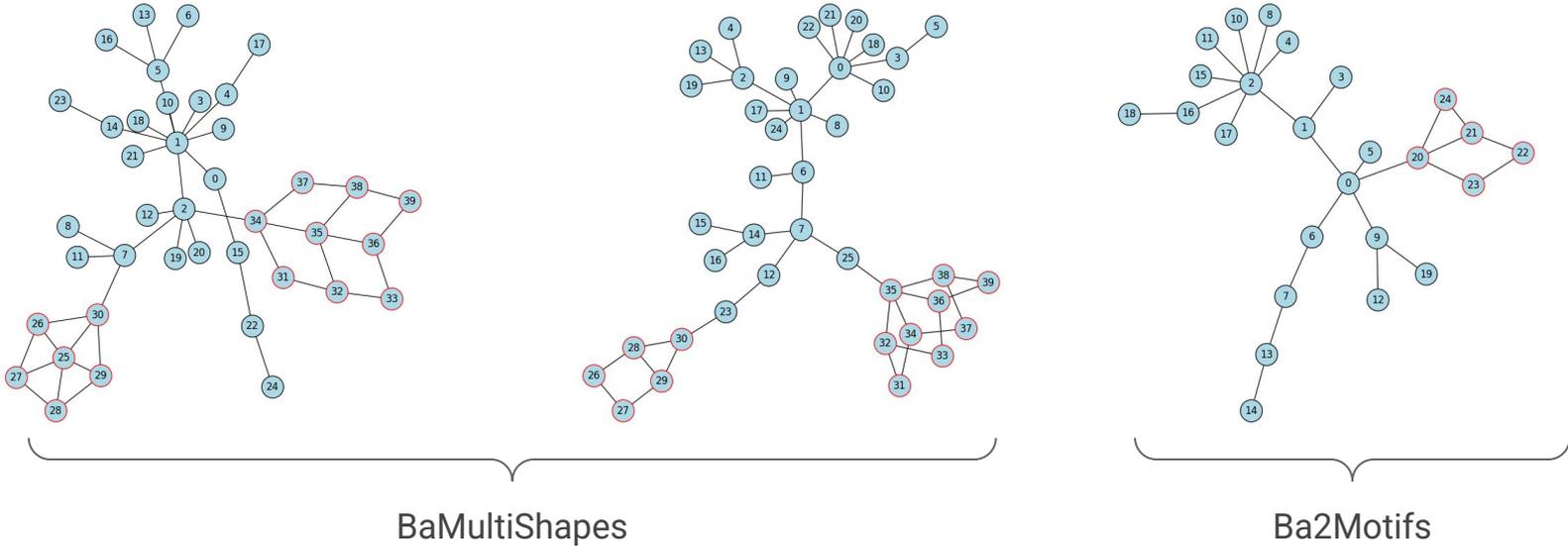
On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Results

Dataset	LogiX-GIN	PiGNN	GIB	KerGNN	GNAN
Ba2Motifs	100.00 ± 0.00	99.89 ± 0.31	100.00 ± 0.00	98.80 ± 0.75	49.10 ± 0.66
BaMultiShapes	100.00 ± 0.00	85.40 ± 5.08	97.60 ± 2.06	83.20 ± 1.94	49.10 ± 0.66
MUTAG	82.63 ± 5.58	82.51 ± 10.48	90.53 ± 6.14	82.11 ± 9.18	55.79 ± 16.43
Mutagenicity	79.31 ± 1.25	82.39 ± 1.68	80.14 ± 0.98	73.32 ± 2.93	55.36 ± 0.52
NCI1	78.93 ± 1.51	78.54 ± 2.74	78.15 ± 1.32	69.00 ± 1.38	50.80 ± 1.15
PROTEINS	72.05 ± 5.77	70.00 ± 2.44	68.47 ± 5.00	72.97 ± 4.87	57.67 ± 2.62
BBBP	85.90 ± 0.99	83.54 ± 0.37	84.78 ± 2.57	84.12 ± 2.09	22.80 ± 0.86

On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Can Logic GIN identify relevant subgraphs?



On Logic-based Self-Explainable Graph Neural Networks (Ragno et al., 2025, NeurIPS)

# Limitation and Future Work

- Due to GML limitations, LogiX-GIN expressiveness is limited to counting nodes in neighborhoods.
- Training takes a lot of time due to the distillation procedure (this is TELL's fault)

## Future Work:

Limitations + Real world domains such as chemistry

# Preliminary Results: Higher Expressivity

Dataset	Gumbel-GIN	Gumbel-Me	LogiX-GIN	LogiX-Me
BaMultiShapes	99.90 ± 0.32	100.00 ± 0.00	100.00 ± 0.00	100.00 ± 0.00
Ba2Motifs	75.00 ± 26.48	99.90 ± 0.32	100.00 ± 0.00	100.00 ± 0.00
BBBP	88.54 ± 1.89	86.20 ± 2.47	85.90 ± 0.99	86.44 ± 2.02
MUTAG	85.26 ± 8.88	78.95 ± 9.28	82.63 ± 5.58	85.26 ± 4.40
NCI1	80.95 ± 1.19	80.36 ± 1.55	78.93 ± 1.51	77.57 ± 1.70
PROTEINS	75.00 ± <i>nan</i>	73.39 ± 4.47	72.05 ± 5.77	75.18 ± 6.23
Mutagenicity	81.75 ± 1.75	81.64 ± 1.93	79.31 ± 1.25	78.62 ± 3.02
BaShapes	95.00 ± 1.68	96.86 ± 0.60	94.29 ± 2.52	97.43 ± 1.56
BaCommunity	84.71 ± 2.36	95.07 ± 1.63	84.14 ± 4.55	94.29 ± 1.01
TreeGrid	96.94 ± 1.97	98.71 ± 1.58	98.71 ± 0.04	99.35 ± 0.36

# Preliminary Results: Chemistry

## Functional groups in organic chemistry

Functional groups are the characteristic groups in organic molecules that give them their reactivity. In the formulae below, R represents the rest of the molecule and X represents any halogen atom.

● Hydrocarbons 
 ● Halogen-containing groups 
 ● Oxygen-containing groups 
 ● Nitrogen-containing groups 
 ● Sulfur-containing groups 
 ● Phosphorus-containing groups

<b>Alkane</b> Naming: -ane e.g. ethane	<b>Alkene</b> Naming: -ene e.g. ethene	<b>Alkyne</b> Naming: -yne e.g. ethyne	<b>Arene</b> Naming: -yl benzene e.g. ethyl benzene	<b>Haloalkane</b> Naming: halo- e.g. chloroethane	<b>Alcohol</b> Naming: -ol e.g. ethanol	<b>Aldehyde</b> Naming: -al e.g. ethanal	<b>Ketone</b> Naming: -one e.g. propanone	<b>Carboxylic acid</b> Naming: -oic acid e.g. ethanoic acid	<b>Acid anhydride</b> Naming: -oic anhydride e.g. ethanoic anhydride
<b>Acyl halide</b> Naming: -oyl halide e.g. ethanoyl chloride	<b>Ester</b> Naming: -yl -oate e.g. ethyl ethanoate	<b>Ether</b> Naming: -oxy -ane e.g. ethoxyethane	<b>Epoxide</b> Naming: -ene oxide e.g. ethene oxide	<b>Amine</b> Naming: -amine e.g. ethanamine	<b>Amide</b> Naming: -amide e.g. ethanamide	<b>Nitrate</b> Naming: -yl nitrate e.g. ethyl nitrate	<b>Nitrite</b> Naming: -yl nitrite e.g. ethyl nitrite	<b>Nitrile</b> Naming: -nitrile e.g. ethanenitrile	<b>Nitro</b> Naming: nitro- e.g. nitromethane
<b>Nitroso</b> Naming: nitroso- e.g. nitrosobenzene	<b>Imine</b> Naming: -imine e.g. ethanimine	<b>Imide</b> Naming: -imide e.g. succinimide	<b>Azide</b> Naming: -yl azide e.g. phenyl azide	<b>Cyanate</b> Naming: -yl cyanate e.g. methyl isocyanate	<b>Isocyanate</b> Naming: -yl isocyanate e.g. methyl isocyanate	<b>Azo compound</b> Naming: azo- e.g. azobenzene	<b>Thiol</b> Naming: -thiol e.g. methanethiol	<b>Sulfide</b> Naming: sulfide e.g. dimethyl sulfide	<b>Disulfide</b> Naming: disulfide e.g. dimethyl disulfide
<b>Sulfoxide</b> Naming: sulfoxide e.g. dimethyl sulfoxide	<b>Sulfone</b> Naming: sulfone e.g. dimethyl sulfone	<b>Sulfonic acid</b> Naming: sulfonic acid e.g. benzenesulfonic acid	<b>Sulfonic acid</b> Naming: sulfonic acid e.g. benzenesulfonic acid	<b>Sulfonate ester</b> Naming: -yl sulfonate e.g. methyl methanesulfonate	<b>Thiocyanate</b> Naming: thiocyanate e.g. ethyl thiocyanate	<b>Isothiocyanate</b> Naming: isothiocyanate e.g. ethyl isothiocyanate	<b>Thial</b> Naming: -thial e.g. ethanethial	<b>Thioketone</b> Naming: -thione e.g. propanethione	<b>Phosphine</b> Naming: phosphine e.g. methylphosphane

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	dataset	acc	rocauc	exp	model	grouping_method
0	HIV	96.98 ± 0.38	75.31 ± 2.71	256	GIN	NaN
1	HIV	96.77 ± 0.70	73.85 ± 3.52	64	FG_GIN	functional
2	HIV	97.08 ± 0.35	72.70 ± 2.97	64	FG_GIN	brics
3	HIV	96.86 ± 0.60	75.65 ± 3.07	64	FG_LOGIXGIN	functional
4	HIV	96.93 ± 0.64	73.30 ± 3.48	64	FG_LOGIXGIN	brics
5	BBBP	81.95 ± 2.18	80.89 ± 6.92	256	GIN	NaN
6	BBBP	81.95 ± 4.46	85.27 ± 4.52	64	FG_GIN	functional
7	BBBP	79.61 ± 3.80	81.86 ± 6.24	64	FG_GIN	brics
8	BBBP	83.32 ± 3.49	85.26 ± 4.09	64	FG_LOGIXGIN	functional
9	BBBP	81.27 ± 3.79	82.67 ± 5.83	64	FG_LOGIXGIN	brics
10	Tox21	71.32 ± 10.40	nan ± nan	106	GIN	NaN
11	Tox21	71.05 ± 10.45	nan ± nan	30	FG_GIN	functional
12	Tox21	71.02 ± 10.31	nan ± nan	32	FG_GIN	brics
13	Tox21	71.09 ± 10.47	nan ± nan	36	FG_LOGIXGIN	functional
14	Tox21	70.70 ± 10.38	nan ± nan	31	FG_LOGIXGIN	brics
19	BACE	76.03 ± 2.12	81.67 ± 2.32	256	GIN	NaN
20	BACE	74.17 ± 3.54	82.13 ± 2.99	64	FG_GIN	functional
21	BACE	76.16 ± 2.77	81.31 ± 0.76	64	FG_GIN	brics
22	BACE	74.44 ± 4.04	79.47 ± 4.03	64	FG_LOGIXGIN	functional
23	BACE	75.10 ± 4.10	81.22 ± 1.98	64	FG_LOGIXGIN	brics

Thank You