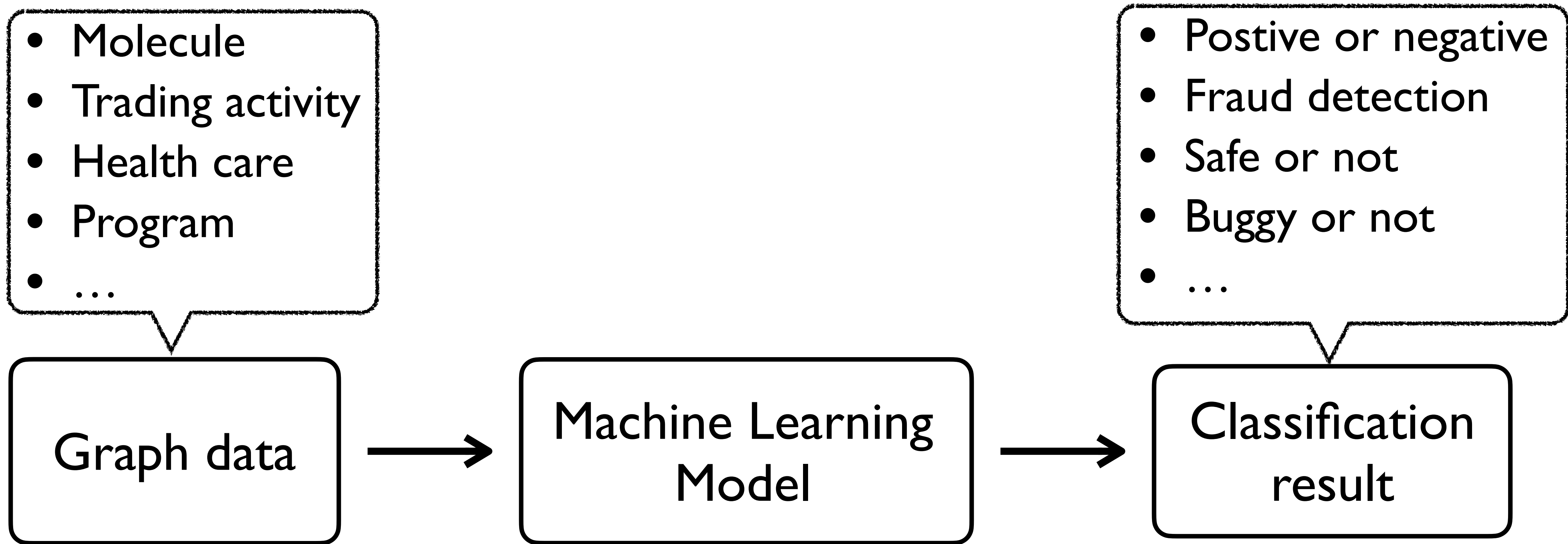




PL4XGL: A Programming Language Approach to Explainable Graph Learning

Minseok Jeon

18 September 2025 @ IC637



- Molecule
- Trading activity
- Health care
- Program
- ...

- Postive or negative
- Fraud detection
- Safe or not
- Buggy or not
- ...

Graph data



Graph
Neural Network



Classification
result

- GNN is the dominant graph machine learning method

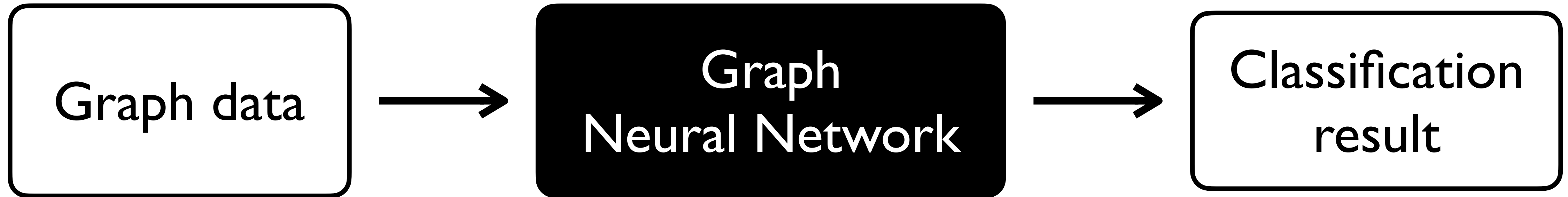


arXiv

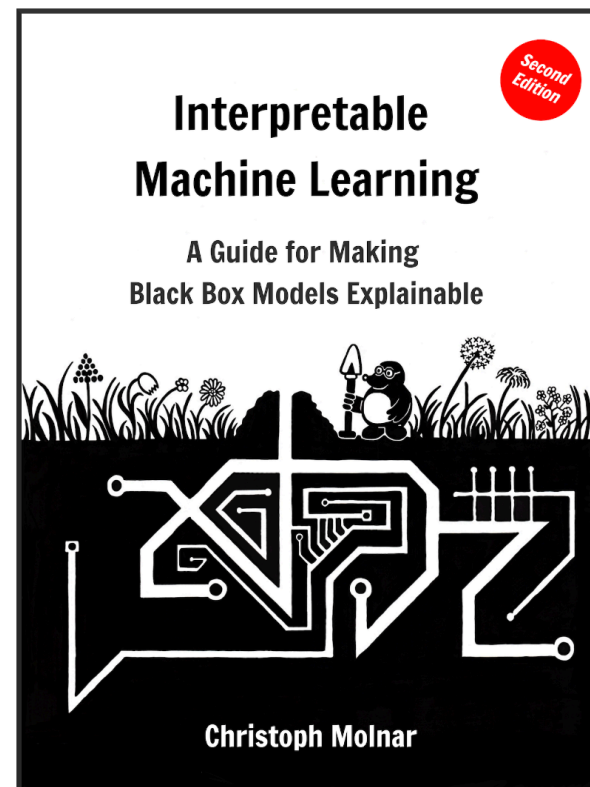
<https://arxiv.org> › cs

Semi-Supervised Classification with Graph Convolutional ...

TN Kipf 저술 2016 · 32974회 인용 — Access Paper: View a PDF of the paper titled Semi-Supervised Classification with Graph Convolutional Networks, by Thomas N. Kipf and 1 other ...



Problem
Does not explain **why**



The value of **why** is growing fast

A correct prediction only partially solves your problem. The model must also explain **why**.

- Molnar [2022]

Graph data



Graph
Neural Network

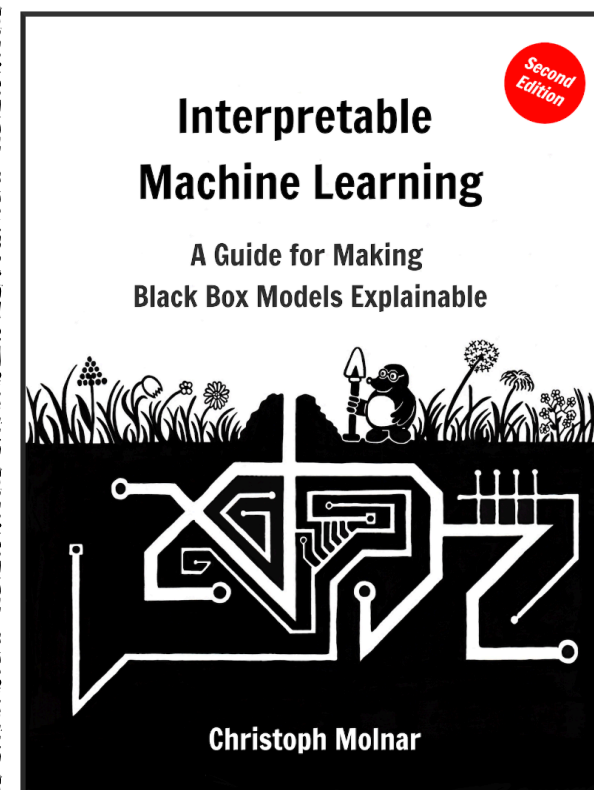


Classification
result

- Health care
- Trading activity
- ...

Problem
Does not explain **why**

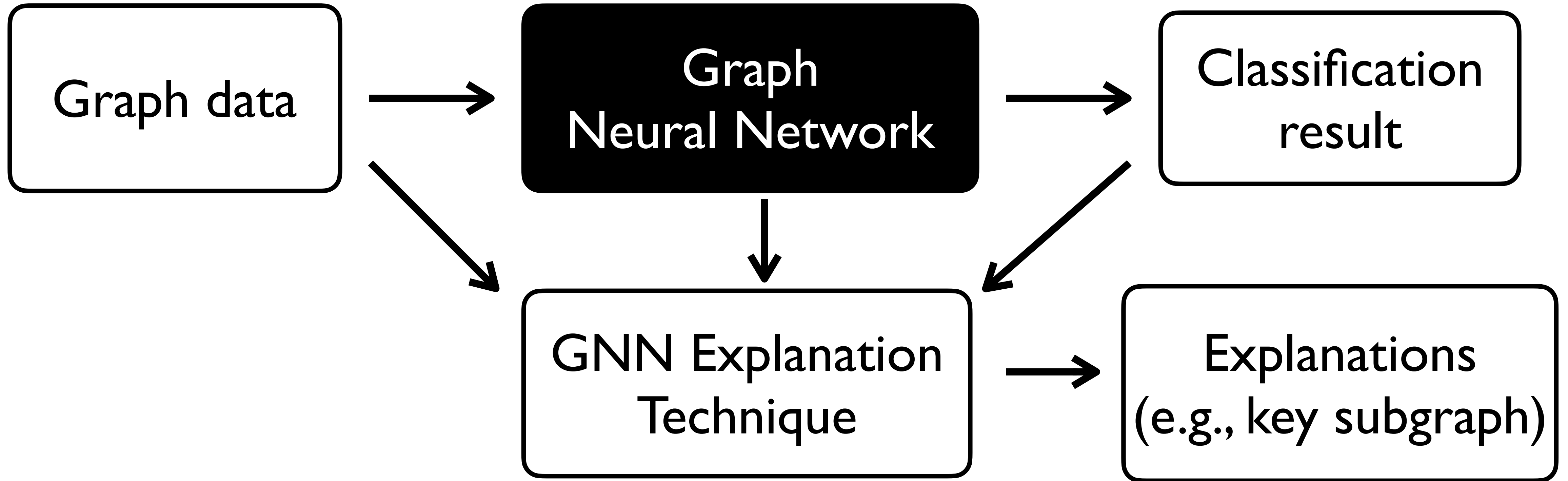
- Safe or not
- Fraud or not
- ...

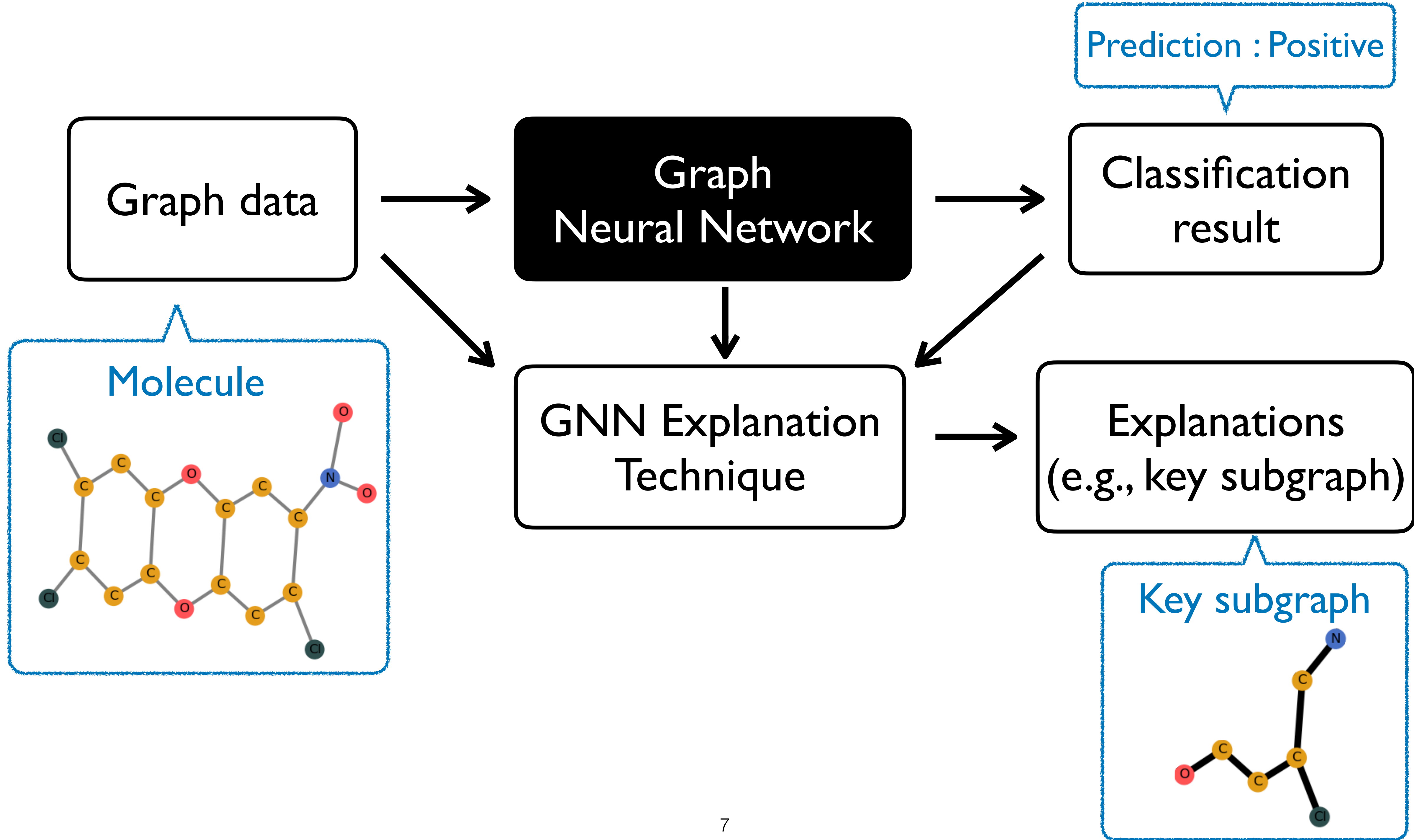


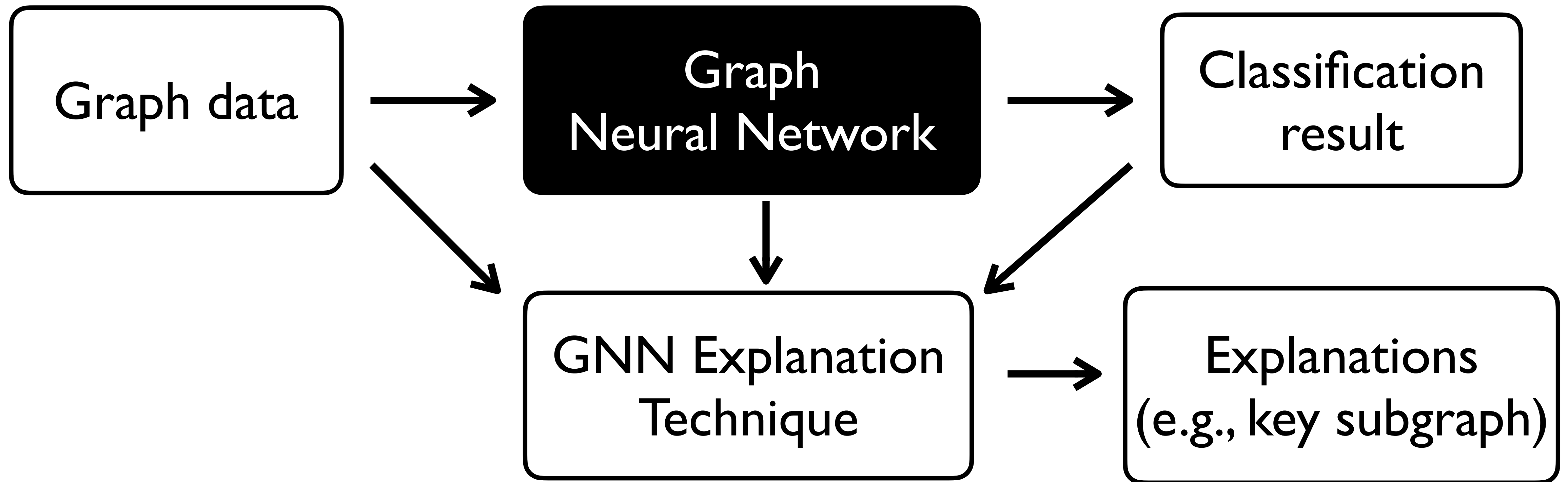
The value of **why** is growing fast

A correct prediction only partially solves your problem. The model must also explain **why**.

- Molnar [2022]







Two key limitations

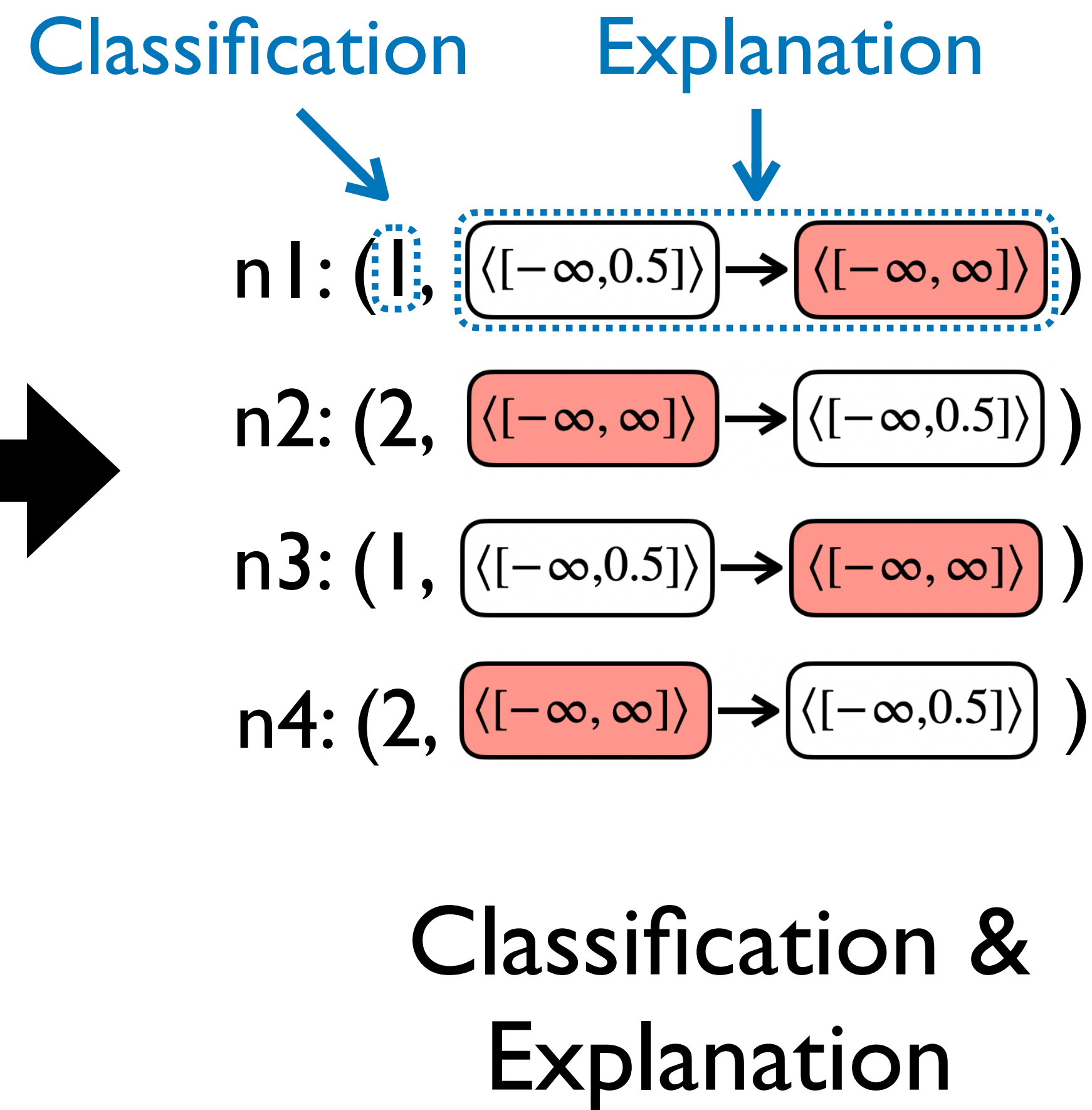
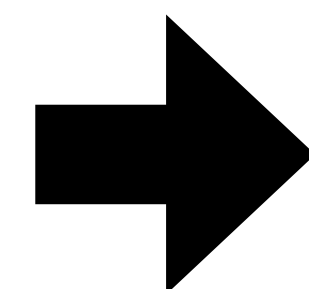
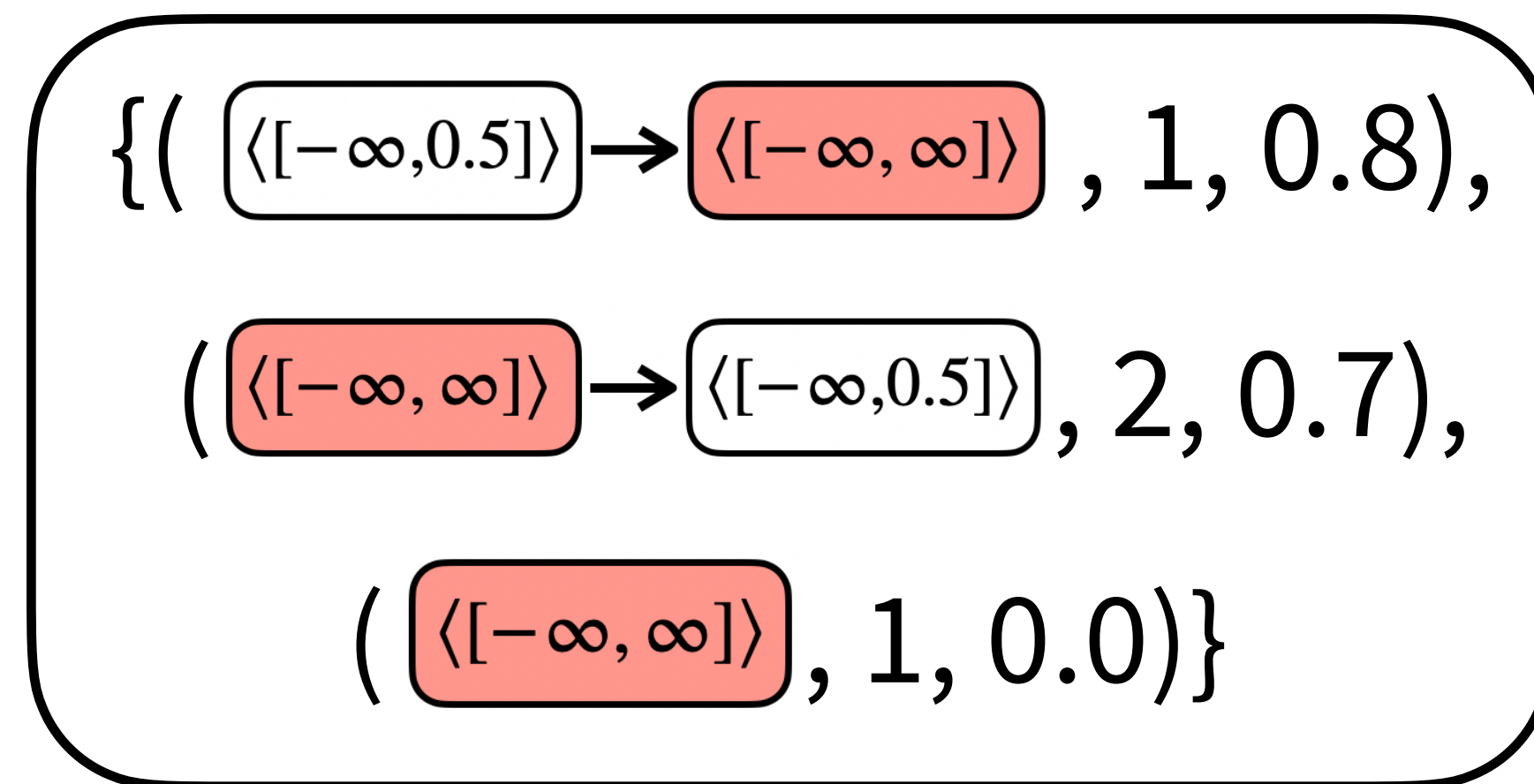
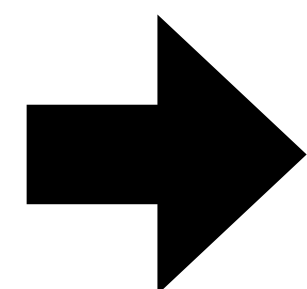
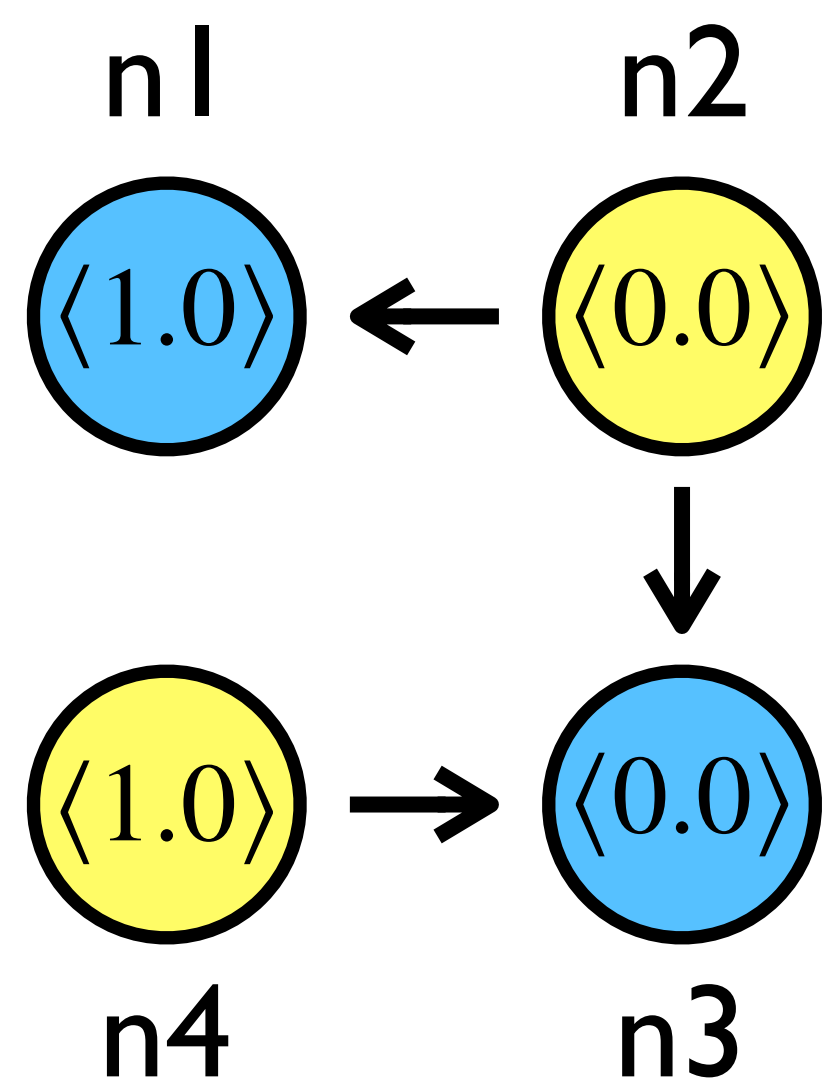
- Additional (expensive) explanation cost is required
- The explanations are not guaranteed to be correct

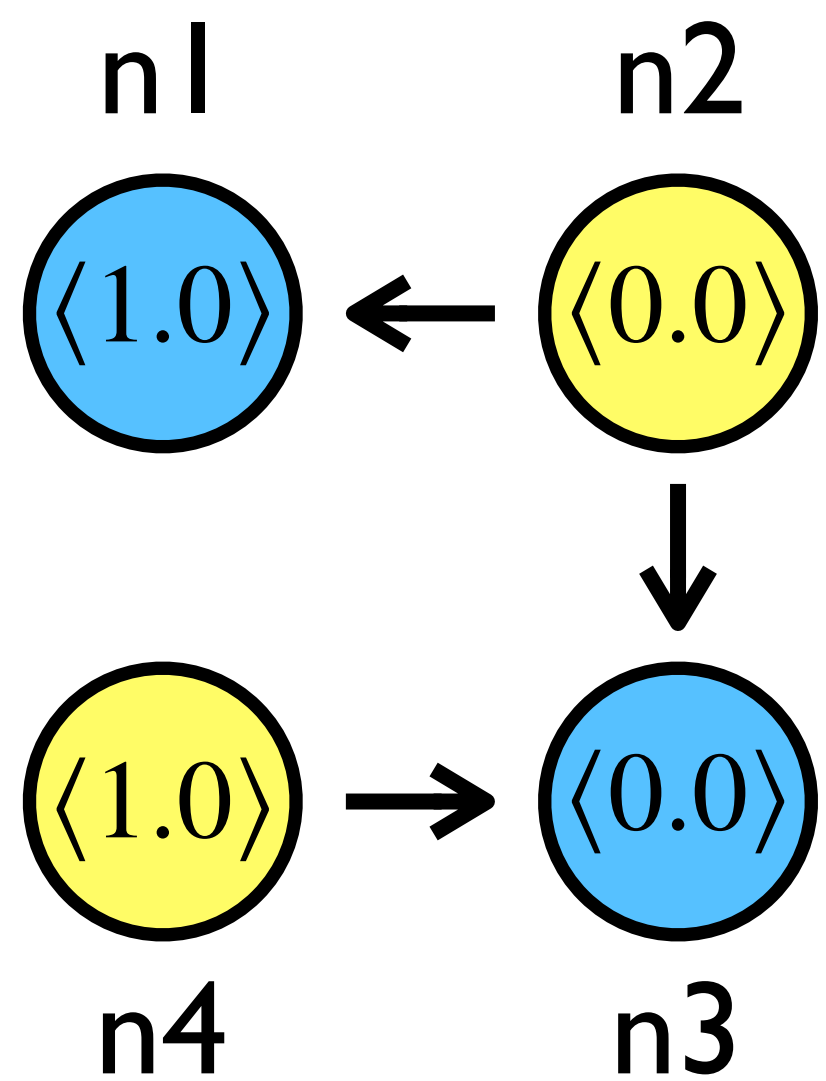
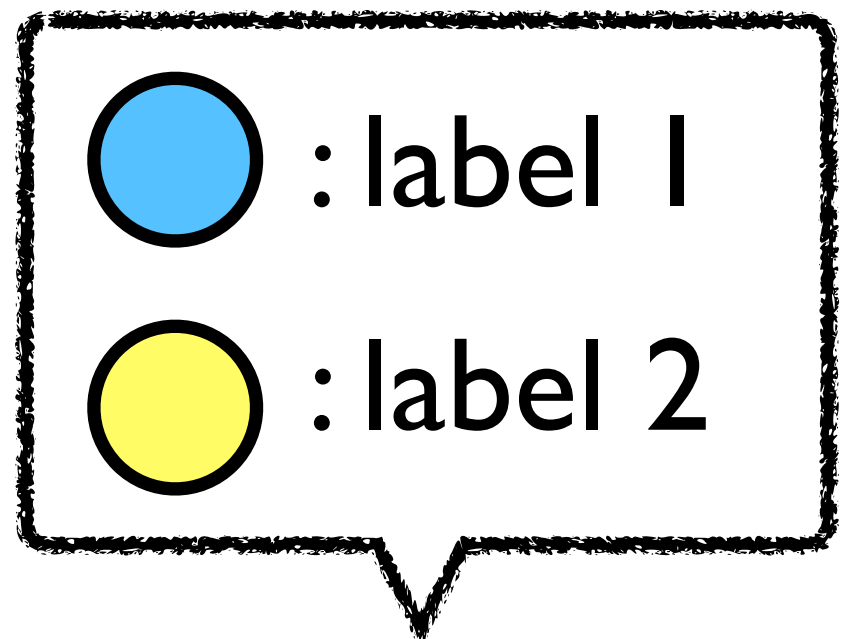
- PL4XGL: inherently explainable graph machine learning method



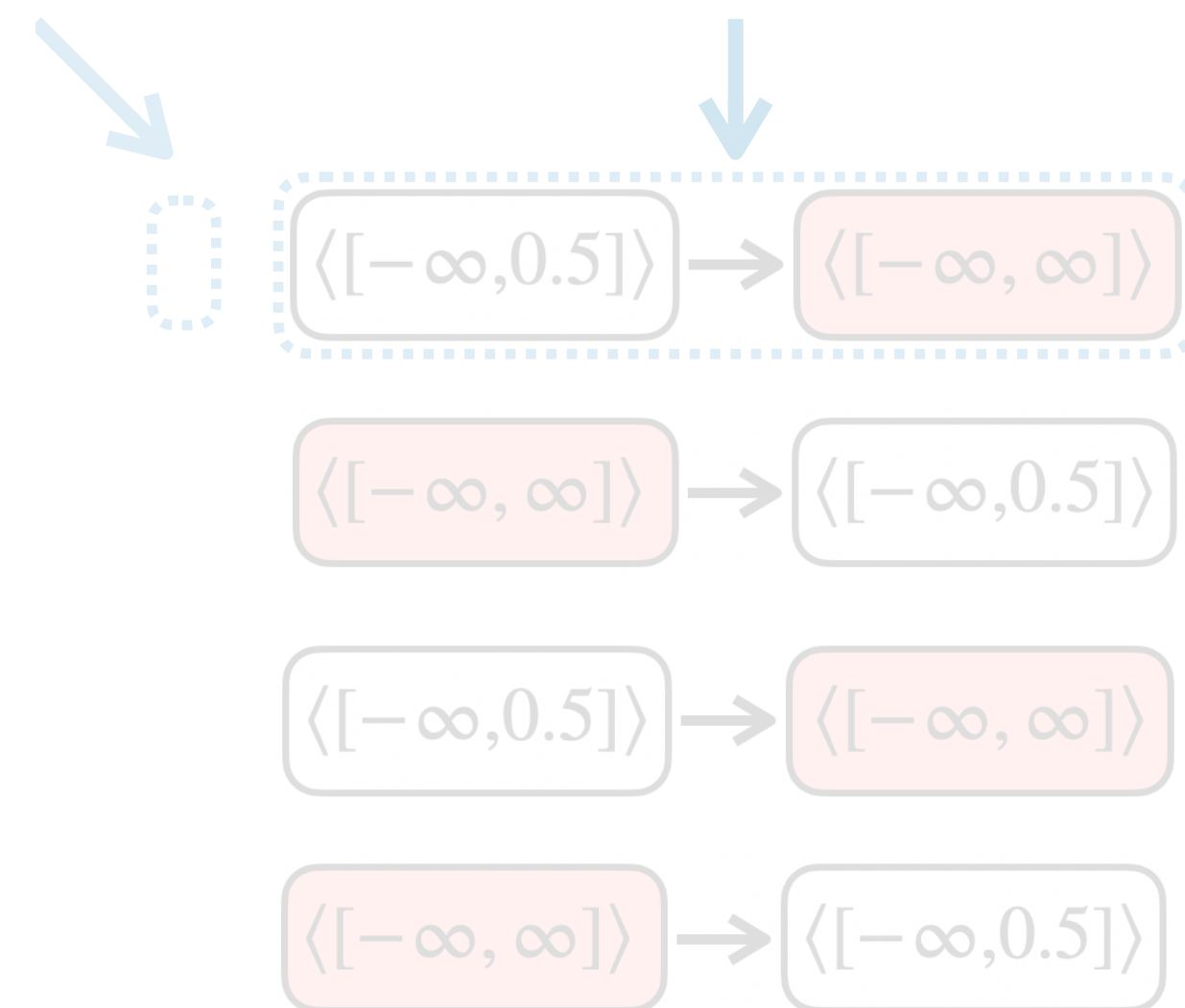
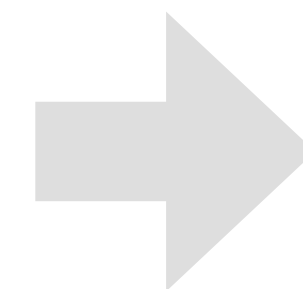
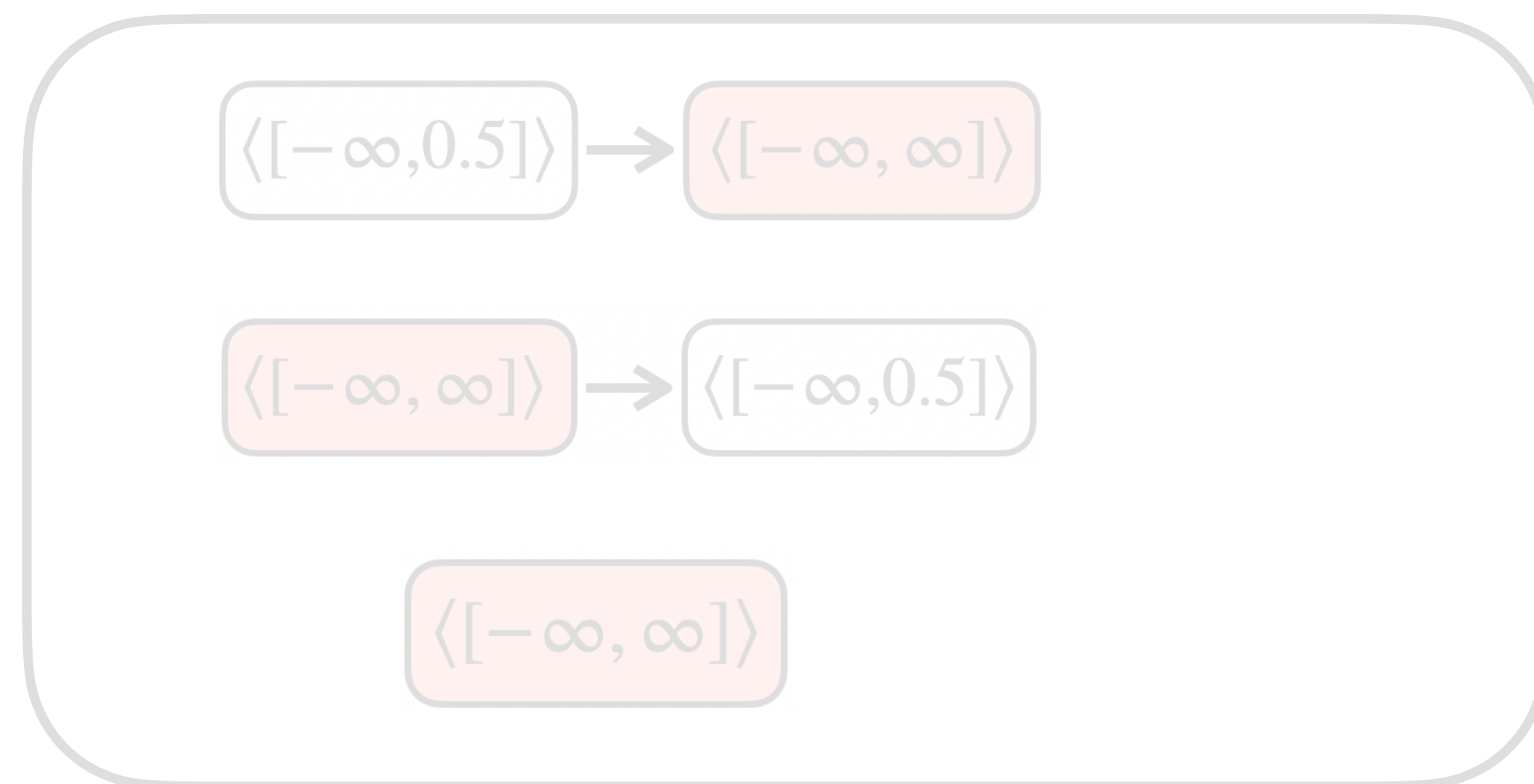
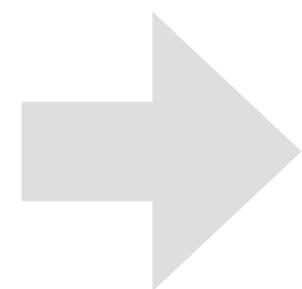
Graph Description Language (GDL)

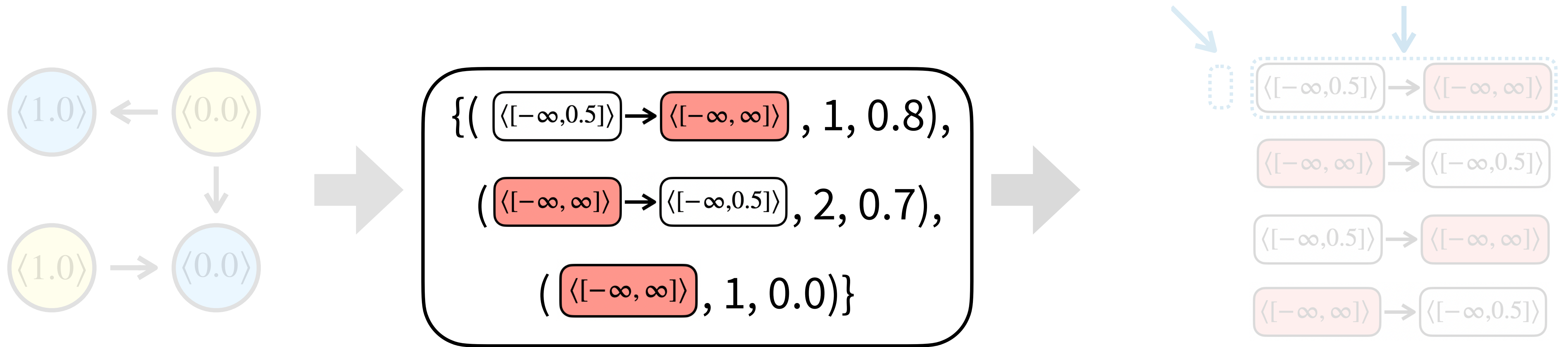
Programs	$P ::= \bar{\delta} \text{ target } t$	$\in \mathcal{P} = \mathcal{D}^* \times \mathcal{T}$
Descriptions	$\delta ::= \delta_V \mid \delta_E$	$\in \mathcal{D} = \mathcal{D}_V \uplus \mathcal{D}_E$
Node Descriptions	$\delta_V ::= \text{node } x < \bar{\phi} > ?$	$\in \mathcal{D}_V = \mathbb{X} \times \Phi^d$
Edge Descriptions	$\delta_E ::= \text{edge } (x, x) < \bar{\phi} > ?$	$\in \mathcal{D}_E = \mathbb{X} \times \mathbb{X} \times \Phi^c$
Target Symbols	$t ::= \text{node } x \mid \text{edge } (x, x) \mid \text{graph}$	$\in \mathcal{T} = \mathbb{X} \uplus (\mathbb{X} \times \mathbb{X}) \uplus \{\epsilon\}$
Intervals	$\phi ::= [n^?, n^?]$	$\in \Phi = (\mathbb{R} \uplus \{-\infty\}) \times (\mathbb{R} \uplus \{\infty\})$
Real Numbers	$n ::= 0.2 \mid 0.7 \mid 6 \mid -8 \dots$	$\in \mathbb{R}$
Variables	$x ::= x \mid y \mid z \mid \dots$	$\in \mathbb{X}$



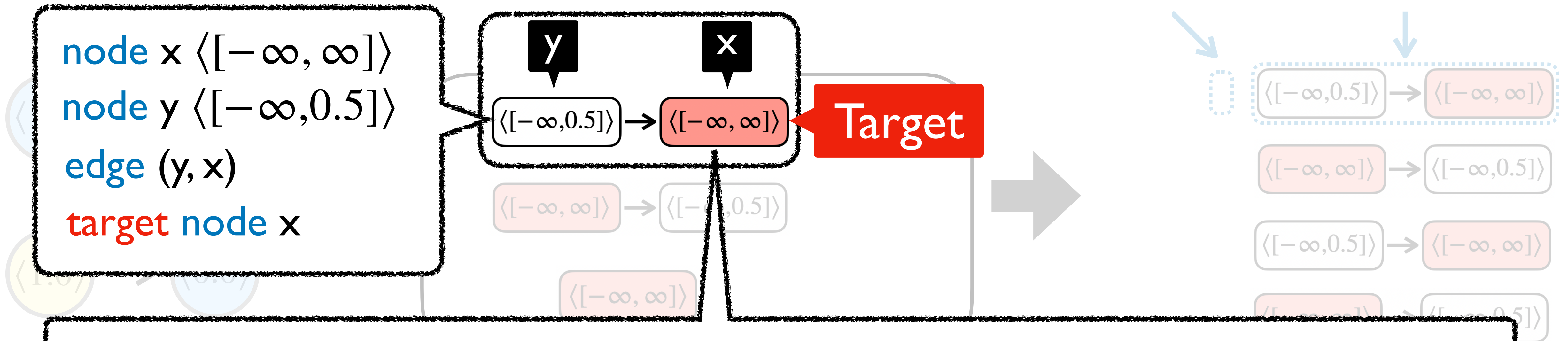


Graph data





Our model



The GDL program is describing:

“**Nodes** having a predecessor whose feature value is equal or less than 0.5”

Such nodes will be classified into label 1

node $x \langle [-\infty, \infty] \rangle$
node $y \langle [-\infty, 0.5] \rangle$
edge (y, x)
target node x

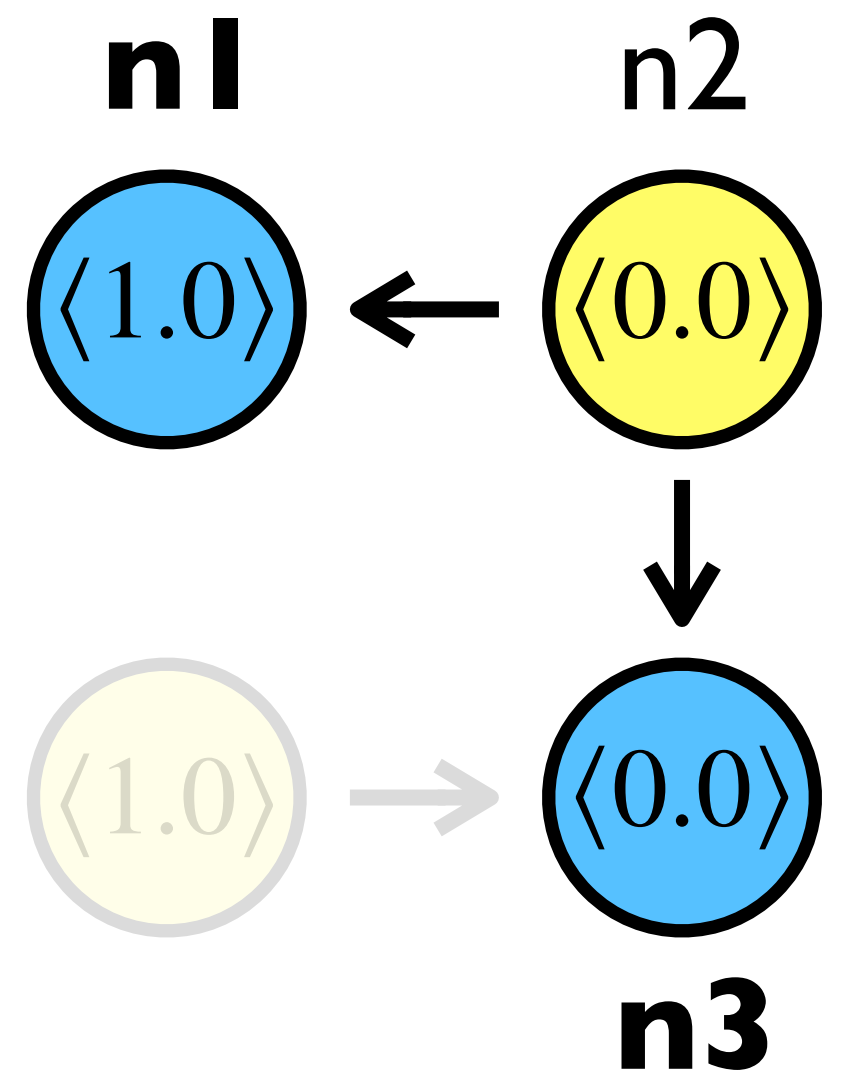
$\langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle, 1, 0.8$

Score of the program is 0.8

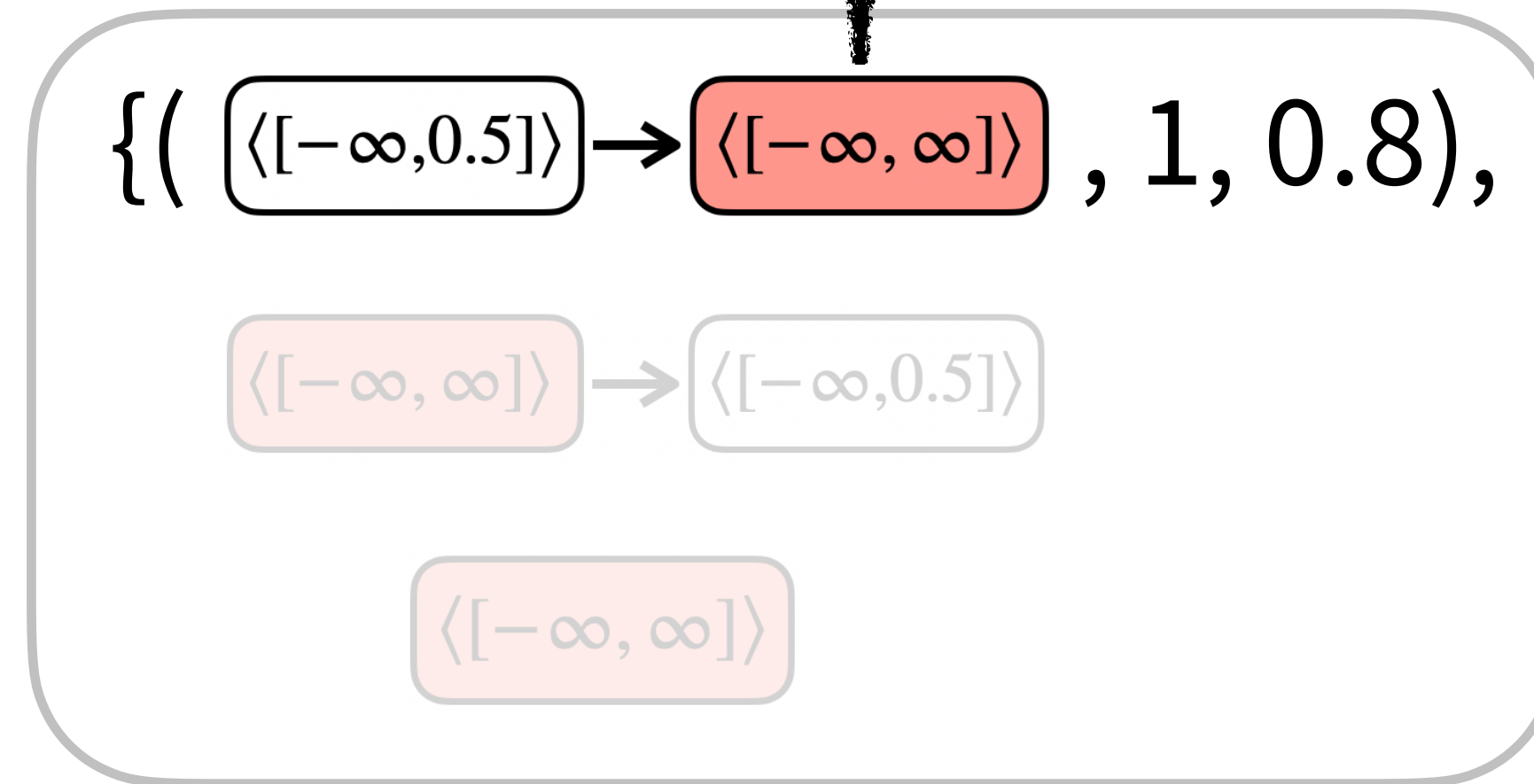
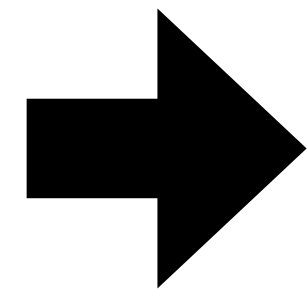
The GDL program is describing:

“Nodes having a predecessor whose feature value is equal or less than 0.5”

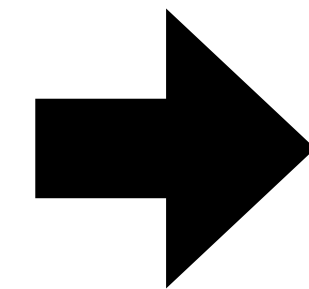
The GDL program is describing:
“**Nodes** having a predecessor whose feature value is equal or less than 0.5”



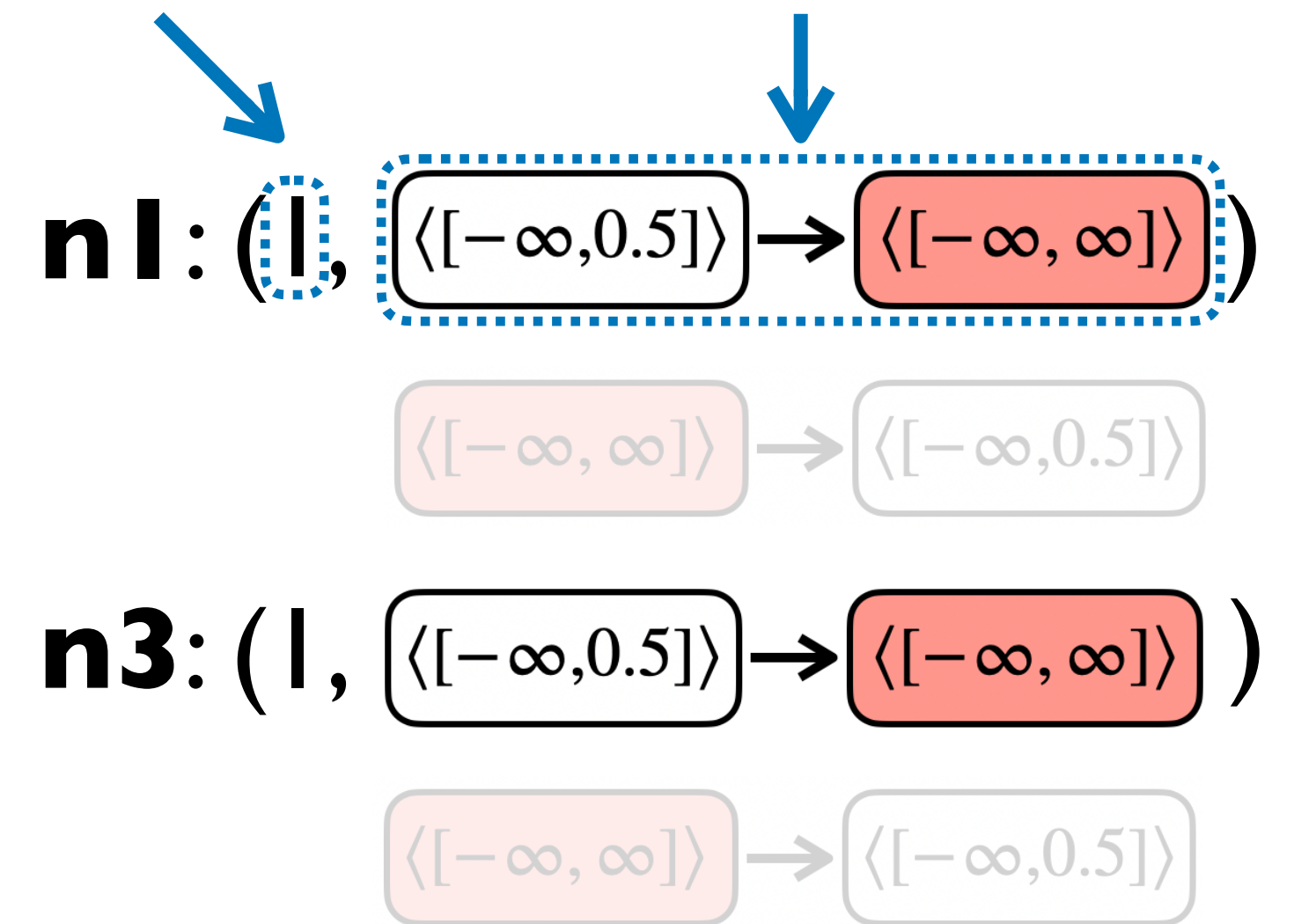
Graph data



Our model



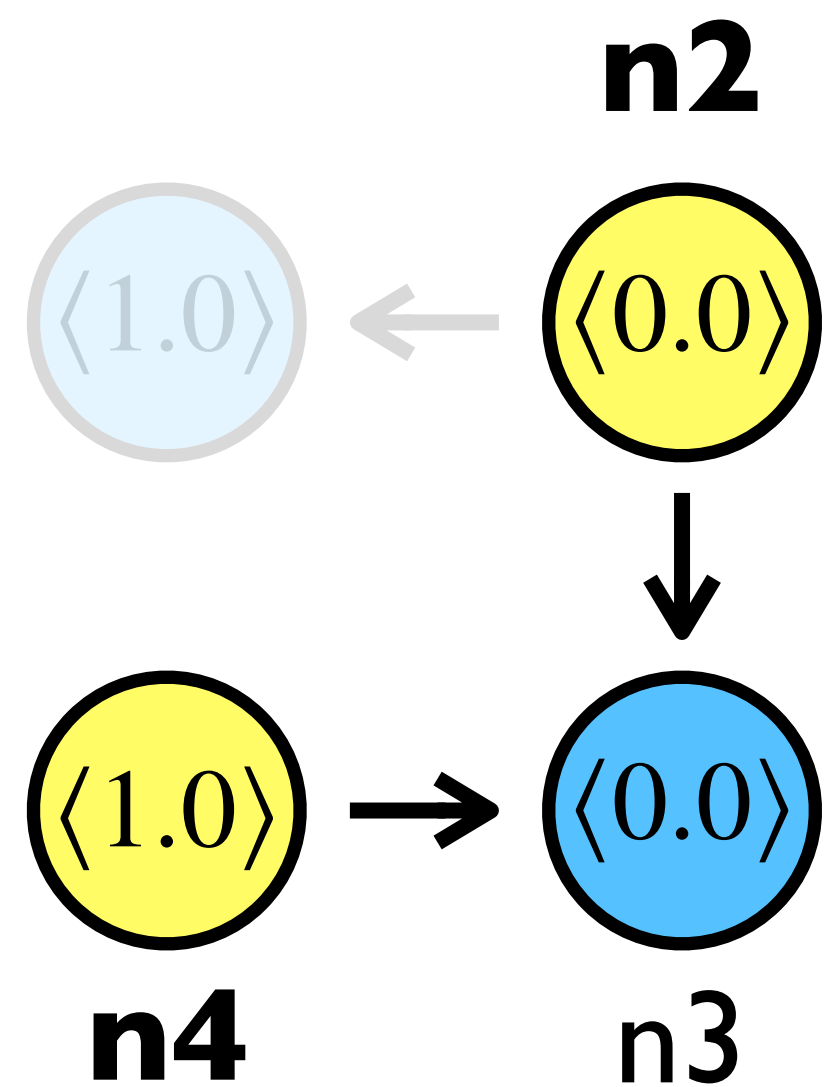
Classification Explanation



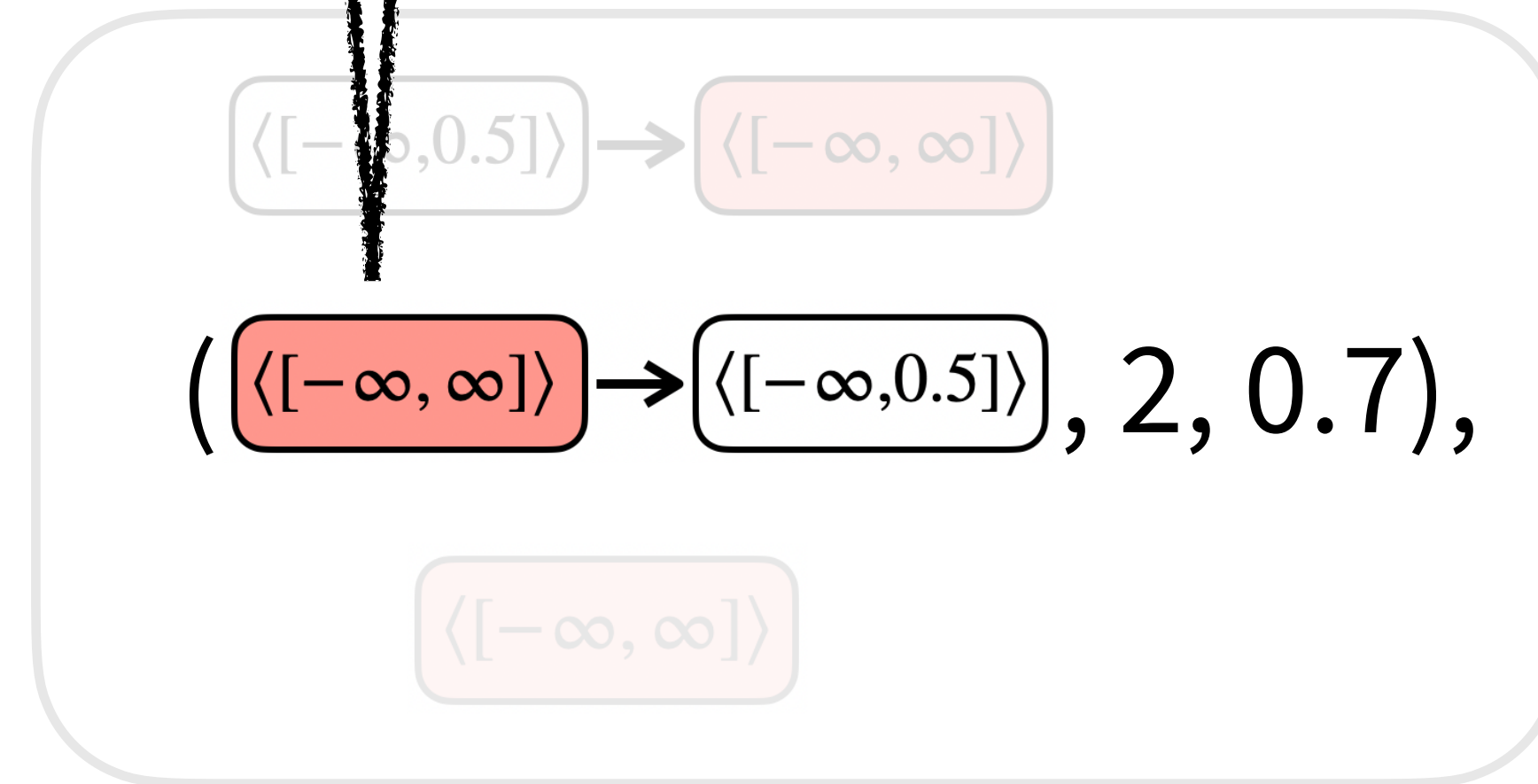
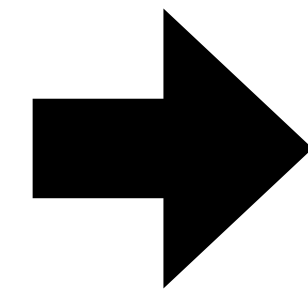
Classification & Explanation

The GDL program is describing:

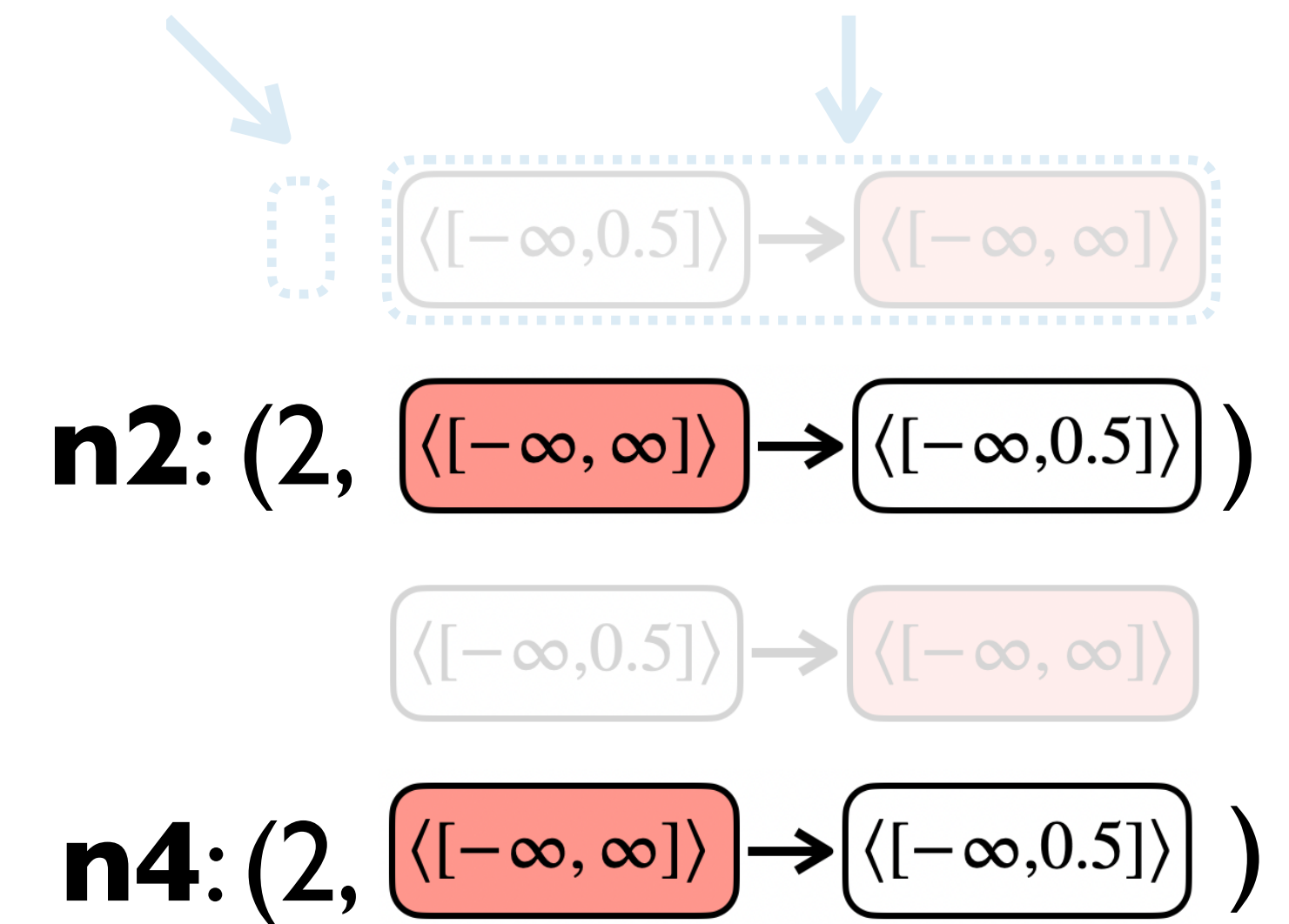
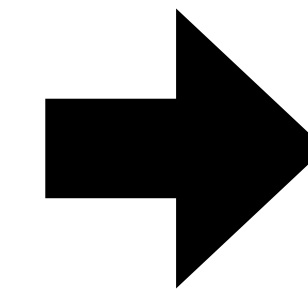
“**Nodes** having a successor whose feature value is equal or less than 0.5”



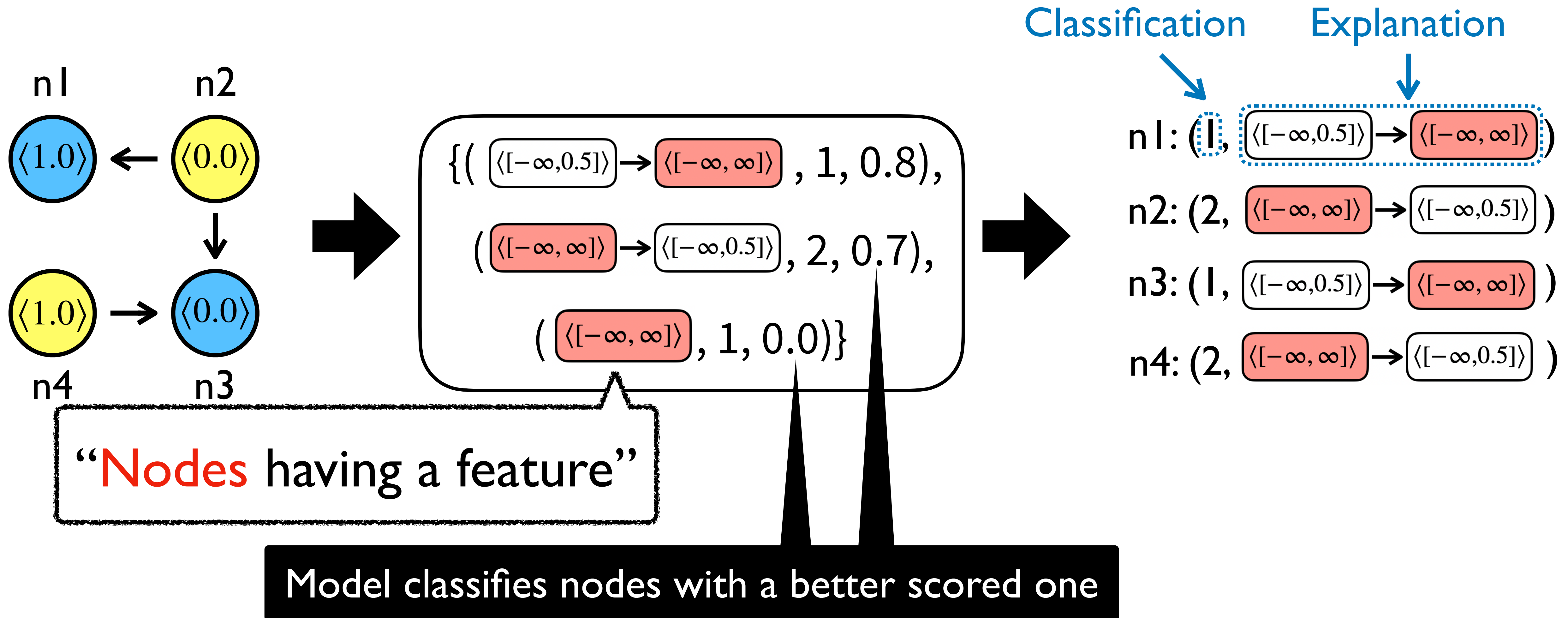
Graph data

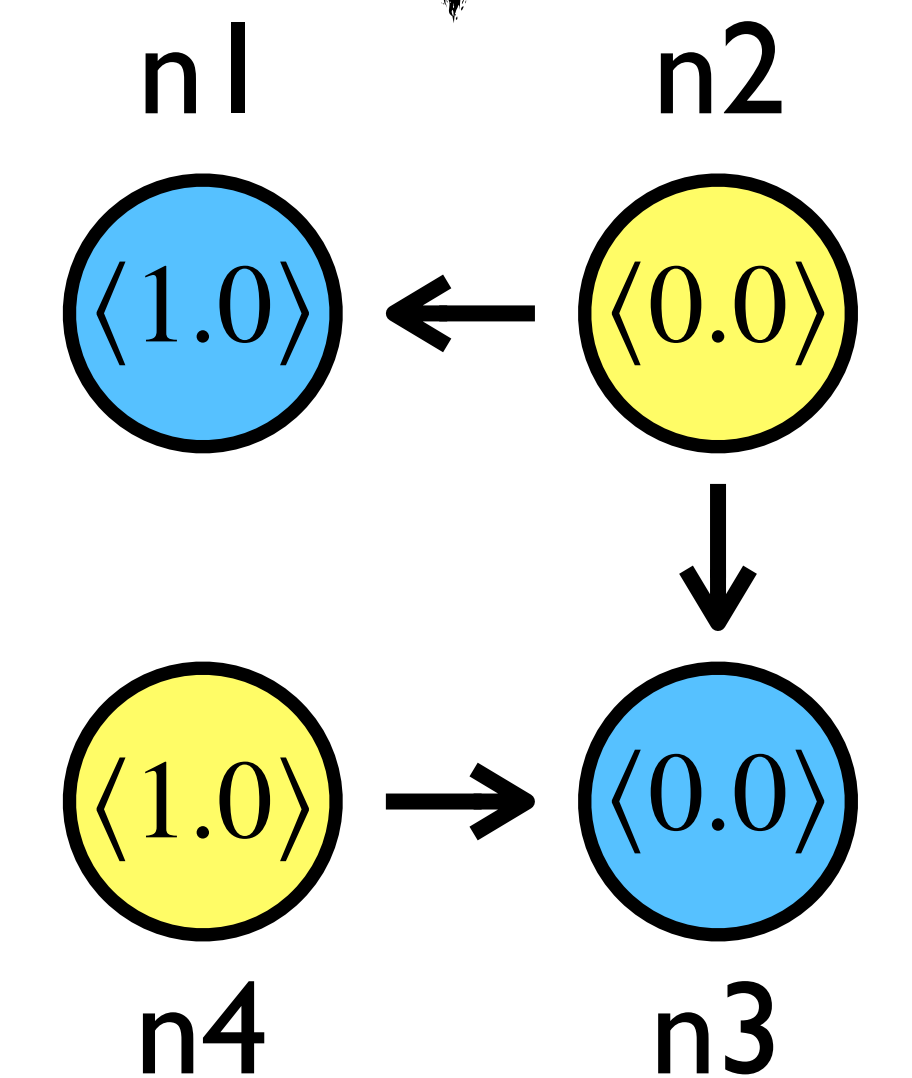
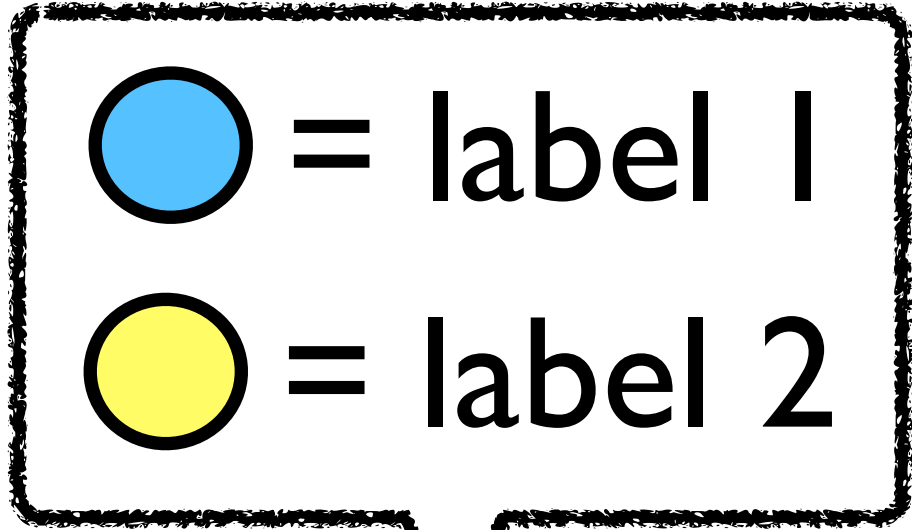


Our model



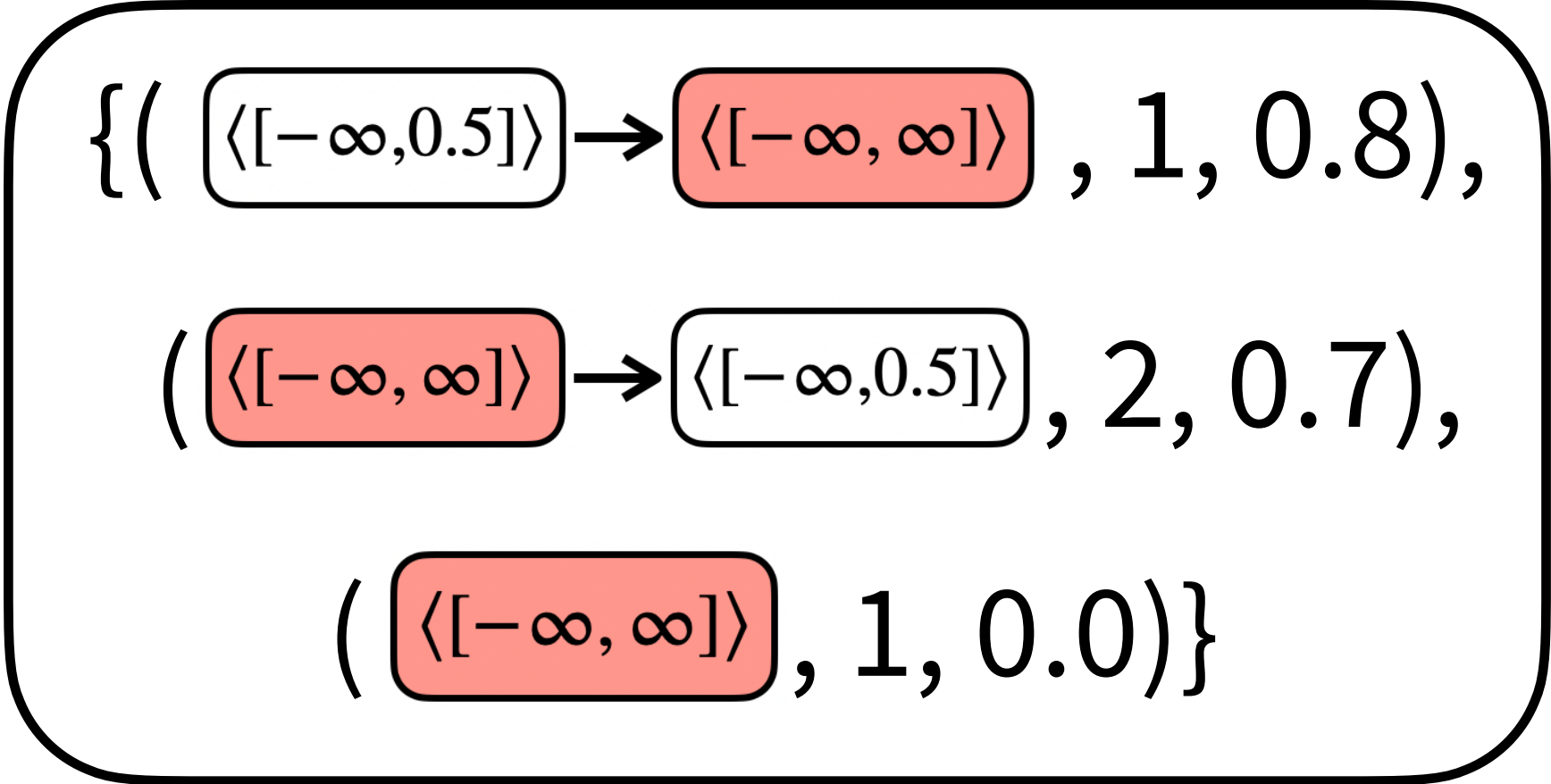
Classification & Explanation





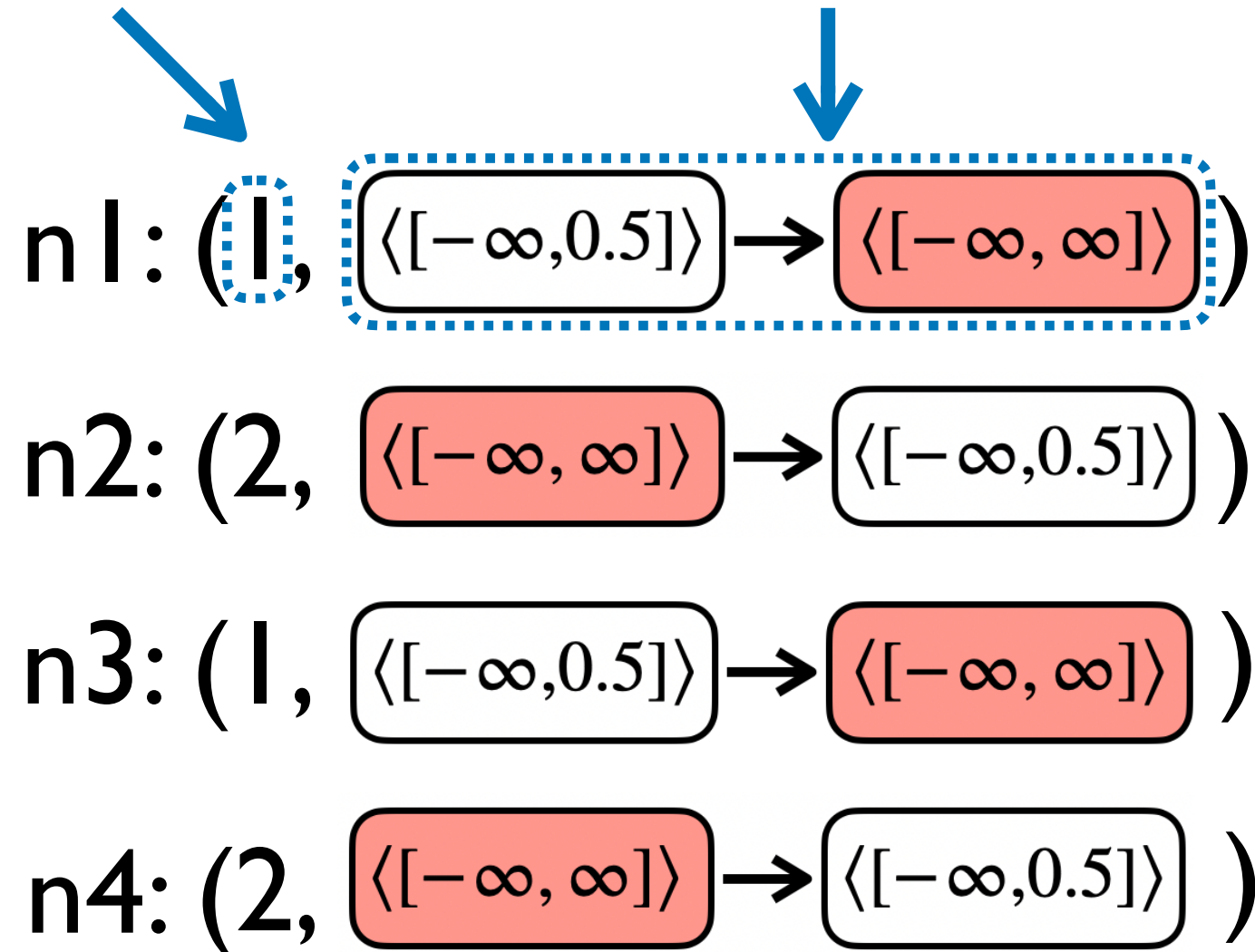
Graph data

- No additional explanation cost
- Explanations are guaranteed to be correct

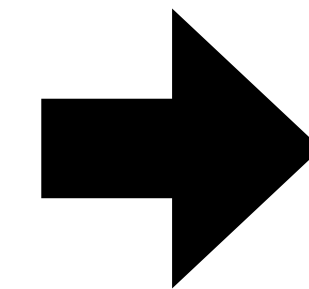
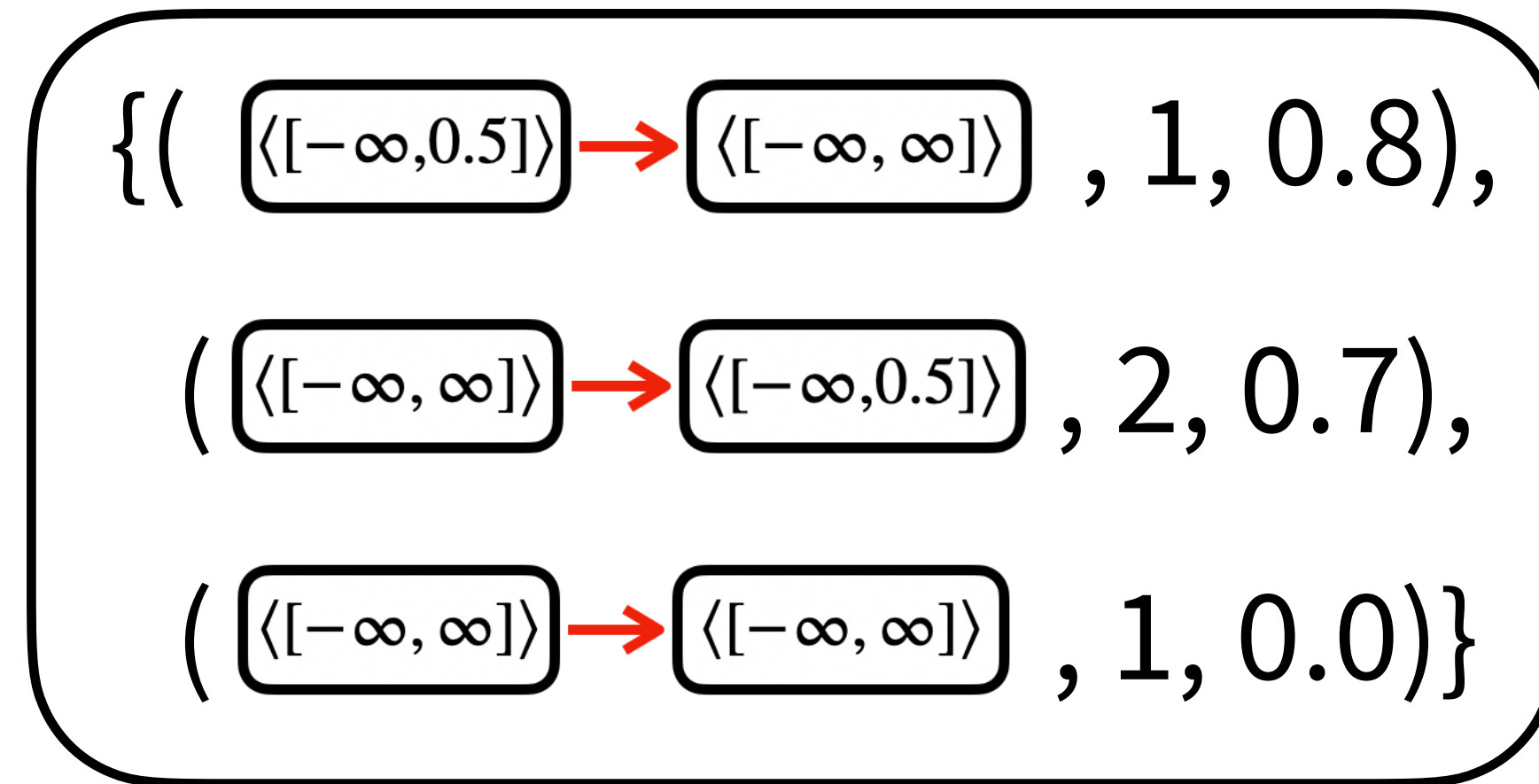
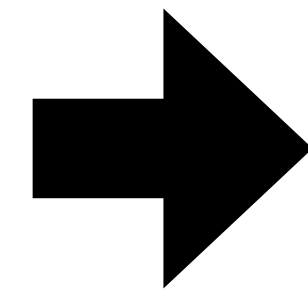
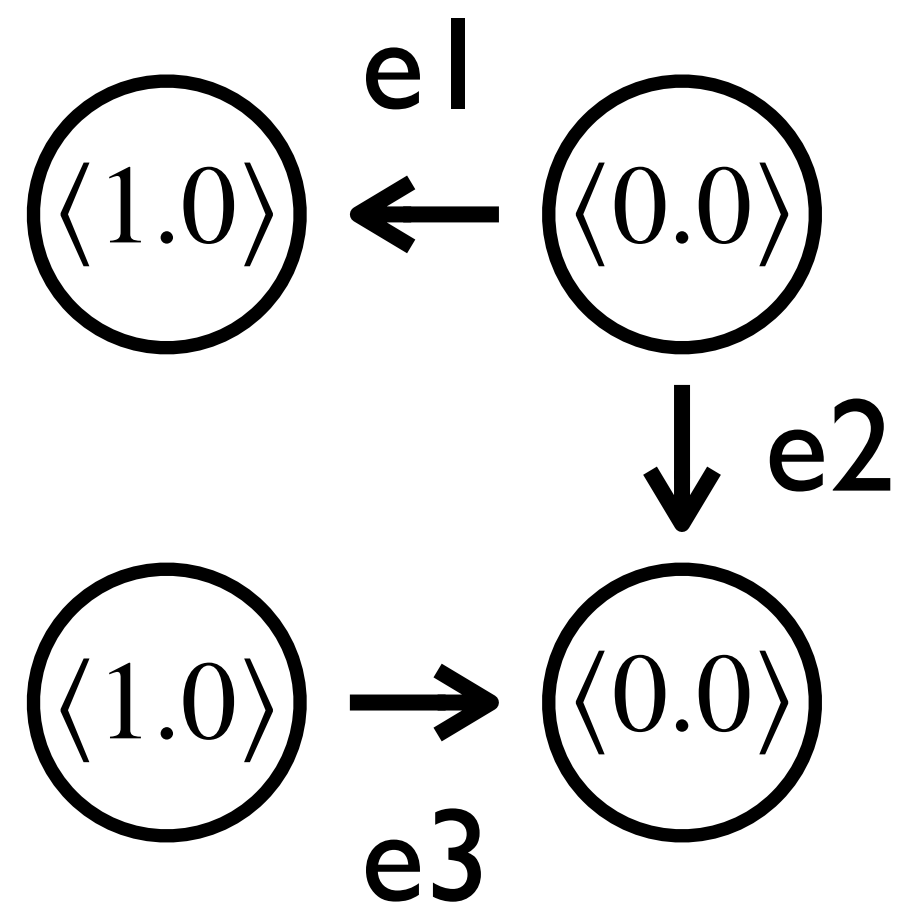


Our model

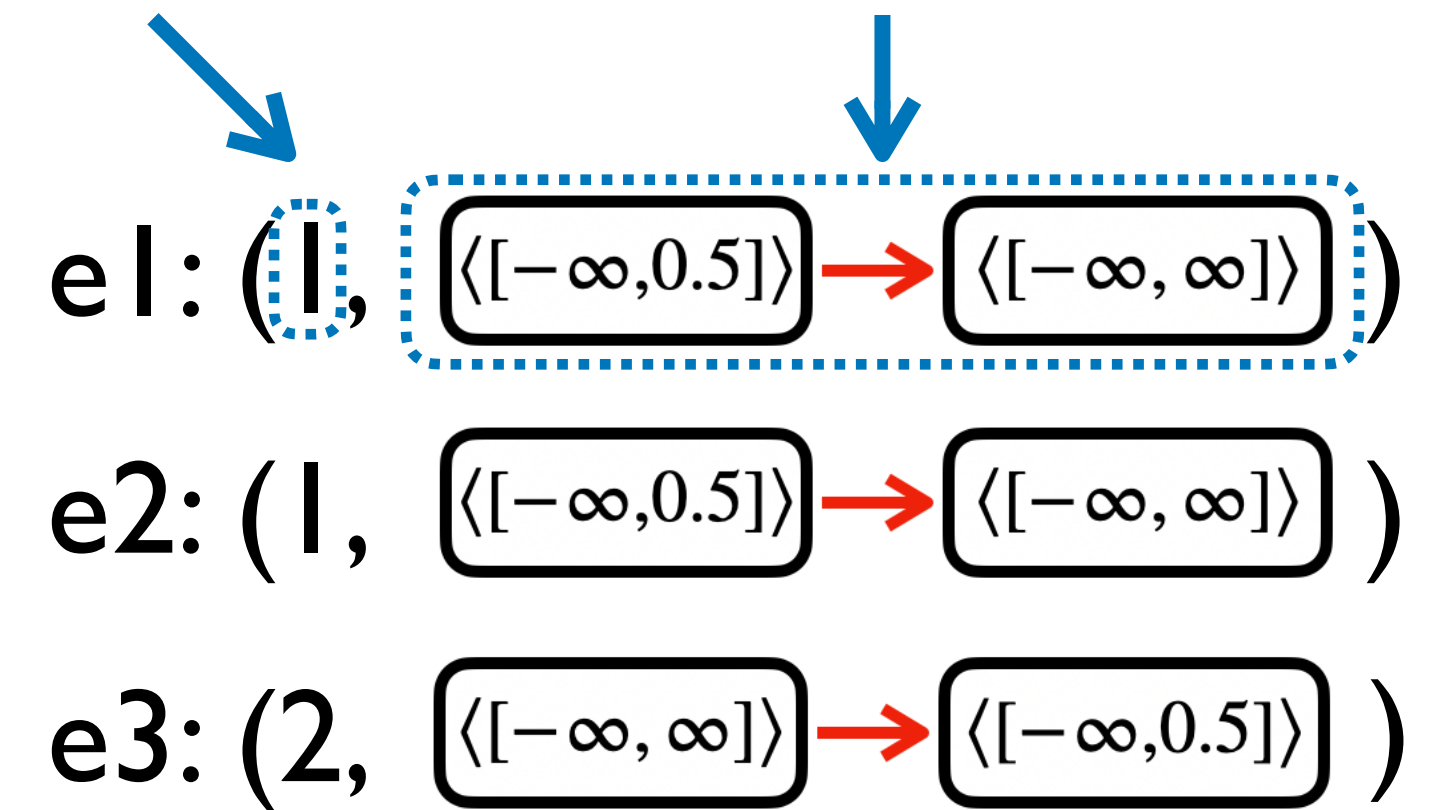
Classification Explanation



Classification & Explanation



Classification Explanation



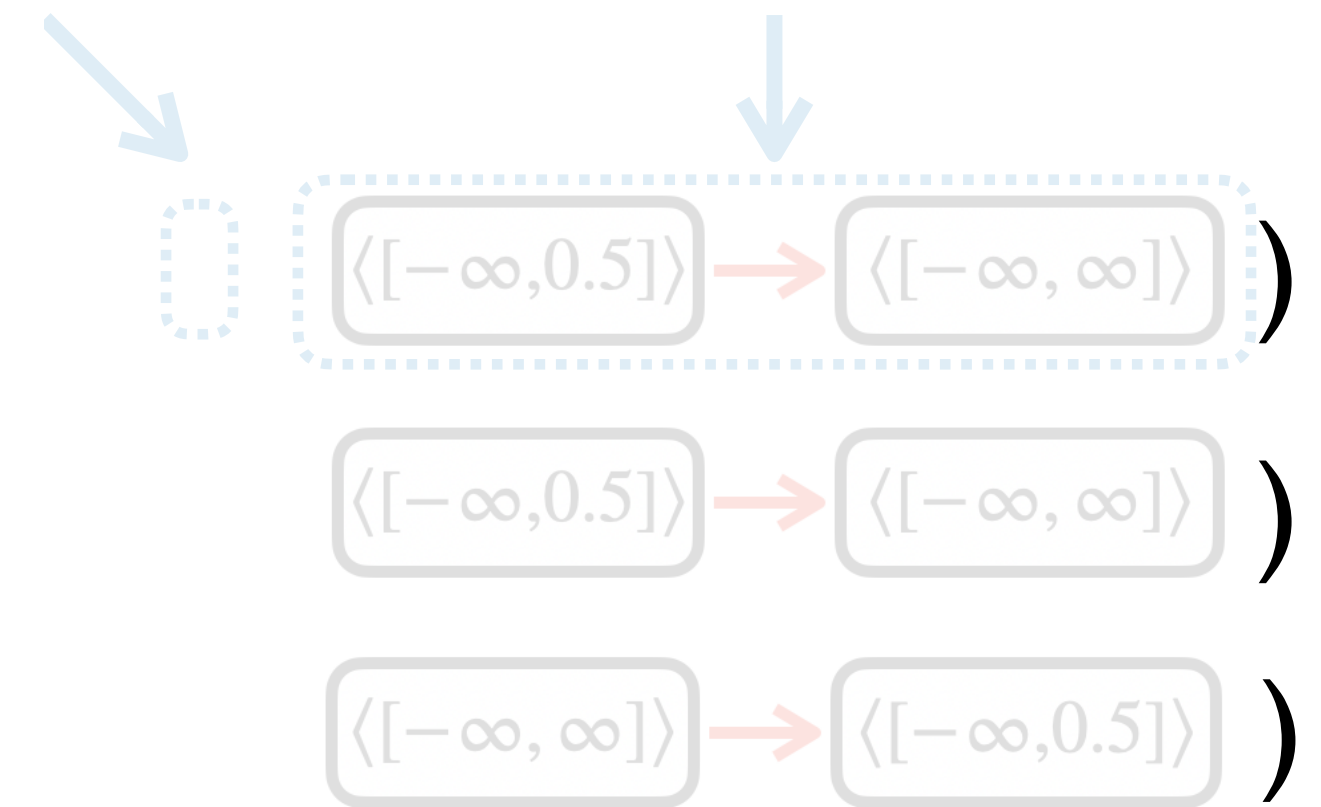
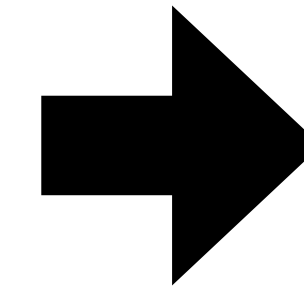
Classification &
Explanation

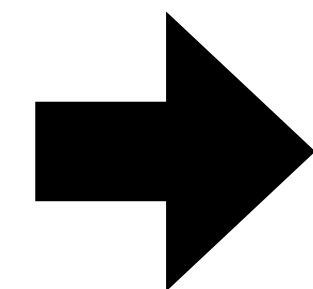
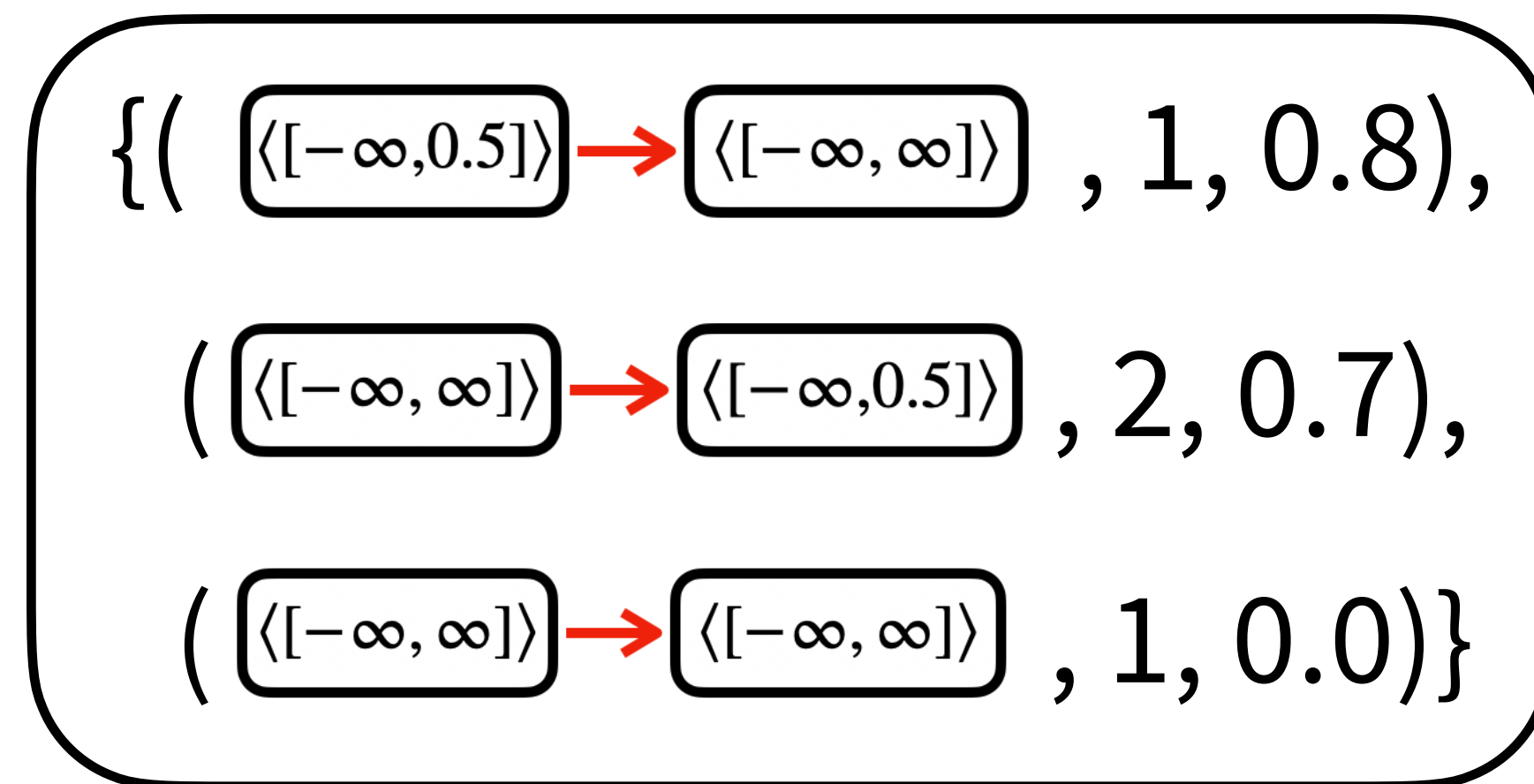
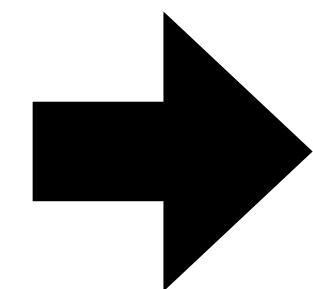
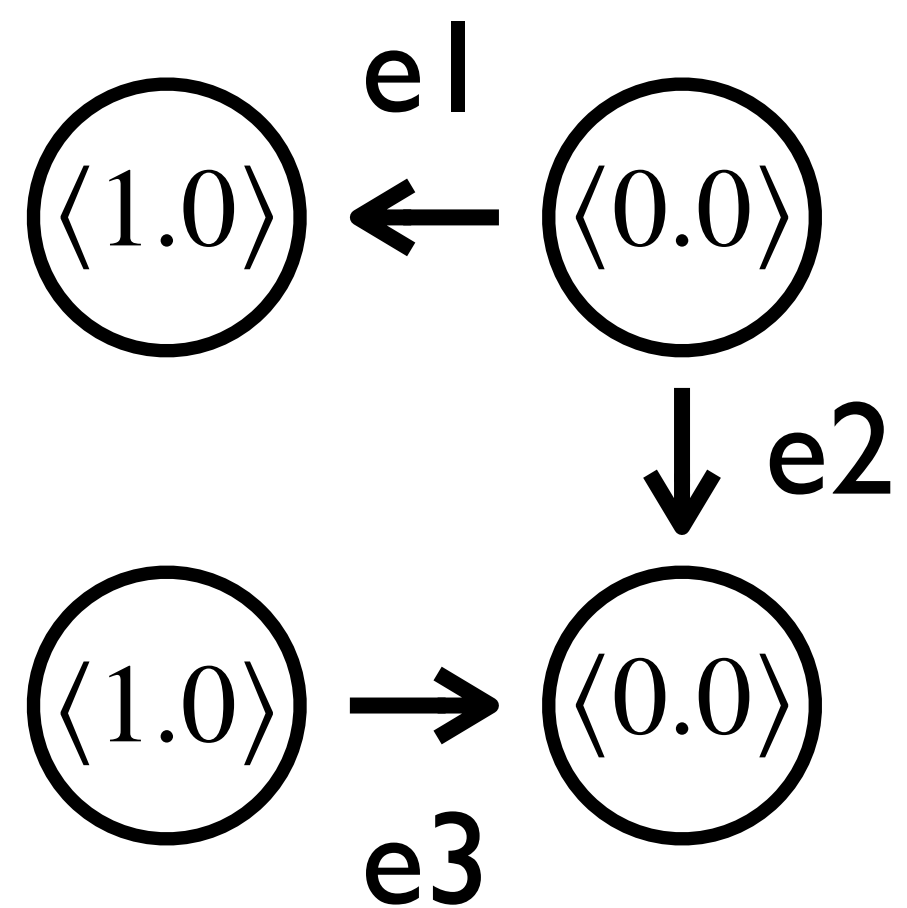
node $x \langle [-\infty, 0.5] \rangle$
 node $y \langle [-\infty, \infty] \rangle$
 edge (x, y)
 target edge (x, y)

node $x \langle [-\infty, \infty] \rangle$
 node $y \langle [-\infty, 0.5] \rangle$
 edge (x, y)
 target edge (x, y)

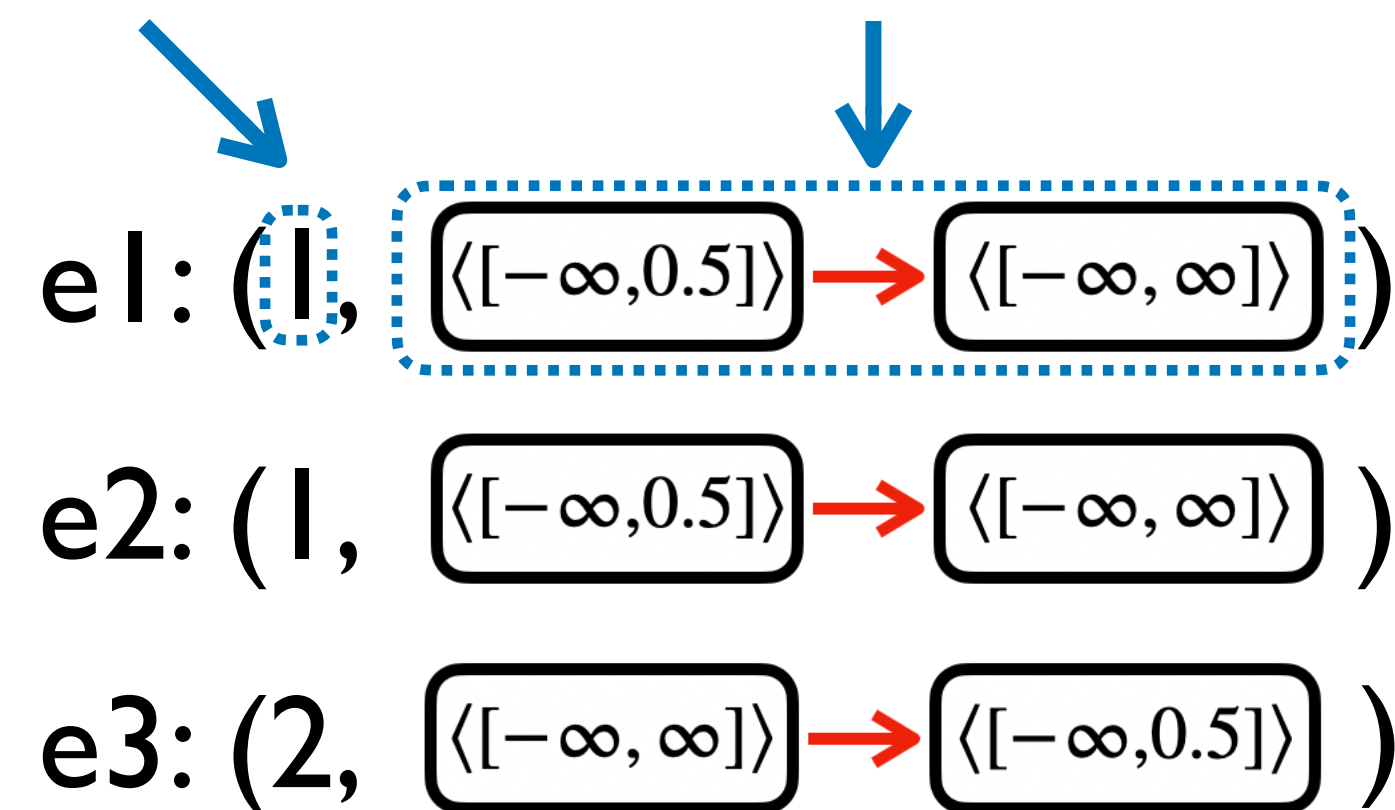
$\{ (\langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle , 1, 0.8),$
 $(\langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, 0.5] \rangle , 2, 0.7),$
 $(\langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, \infty] \rangle , 1, 0.0) \}$

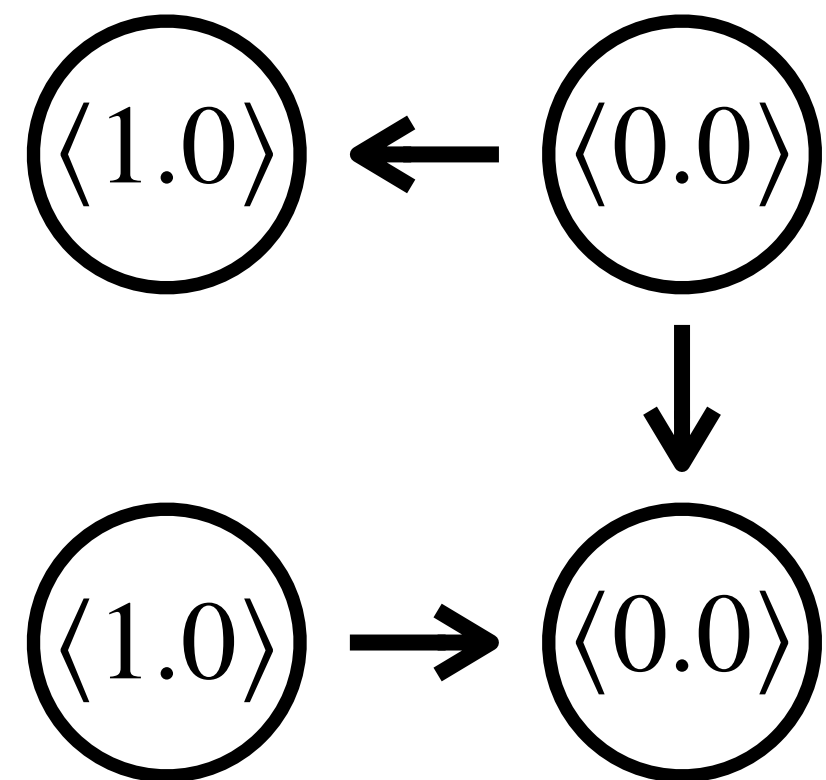
node $x \langle [-\infty, \infty] \rangle$
 node $y \langle [-\infty, \infty] \rangle$
 edge (x, y)
 target edge (x, y)



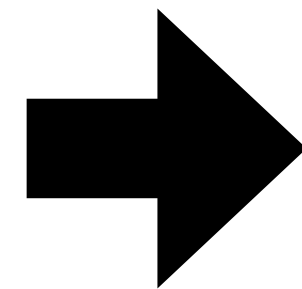


Classification Explanation





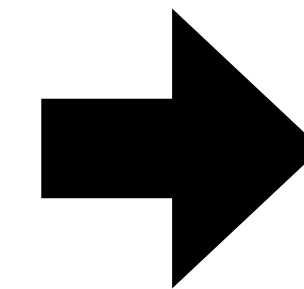
Graph G



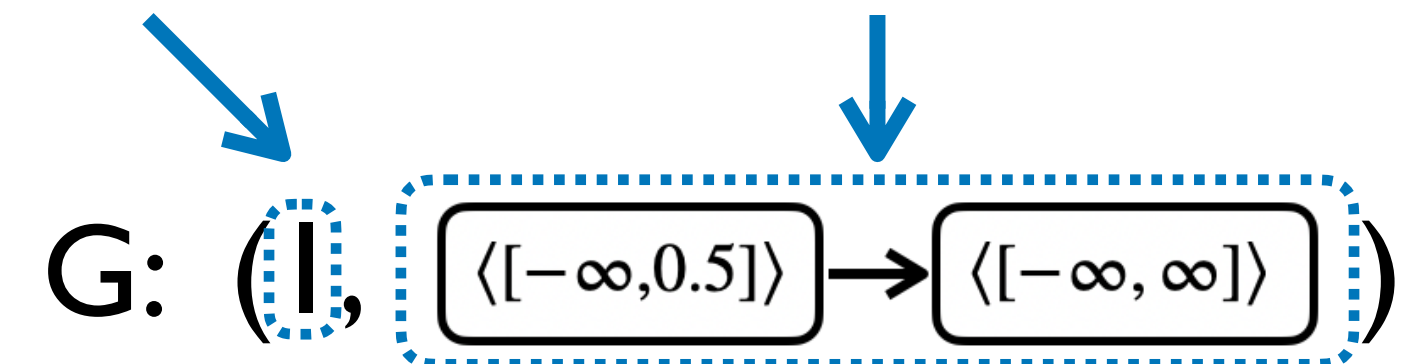
node $x \langle [-\infty, 0.5] \rangle$
 node $y \langle [-\infty, \infty] \rangle$
 edge (x, y)
 target graph

$\{ (\langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle, 1, 0.8),$
 $(\langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, \infty] \rangle, 2, 0.0) \}$

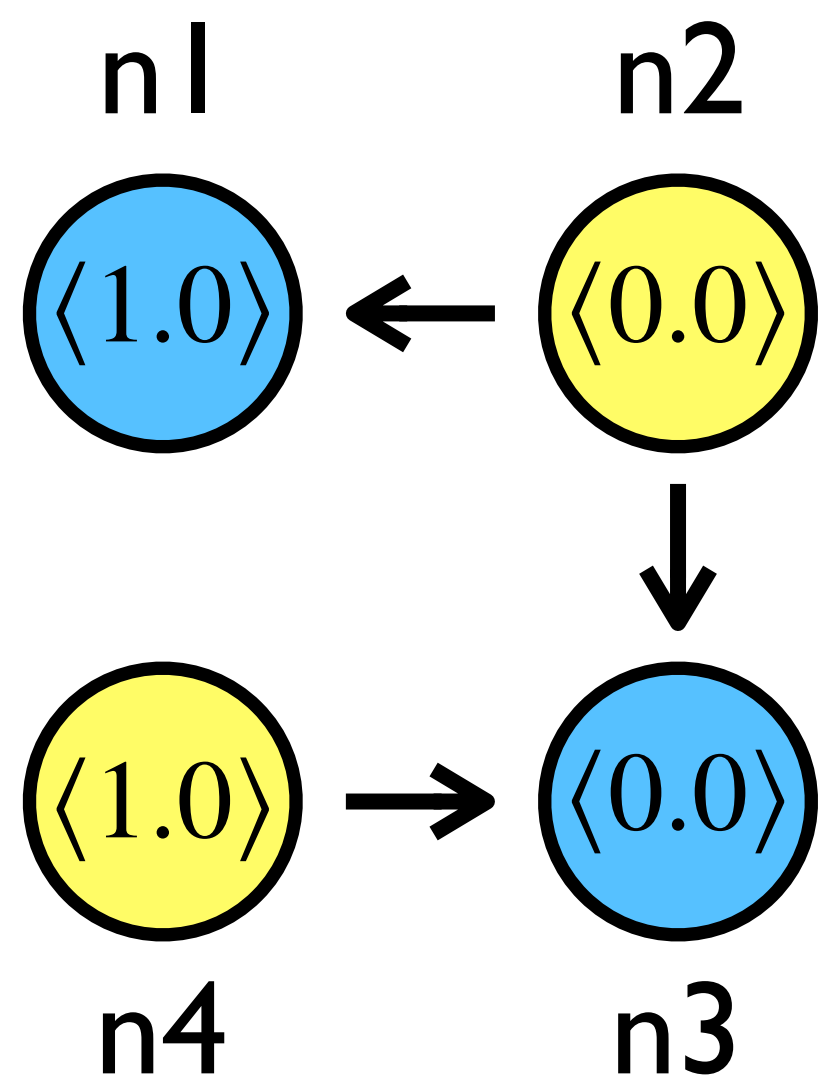
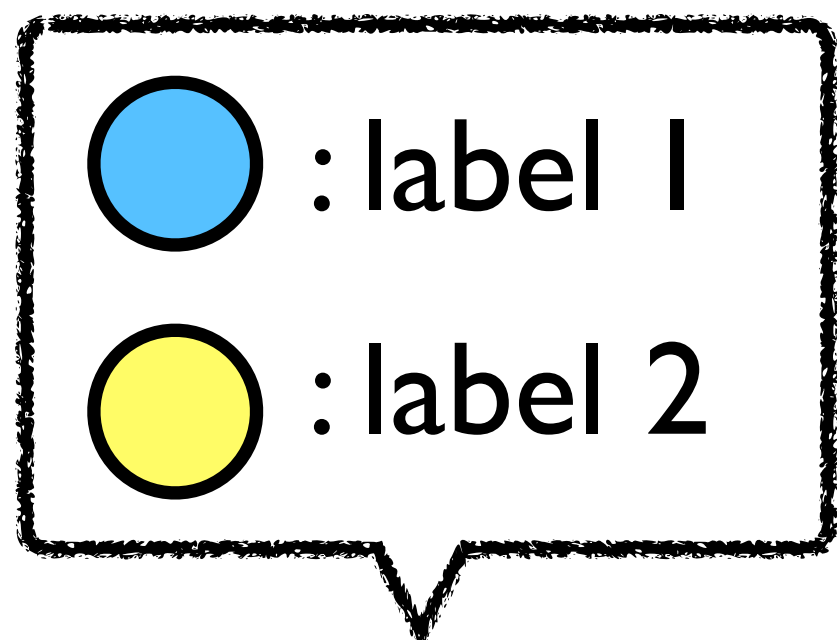
Our model
 (**graph** classification)



Classification Explanation



Classification &
 Explanation



Graph data

Quality of the programs determines the accuracy

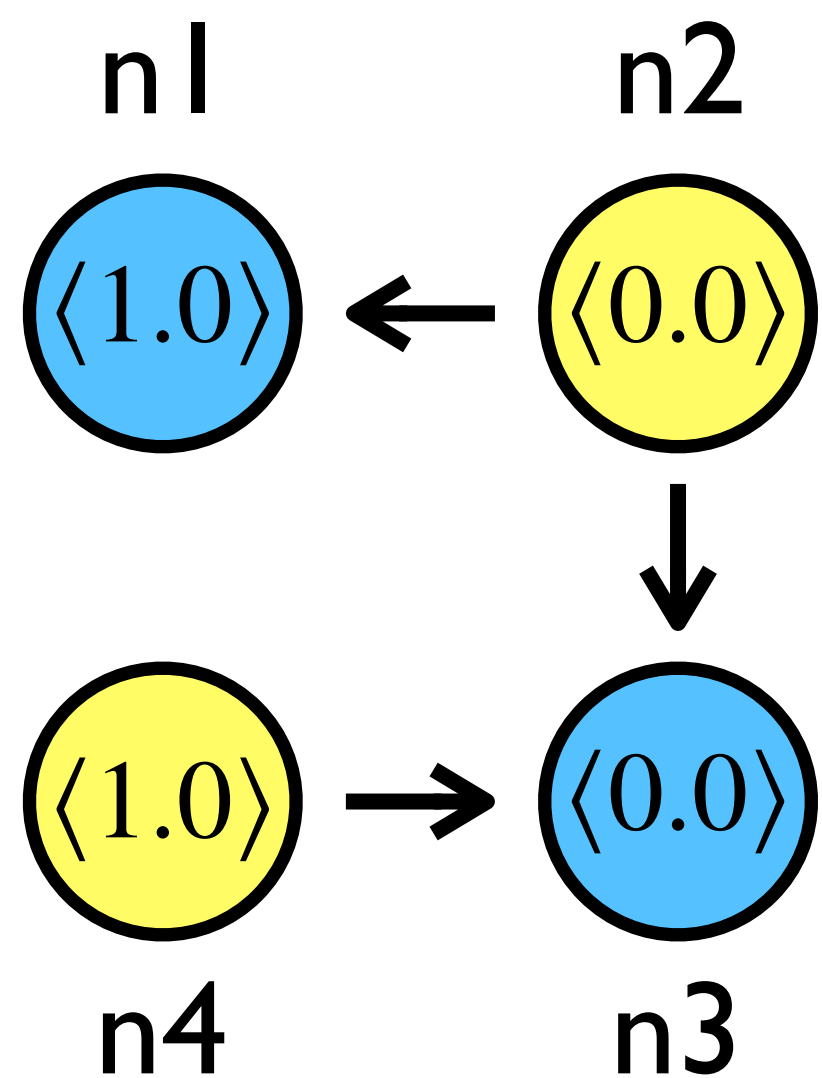
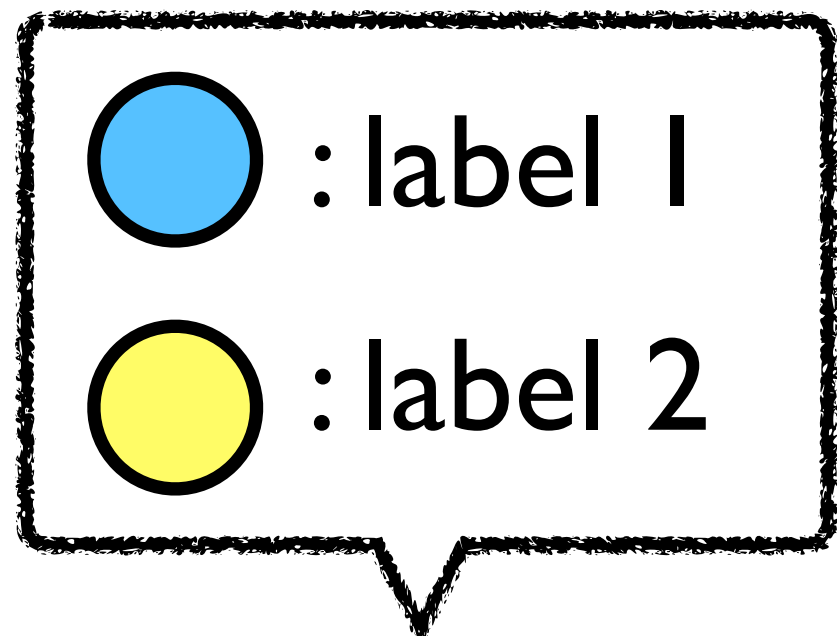
$\{ (\langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle, 1, 0.8),$
 $(\langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, 0.5] \rangle, 2, 0.7),$
 $(\langle [-\infty, \infty] \rangle, 1, 0.0) \}$

Our model
(node classification)

Accuracy : **1.0**

n1: $(1, \langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle)$
 n2: $(2, \langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, 0.5] \rangle)$
 n3: $(1, \langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle)$
 n4: $(2, \langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, 0.5] \rangle)$

Classification &
Explanation



Graph data

Quality of the programs determines the accuracy

$\{$ ($\langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, 0.5] \rangle$, 1, 0.8),
 ($\langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle$, 2, 0.7),
 ($\langle [-\infty, \infty] \rangle$, 1, 0.0) $\}$

Our model
(node classification)

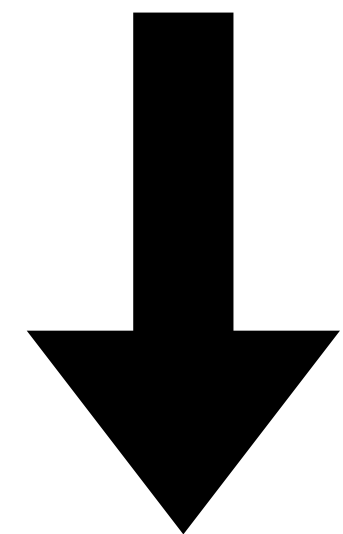
Accuracy : **0.0**

n1: (**2**, $\langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle$)
 n2: (**1**, $\langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, 0.5] \rangle$)
 n3: (**2**, $\langle [-\infty, 0.5] \rangle \rightarrow \langle [-\infty, \infty] \rangle$)
 n4: (**1**, $\langle [-\infty, \infty] \rangle \rightarrow \langle [-\infty, 0.5] \rangle$)

Classification &
Explanation

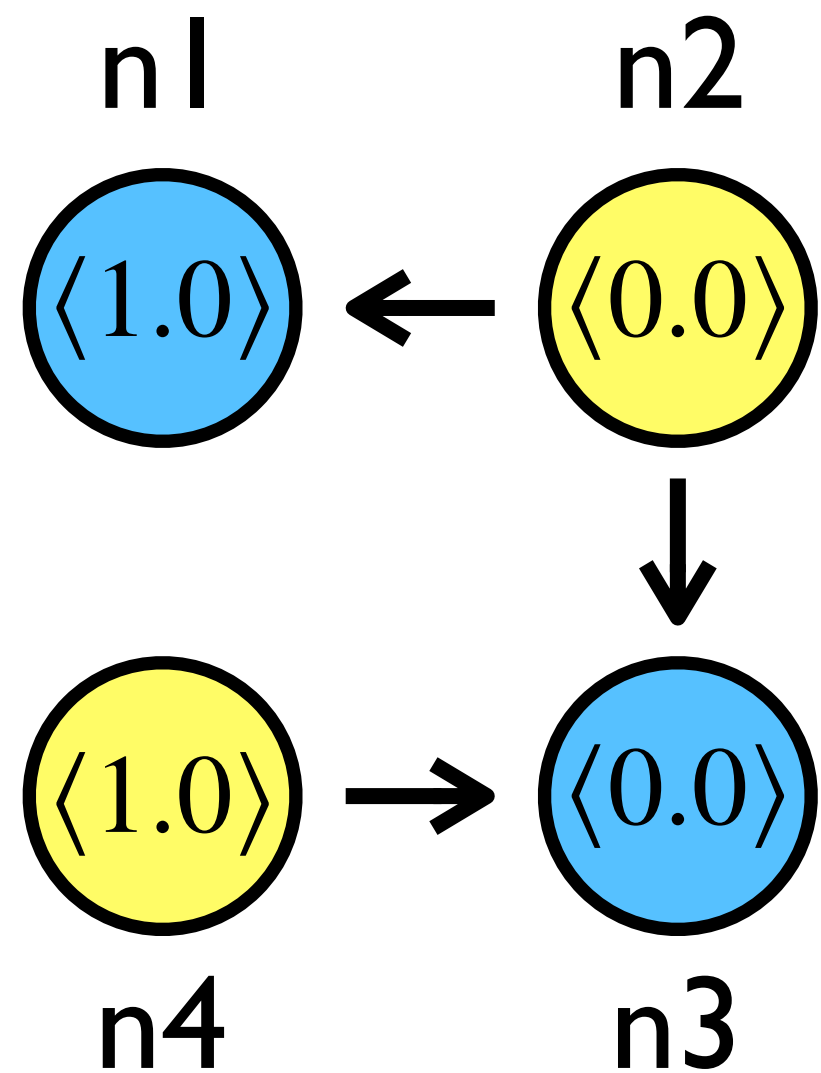


Training data

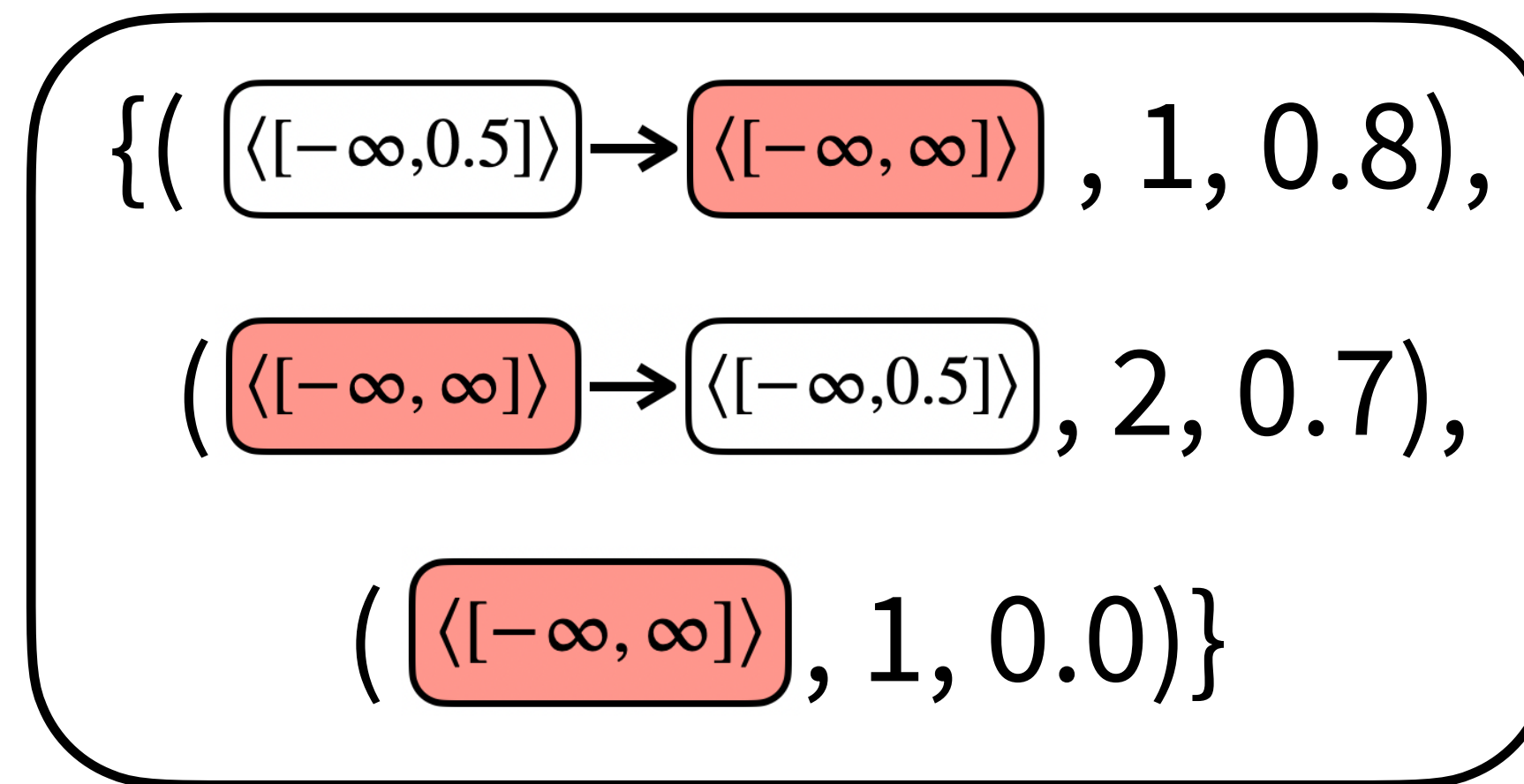
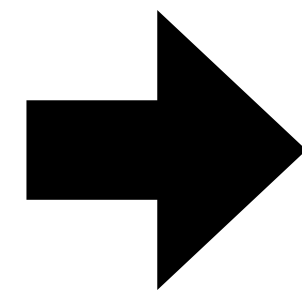


Learning algorithm

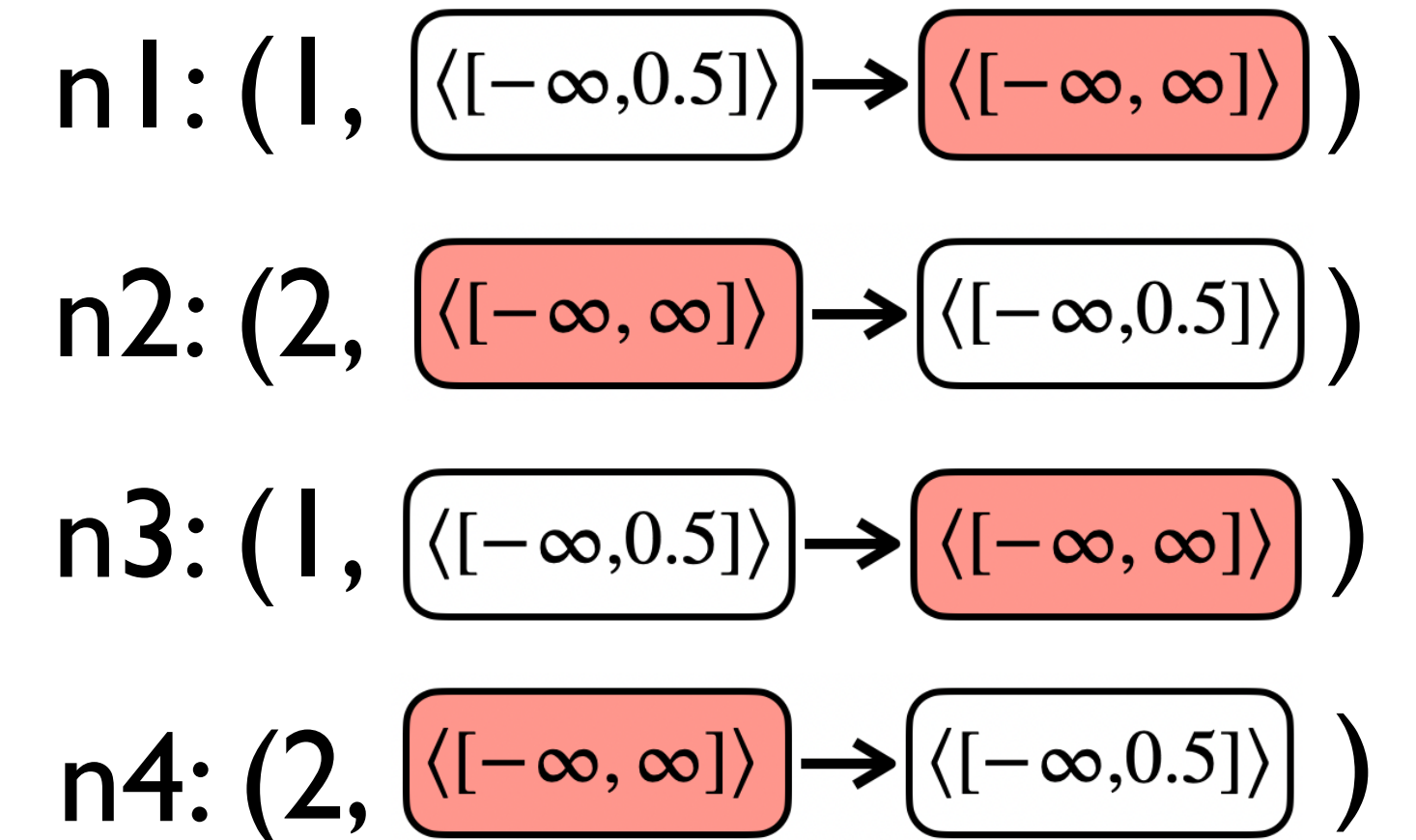
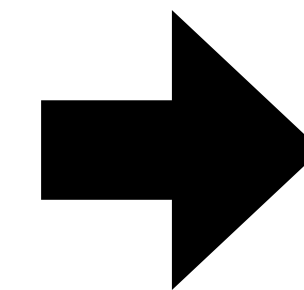
Learning objective:
Learn high-quality GDL programs



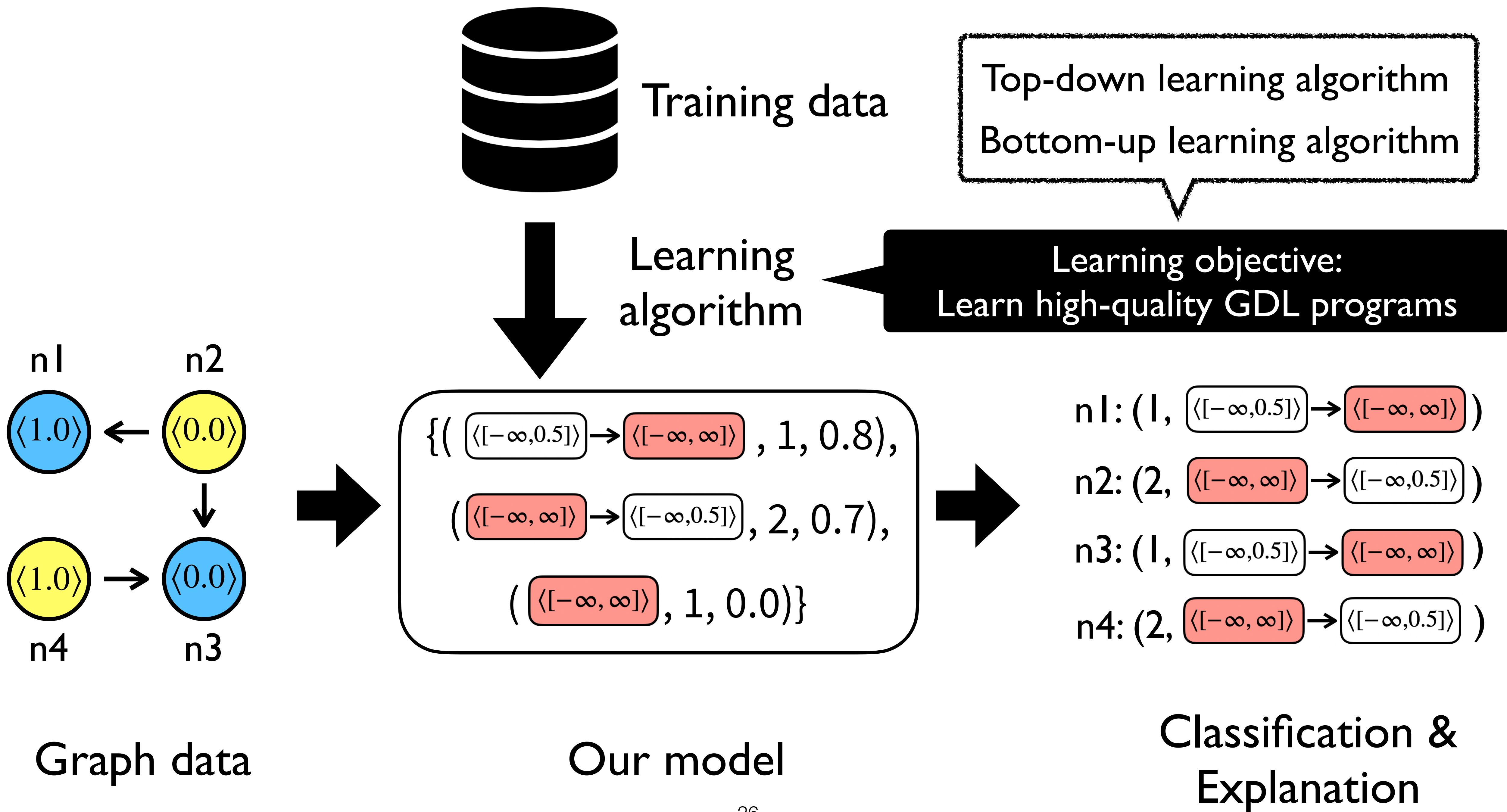
Graph data



Our model

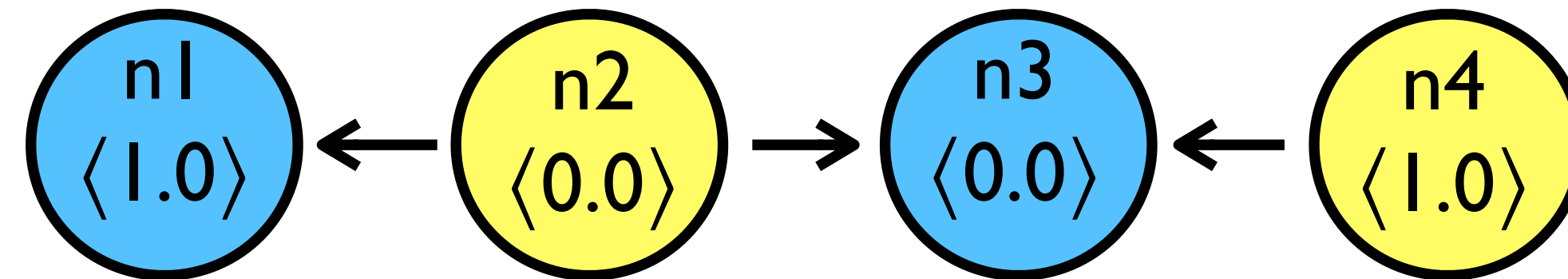


Classification &
Explanation



GDL Program Learning Algorithm

Training graph :



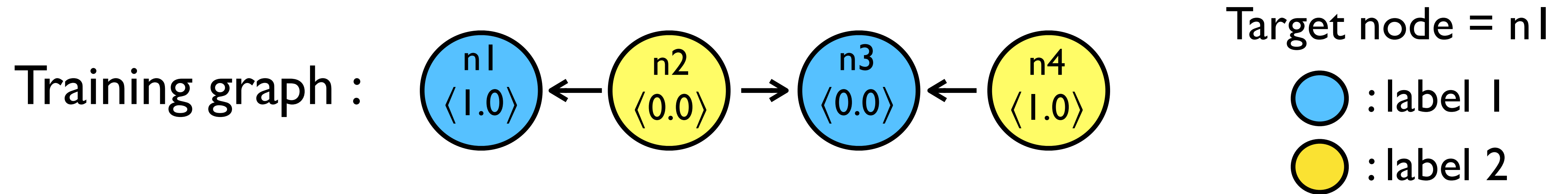
Target node = n1

● : label 1
● : label 2

Learning Objective

Generate a GDL program that includes the target node n1 and precisely describes the nodes belong to the label 1 (●)

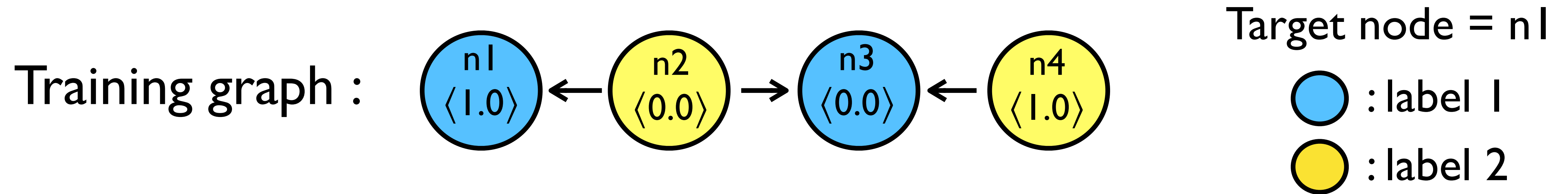
Top-down Learning Algorithm



(I) Starts from the most general program

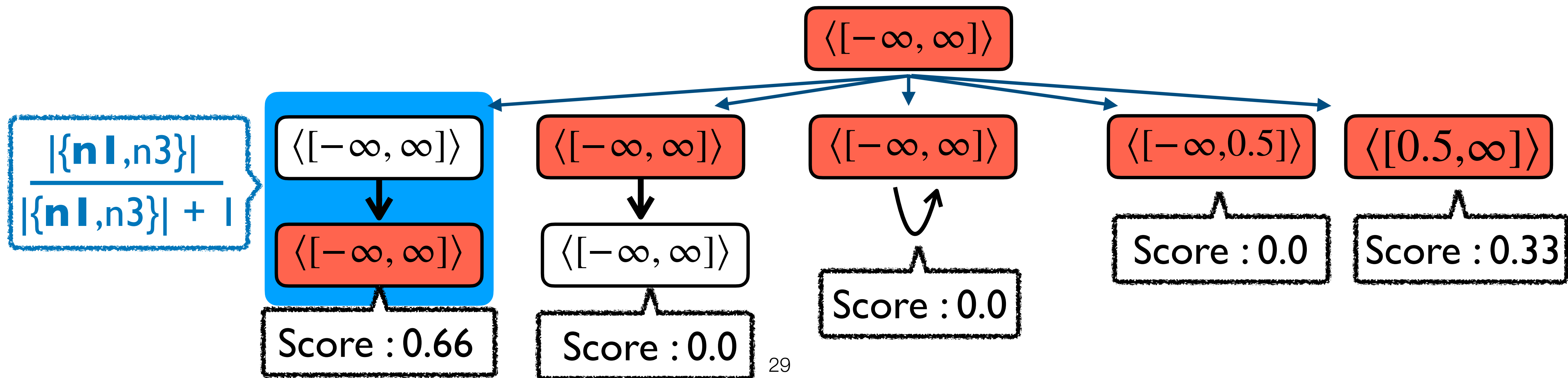


Top-down Learning Algorithm

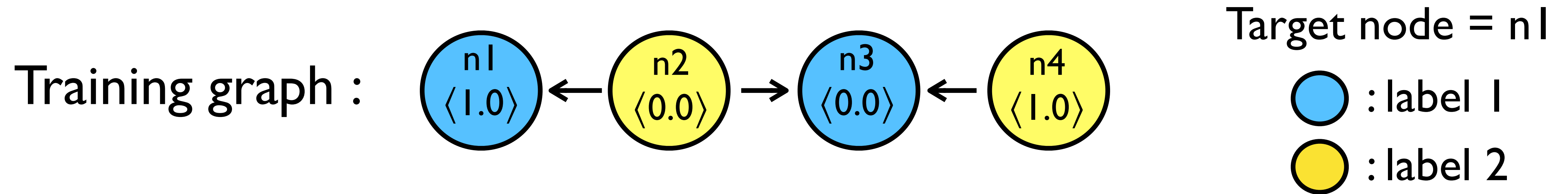


(1) Starts from the most general program $\langle [-\infty, \infty] \rangle$ Score : 0.4

(2) Enumerate possible specified programs and choose a better scored one.

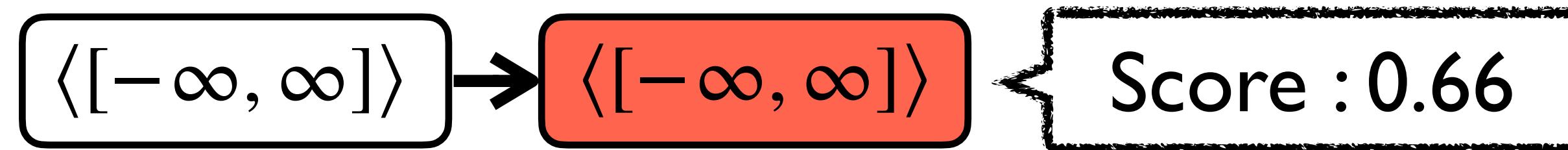


Top-down Learning Algorithm



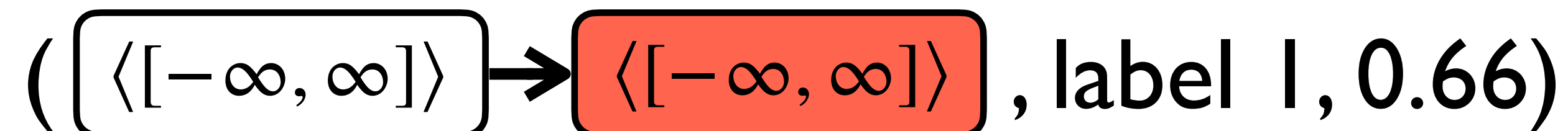
(1) Starts from the most general program $\langle [-\infty, \infty] \rangle$ Score : 0.4

(2) Enumerate possible specified programs and choose a better scored one.

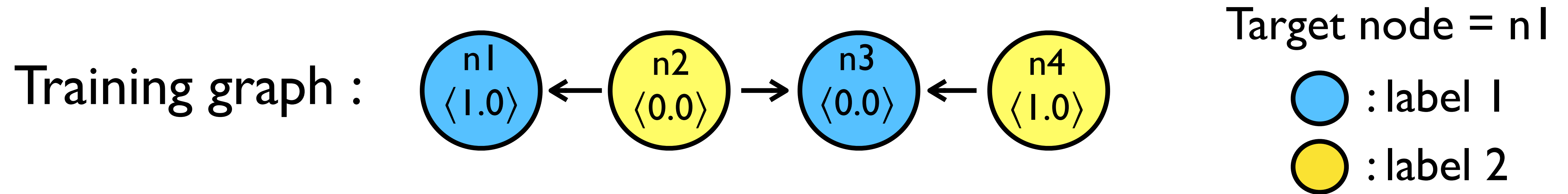


(3) Repeat (2) until no better program is enumerated

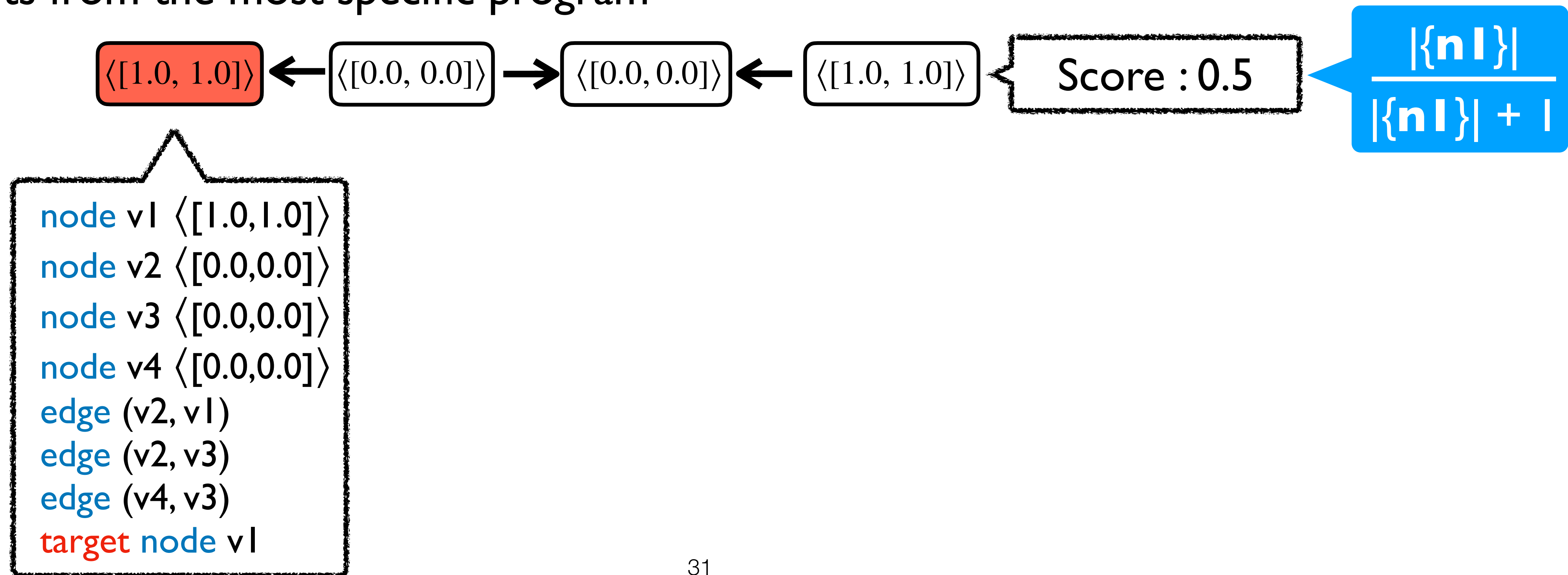
(4) Return the current program



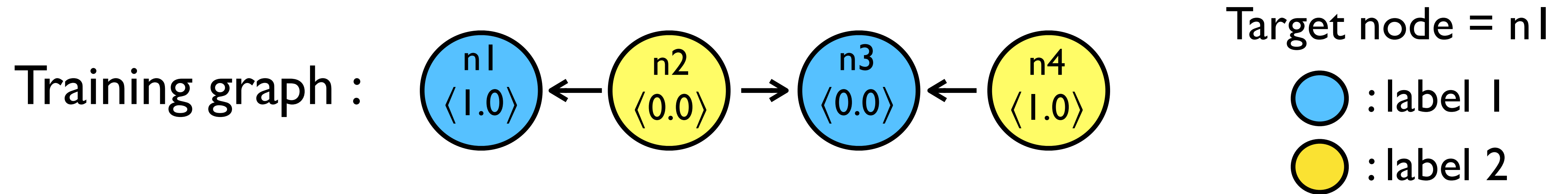
Bottom-up Learning Algorithm



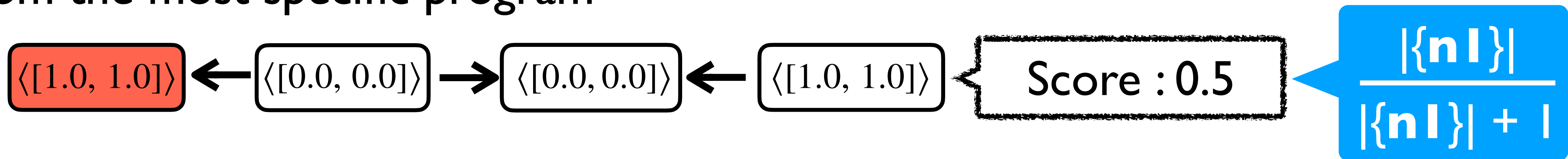
(I) Starts from the most specific program



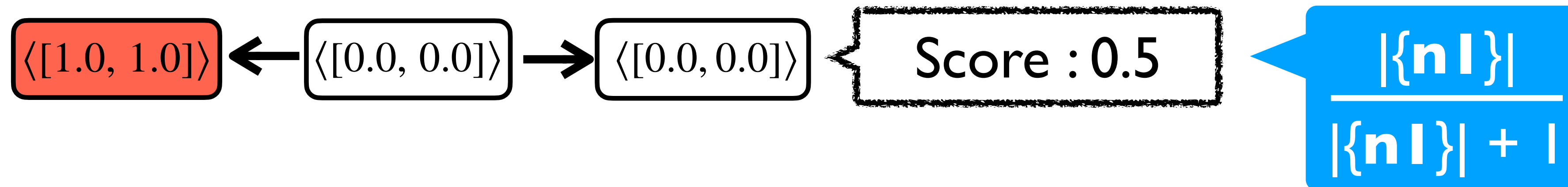
Bottom-up Learning Algorithm



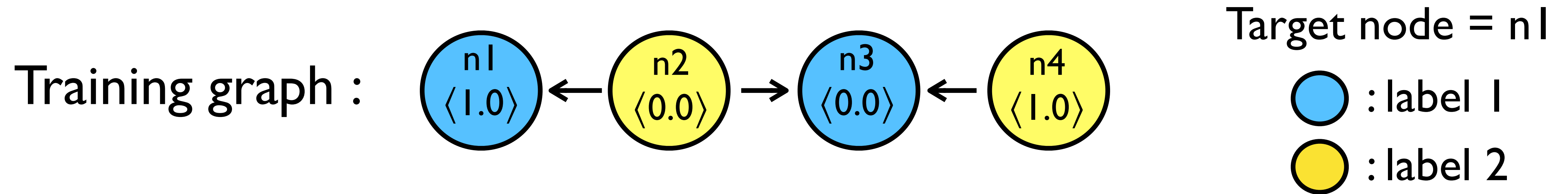
(1) Starts from the most specific program



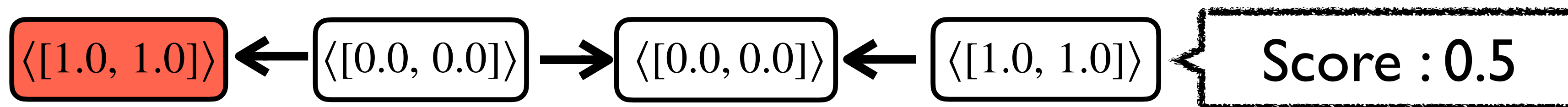
(2) Enumerate possible generalized programs and choose an equal or better scored one



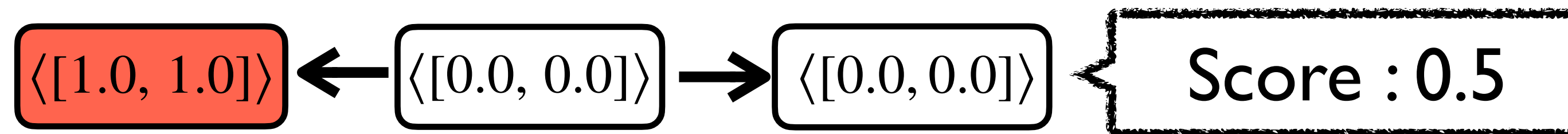
Bottom-up Learning Algorithm



(1) Starts from the most specific program

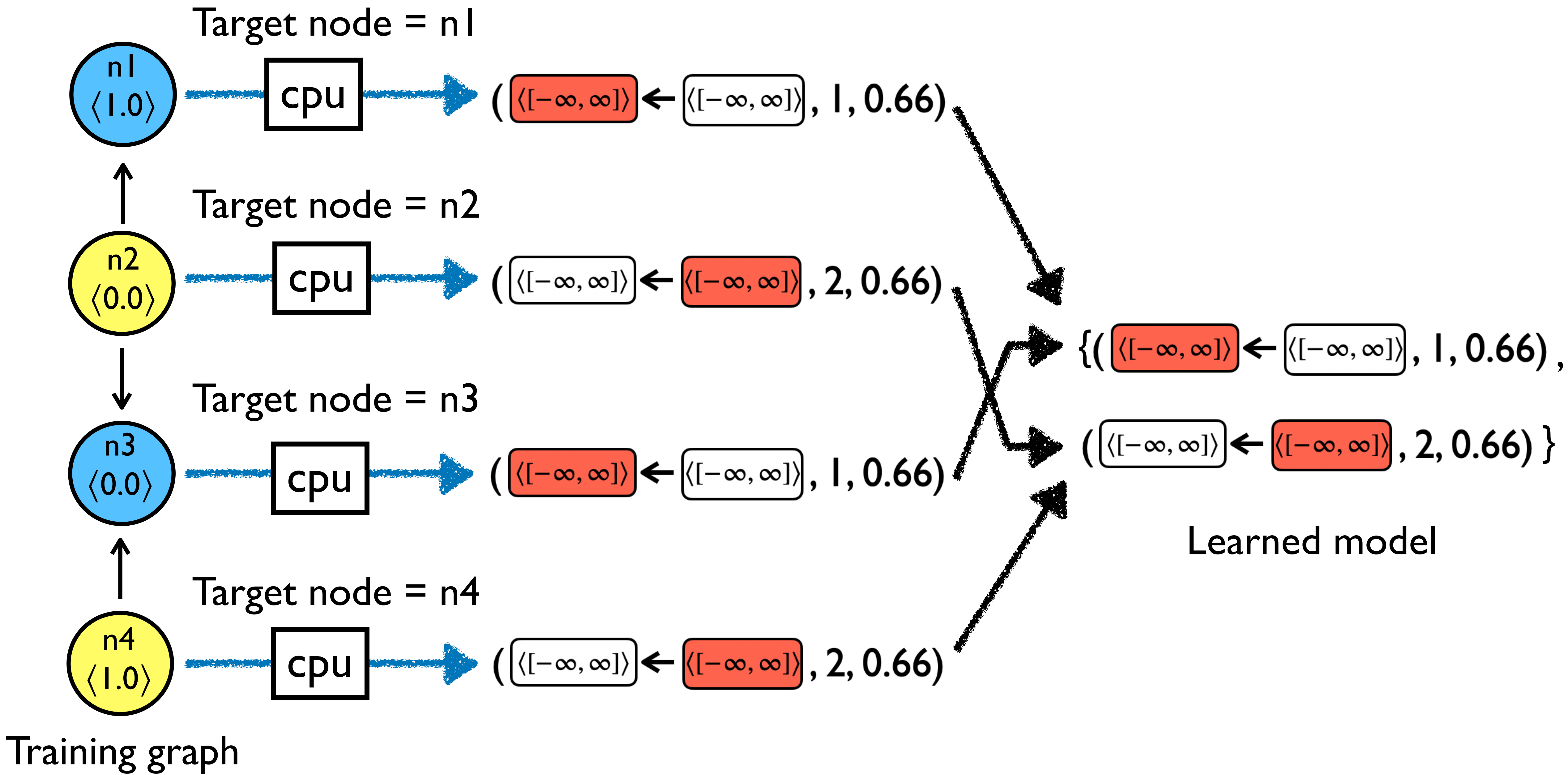


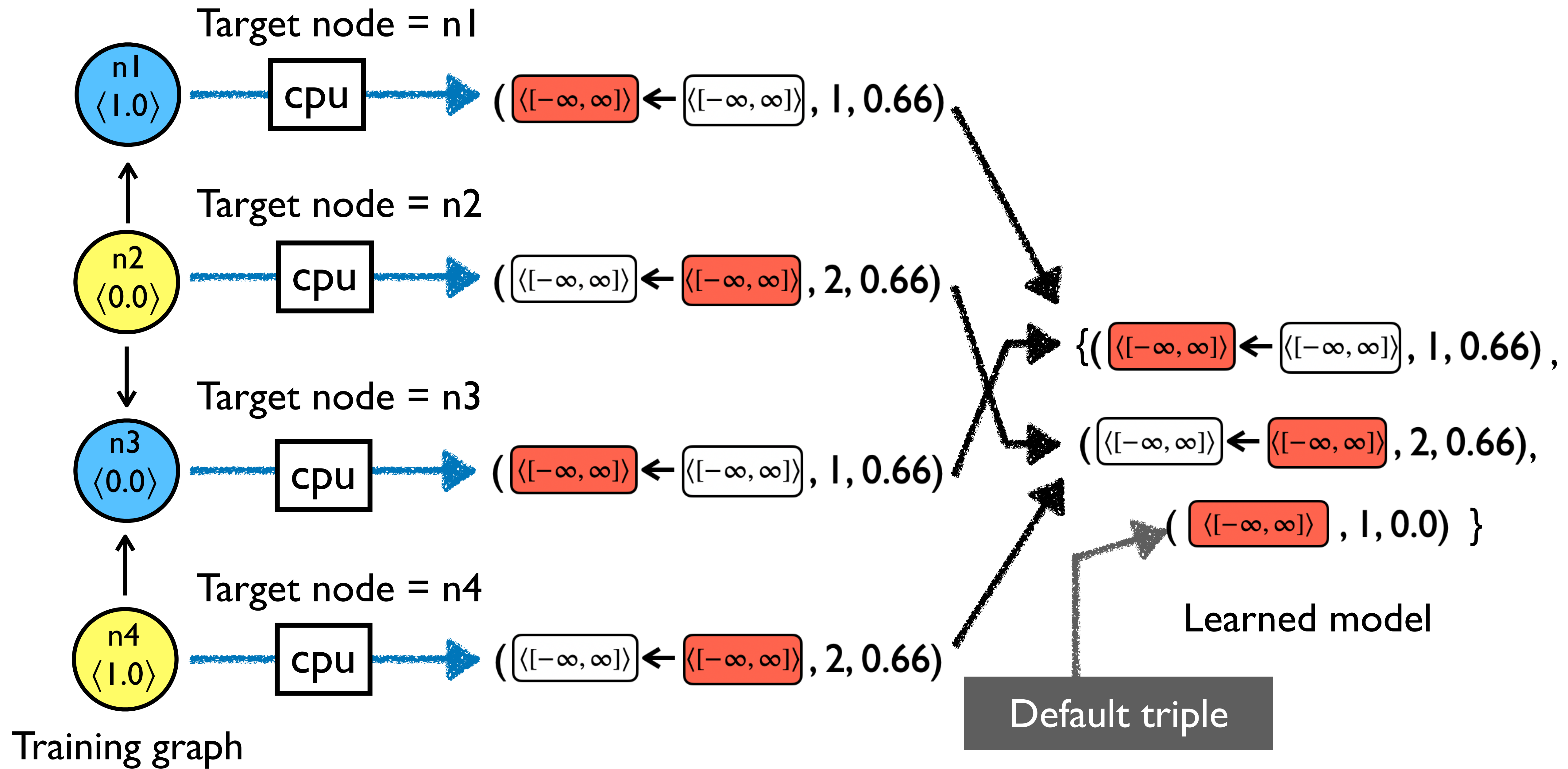
(2) Enumerate possible generalized programs and choose an equal or better scored one



(3) Repeat (2) until all the enumerated programs have lower score

(4) Return the current program ($\langle [-\infty, \infty] \rangle \leftarrow \langle [-\infty, \infty] \rangle$, label 1, 0.66)





Accuracy Comparison

	GCN	GAT	CHEBYNET	JKNET	GRAPHSAGE	GIN	DGCN	PL4XGL
MUTAG	80.0±0.0	89.0±2.2	86.0±4.1	68.0±7.5	78.0±4.4	91.0±5.4	N/A	100.0±0.0
BBBP	83.6±1.4	82.3±1.6	84.6±1.0	85.6±1.9	86.6±0.9	86.2±1.4	N/A	86.8±0.0
BACE	78.4±2.8	52.4±3.3	78.9±1.4	79.9±1.9	79.8±0.8	80.9±0.4	N/A	80.9±0.0
HIV	96.4±0.0	96.4±0.0	96.8±0.2	96.8±0.1	96.9±0.2	96.8±0.1	N/A	N/A
BA-SHAPES	95.1±0.6	76.8±2.3	97.1±0.0	94.3±0.0	97.1±0.0	92.0±1.1	95.1±0.7	95.7±0.0
TREE-CYCLES	97.7±0.0	90.9±0.0	100.0±0.0	98.9±0.0	100.0±0.0	93.2±0.0	99.2±0.5	100.0±0.0
WISCONSIN	64.0±0.0	49.6±3.1	86.4±3.9	64.8±1.5	92.8±2.9	56.0±0.0	96.0±0.0	88.0±0.0
TEXAS	67.7±5.3	50.0±0.0	87.7±2.1	68.8±4.3	86.6±2.6	50.0±0.0	86.6±2.6	83.3±0.0
CORNELL	58.9±2.6	61.1±0.0	81.0±6.5	61.1±0.0	87.7±2.1	61.1±0.0	86.6±2.6	88.8±0.0
CORA	85.6±0.3	86.4±1.8	86.5±5.2	84.9±3.5	86.3±3.2	86.7±0.0	83.2±5.9	80.0± 0.0
CITESEER	75.2±0.0	74.3±0.7	79.1±0.9	73.7±4.2	75.9±2.3	75.2±0.0	71.3±6.0	63.8± 0.0
PUBMED	82.8±1.1	84.7±1.2	88.7±1.0	83.2±0.4	88.0±0.4	86.1±0.6	85.1±0.6	81.4±0.0

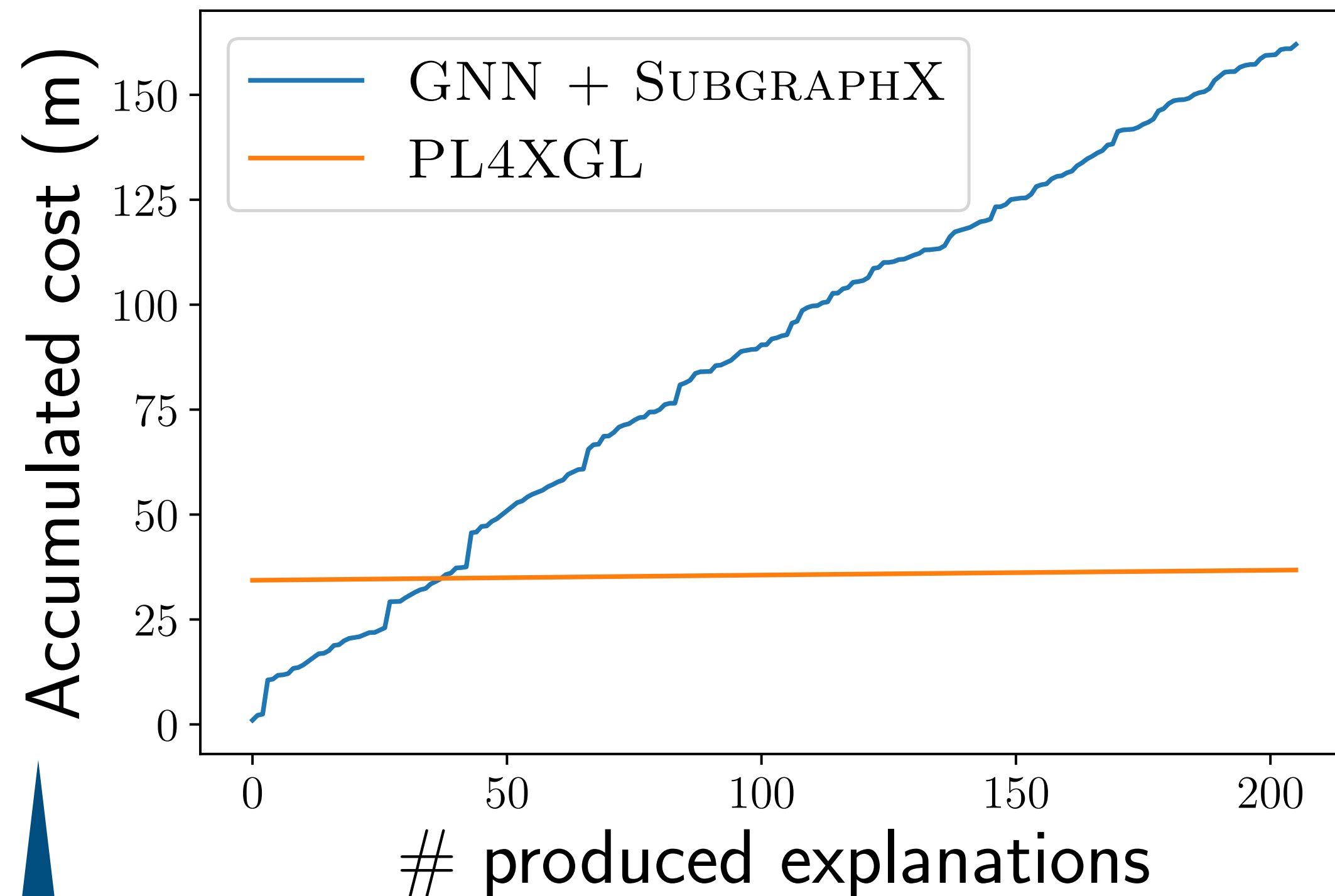
Molecule datasets (graph classification)

	GCN	GAT	CHEBYNET	JKNET	GRAPHSAGE	GIN	DGCN	PL4XGL
MUTAG	80.0±0.0	89.0±2.2	86.0±4.1	68.0±7.5	78.0±4.4	91.0±5.4	N/A	100.0±0.0
BBBP	83.6±1.4	82.3±1.6	84.6±1.0	85.6±1.9	86.6±0.9	86.2±1.4	N/A	86.8±0.0
BACE	78.4±2.8	52.4±3.3	78.9±1.4	79.9±1.9	79.8±0.8	80.9±0.4	N/A	80.9±0.0
HIV	96.4±0.0	96.4±0.0	96.8±0.2	96.8±0.1	96.9±0.2	96.8±0.1	N/A	N/A
BA-SHAPES	95.1±0.6	76.8±2.3	97.1±0.0	94.3	PL4XGL shows the best accuracy			
TREE-CYCLES	97.7±0.0	90.9±0.0	100.0±0.0	98.9				
WISCONSIN	64.0±0.0	49.6±3.1	86.4±3.9	64.8				
TEXAS	67.7±5.3	50.0±0.0	87.7±2.1	68.8±4.3	86.6±2.6	50.0±0.0	86.6±2.6	83.3±0.0
CORNELL	58.9±2.6	61.1±0.0	81.0±6.5	61.1±0.0	87.7±2.1	61.1±0.0	86.6±2.6	88.8±0.0
CORA	85.6±0.3	86.4±1.8	86.5±5.2	84.9±3.5	86.3±3.2	86.7±0.0	83.2±5.9	80.0±0.0
CITSEER	75.2±0.0	74.3±0.7	79.1±0.9	73.7±4.2	75.9±2.3	75.2±0.0	71.3±6.0	63.8±0.0
PUBMED	82.8±1.1	84.7±1.2	88.7±1.0	83.2±0.4	88.0±0.4	86.1±0.6	85.1±0.6	81.4±0.0

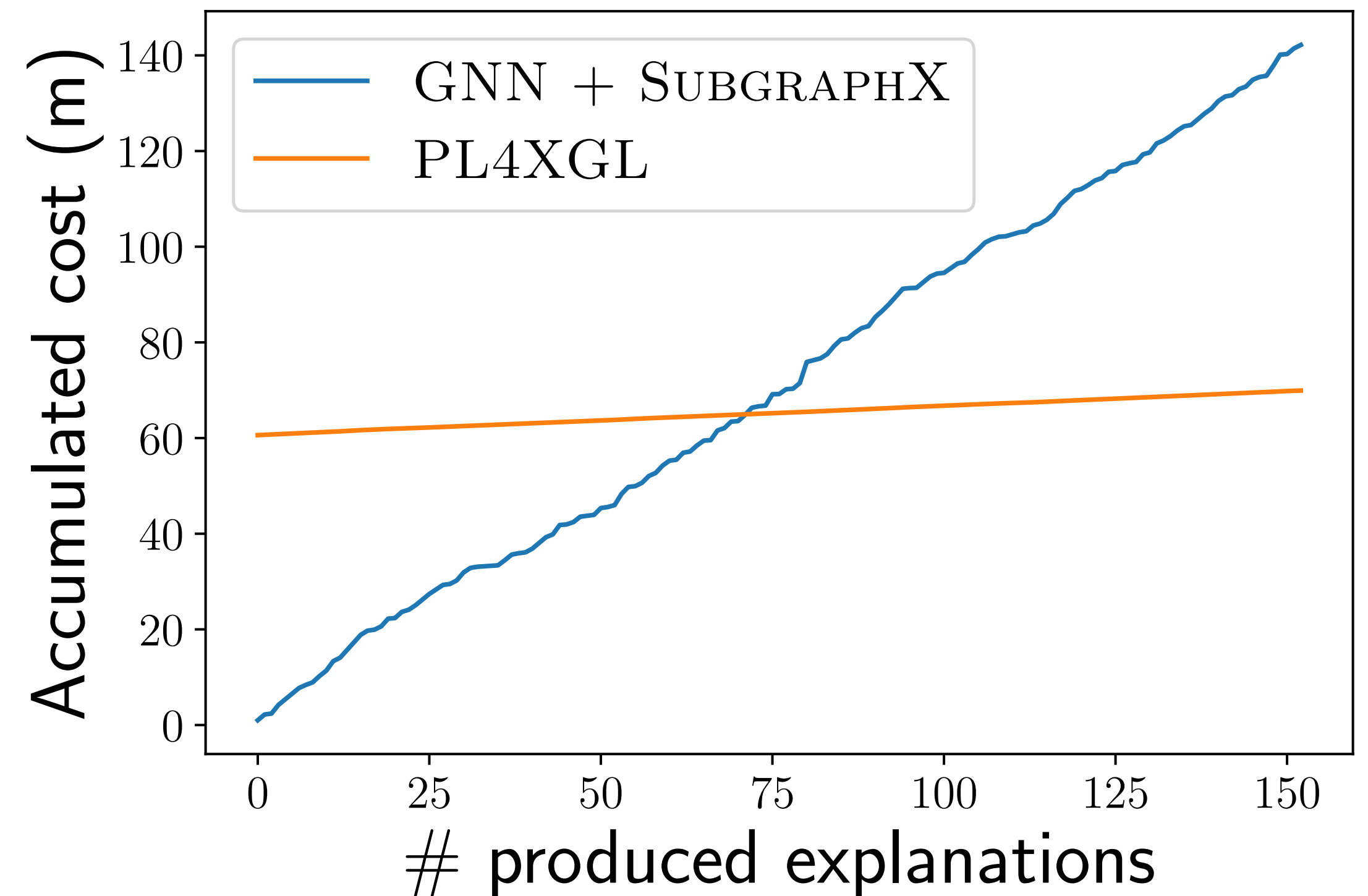
Cost Comparison

- Our approach is fast if explanation cost is included

BBBP



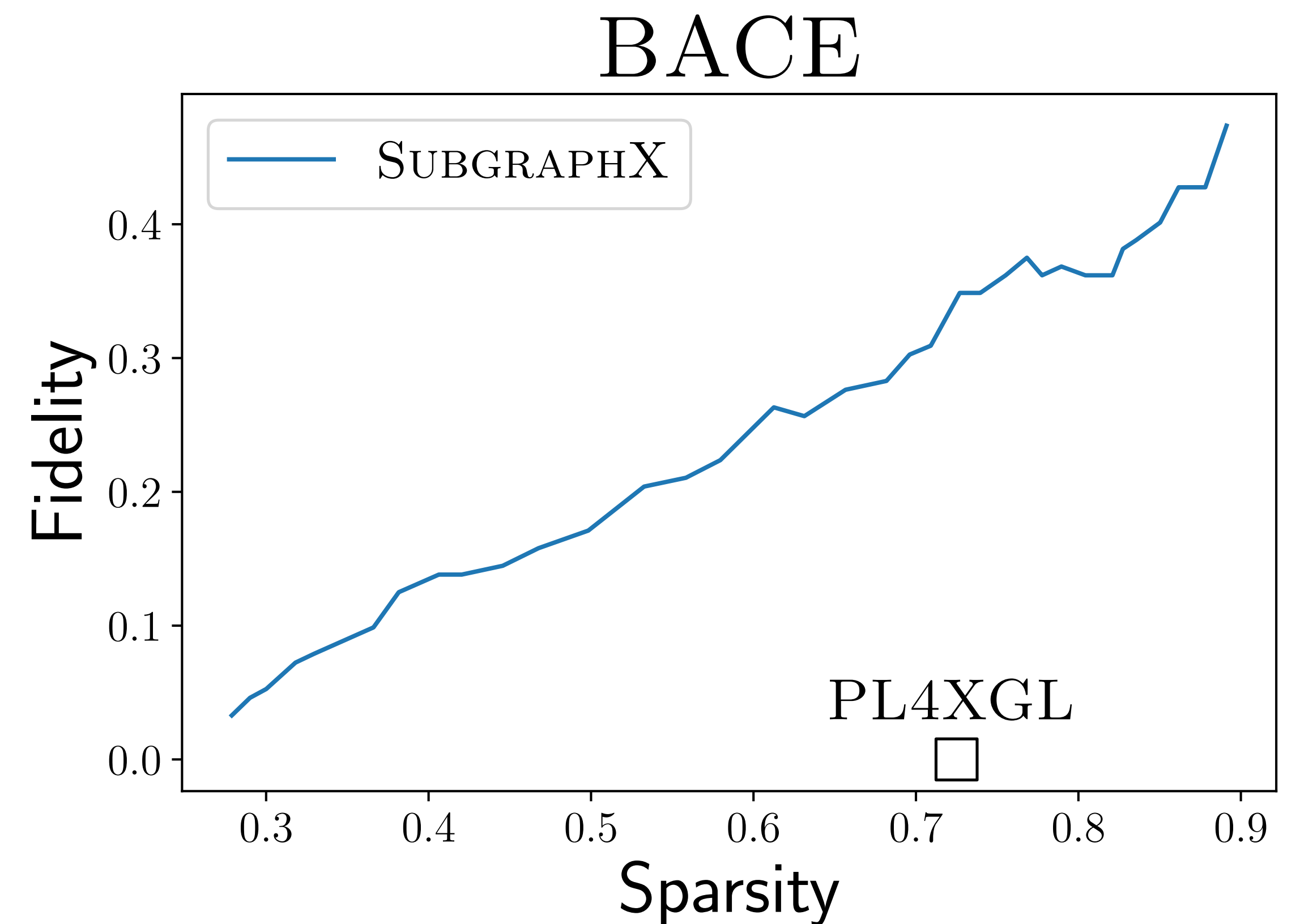
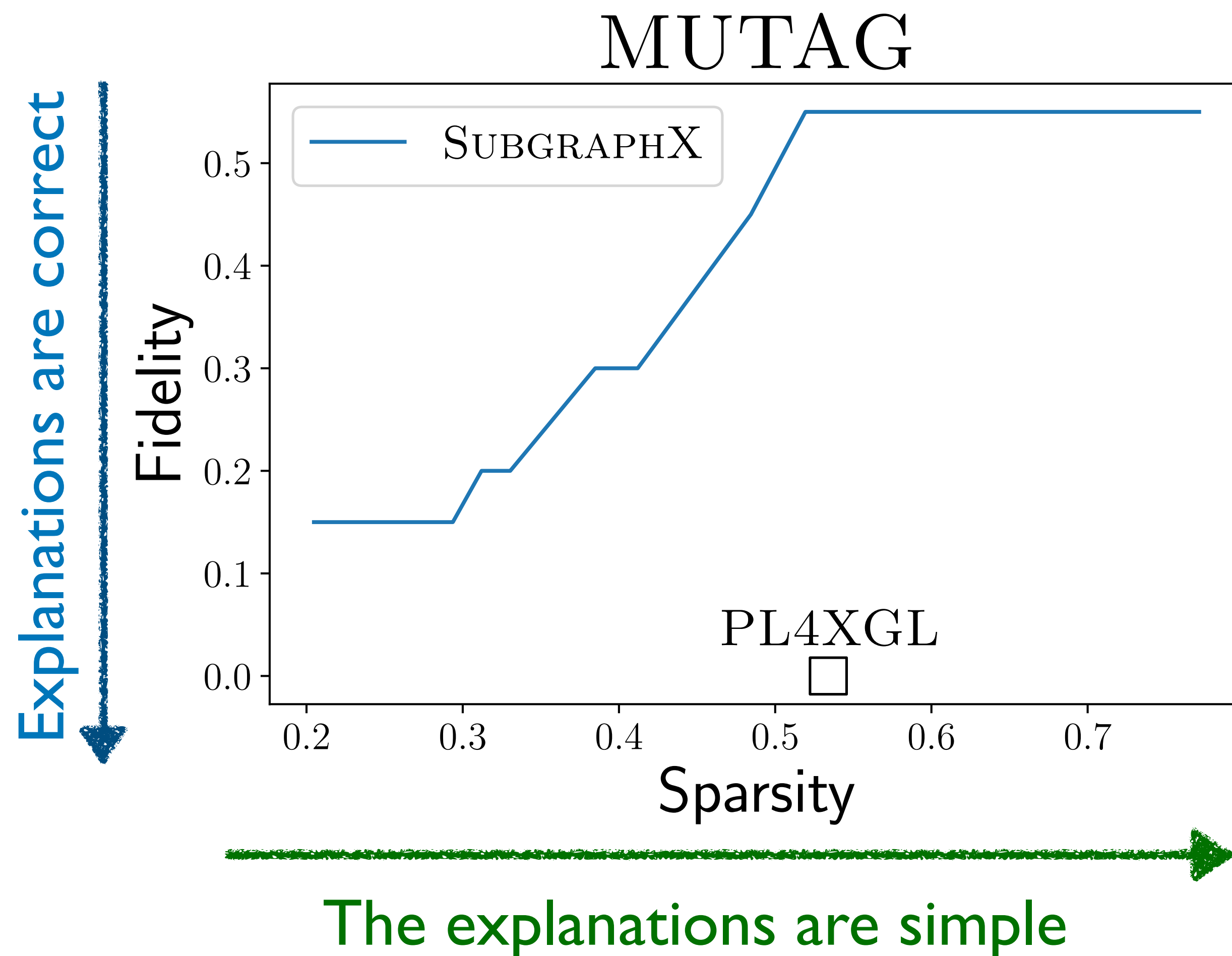
BACE



Training + classification + explanation cost

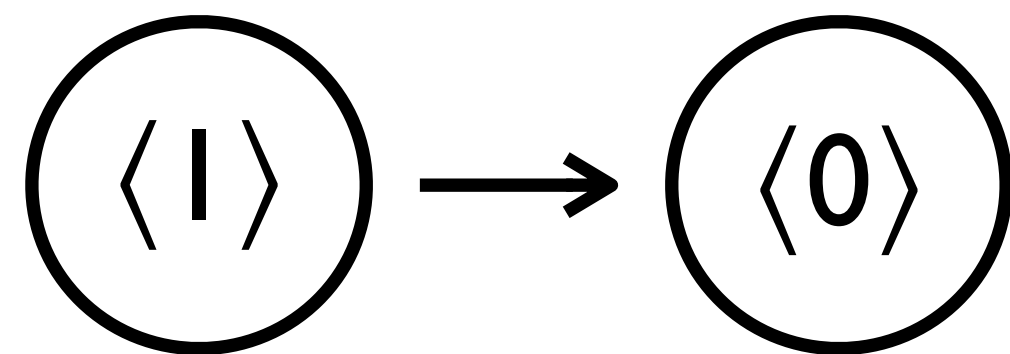
Explainability Comparison

- Our approach provides **correct** & **simple** explanations



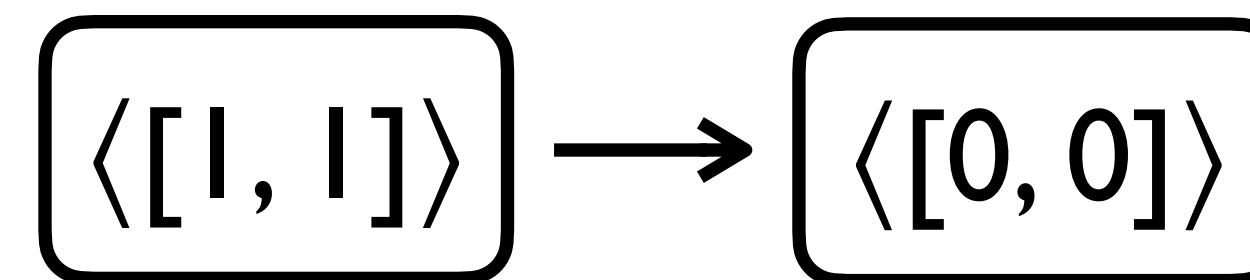
GDL Program vs Subgraph

- GDL is a strictly more expressive than subgraph in graph pattern description

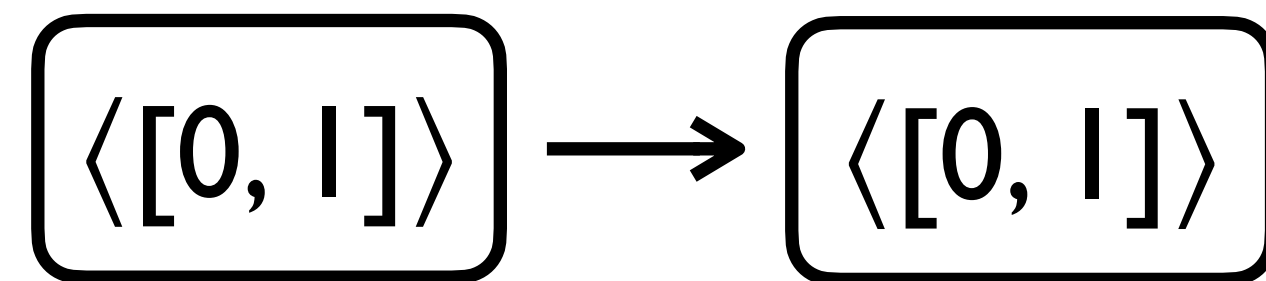


subgraph pattern

=

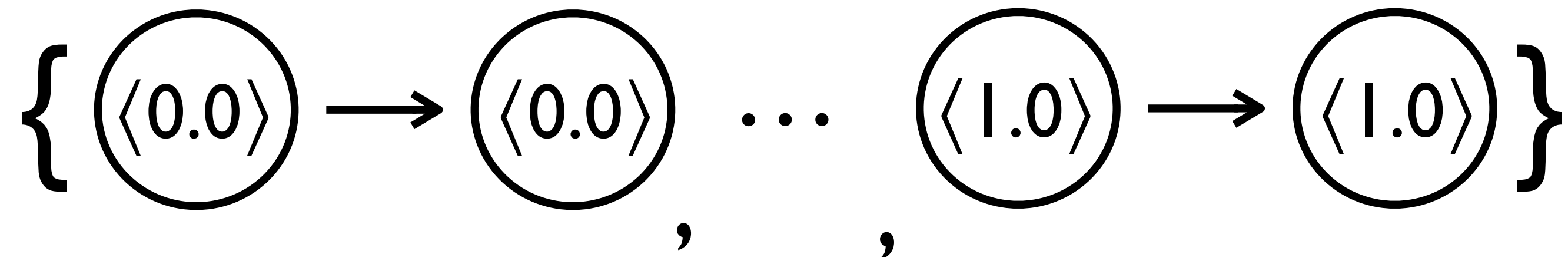


GDL program



GDL program

=



subgraph patterns

OOPSLA' 20

Automatic Feature
Generation for Data-Driven
Static Analysis

OOPSLA' 25

GDL-based
Fault Localization

In progress

Improving GDL &
Synthesis Algorithms

Graph Description Language

Programs	$P ::= \bar{\delta} \text{ target } t$
Descriptions	$\delta ::= \delta_V \mid \delta_E$
Node Descriptions	$\delta_V ::= \text{node } x < \bar{\phi} > ?$
Edge Descriptions	$\delta_E ::= \text{edge } (x, x) < \bar{\phi} > ?$
Target Symbols	$t ::= \text{node } x \mid \text{edge } (x, x) \mid \text{graph}$
Intervals	$\phi ::= [n^?, n^?]$
Real Numbers	$n ::= 0.2 \mid 0.7 \mid 6 \mid -8 \dots$
Variables	$x ::= x \mid y \mid z \mid \dots$

PLDI' 24

Explainable Graph
Machine Learning

In progress

Improving GNN
Using GDL

ToDo

GDL-based
Graph Data-mining

ToDo

GDL-based
GNN Explanation