

PL / SE / ML

그래프 패턴 언어를 활용하여 다양한 분야의 핵심 문제 접근하기

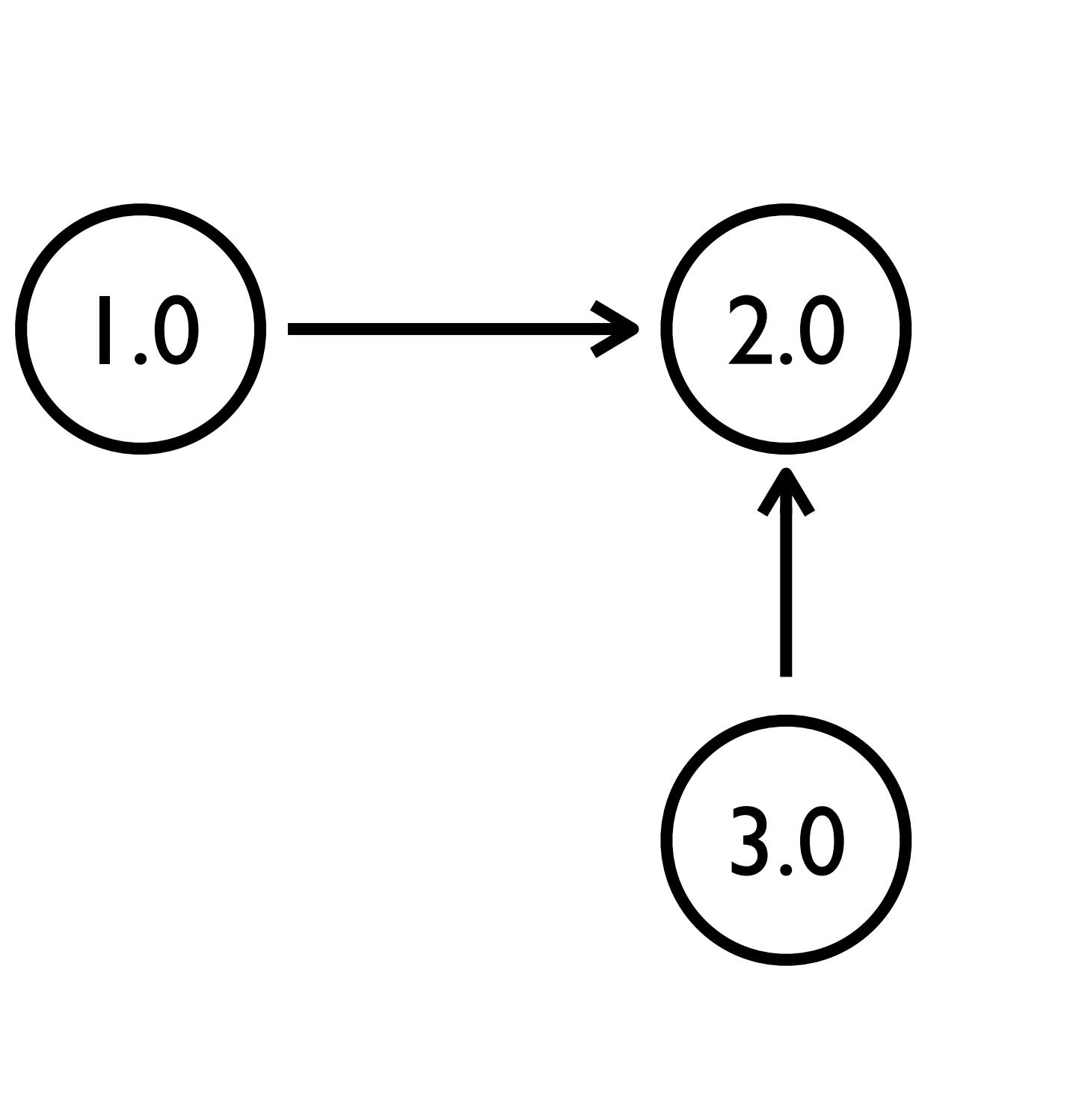
전민석

ERC Workshop @ KAIST, Korea

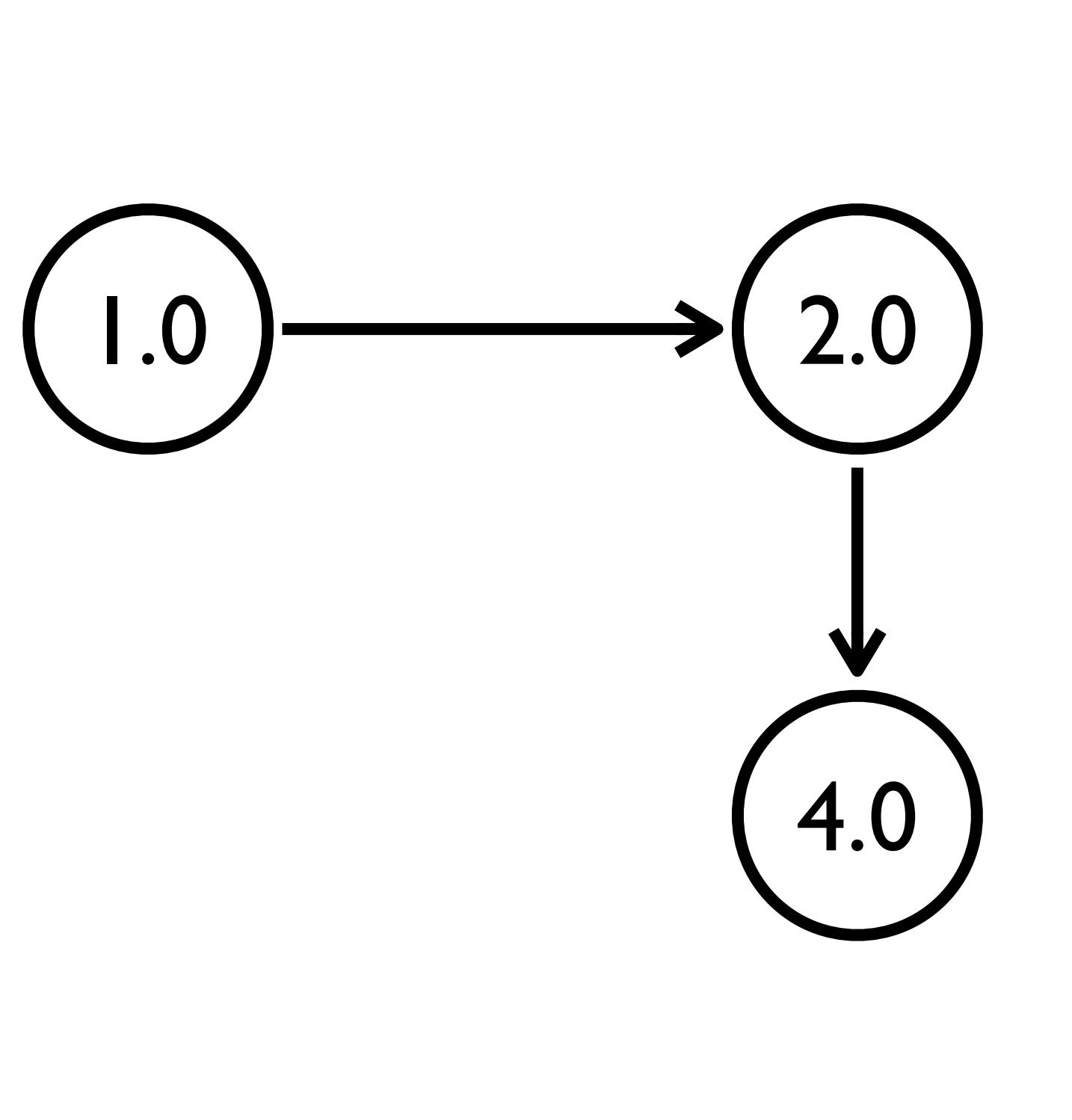


# 그래프 데이터에서의 패턴

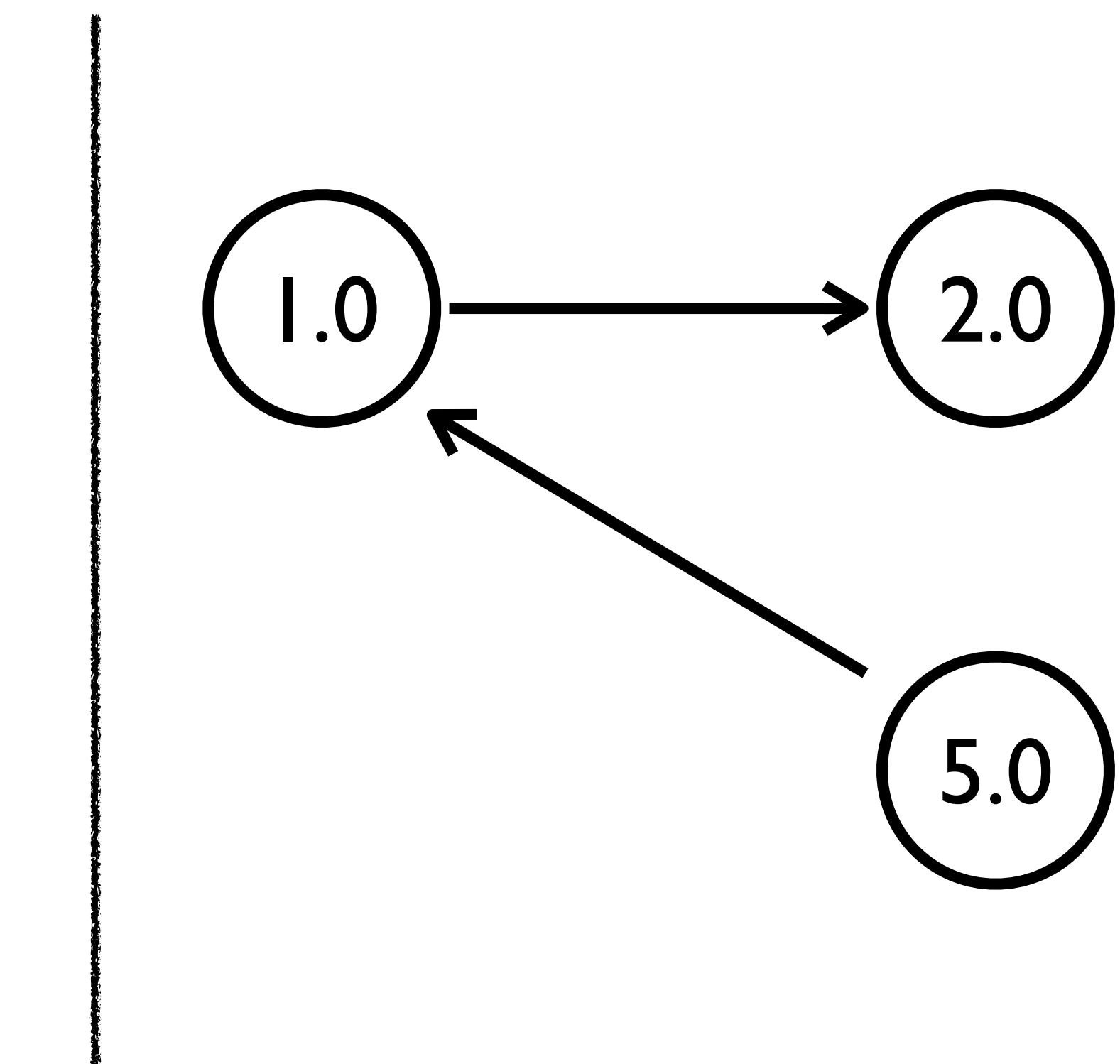
- 세 그래프 데이터의 공통된 패턴은?



그래프 1



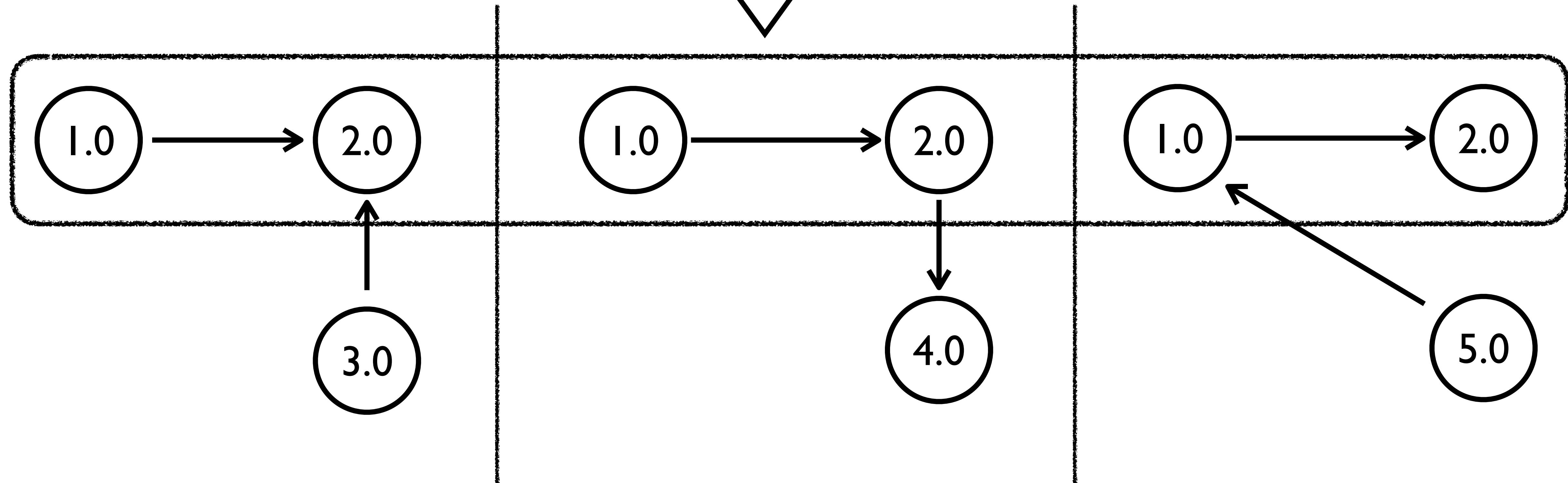
그래프 2



그래프 3

## 공통된 서브그래프(subgraph) 패턴

- 세 그래프



그래프 1

그래프 2

그래프 3

# 기존의 그래프 패턴 표현 언어: 서브그래프

## Application: 그래프 데이터 마이닝

### Graph Mining Algorithms



Inductive Logic Programming (WARMR, King et al. 2001)

- Graphs are represented by Datalog facts

#### Graph Based Approaches

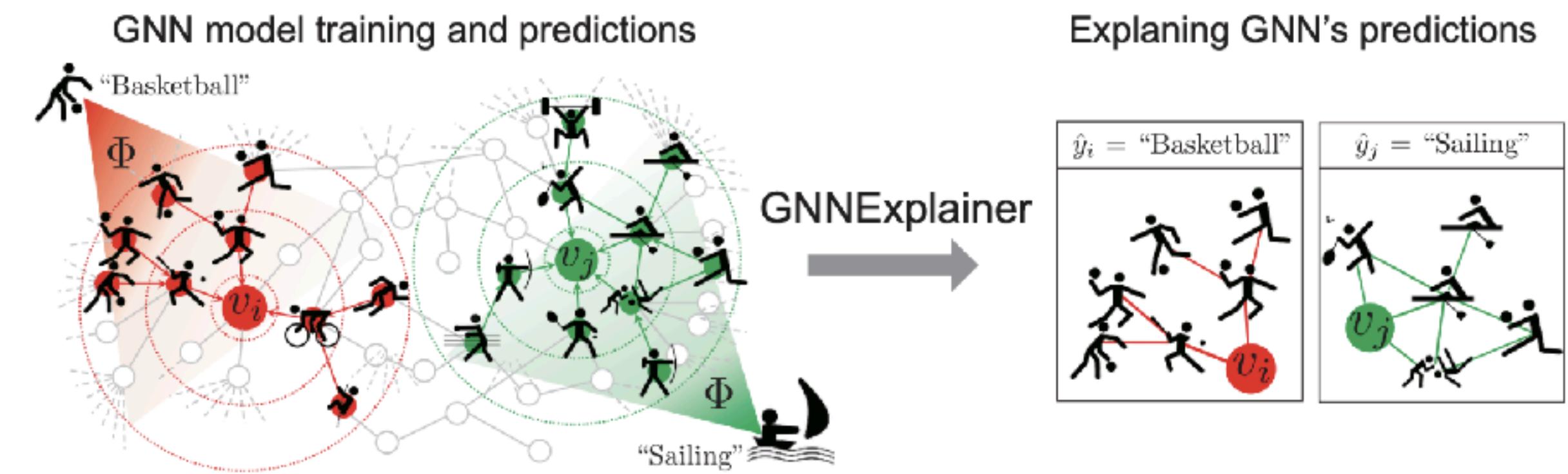
- Apriori-based approach
  - AGM/AcGM: Inokuchi, et al. (PKDD'00)
  - FSG: Kuramochi and Karypis (ICDM'01)
  - PATH#: Vanetik and Gudes (ICDM'02, ICDM'04)
  - FFSM: Huan, et al. (ICDM'03) and SPIN: Huan et al. (KDD'04)
  - FTOSM: Horvath et al. (KDD'06)
- Pattern growth approach
  - Subdue: Holder et al. (KDD'94)
  - MoFa: Borgelt and Berthold (ICDM'02)
  - gSpan: Yan and Han (ICDM'02)
  - Gaston: Nijssen and Kok (KDD'04)
  - CMTreeMiner: Chi et al. (TKDE'05), LEAP: Yan et al. (SIGMOD'08)

서브그래프  
마이닝  
알고리즘

## Application: GNN 설명 기술

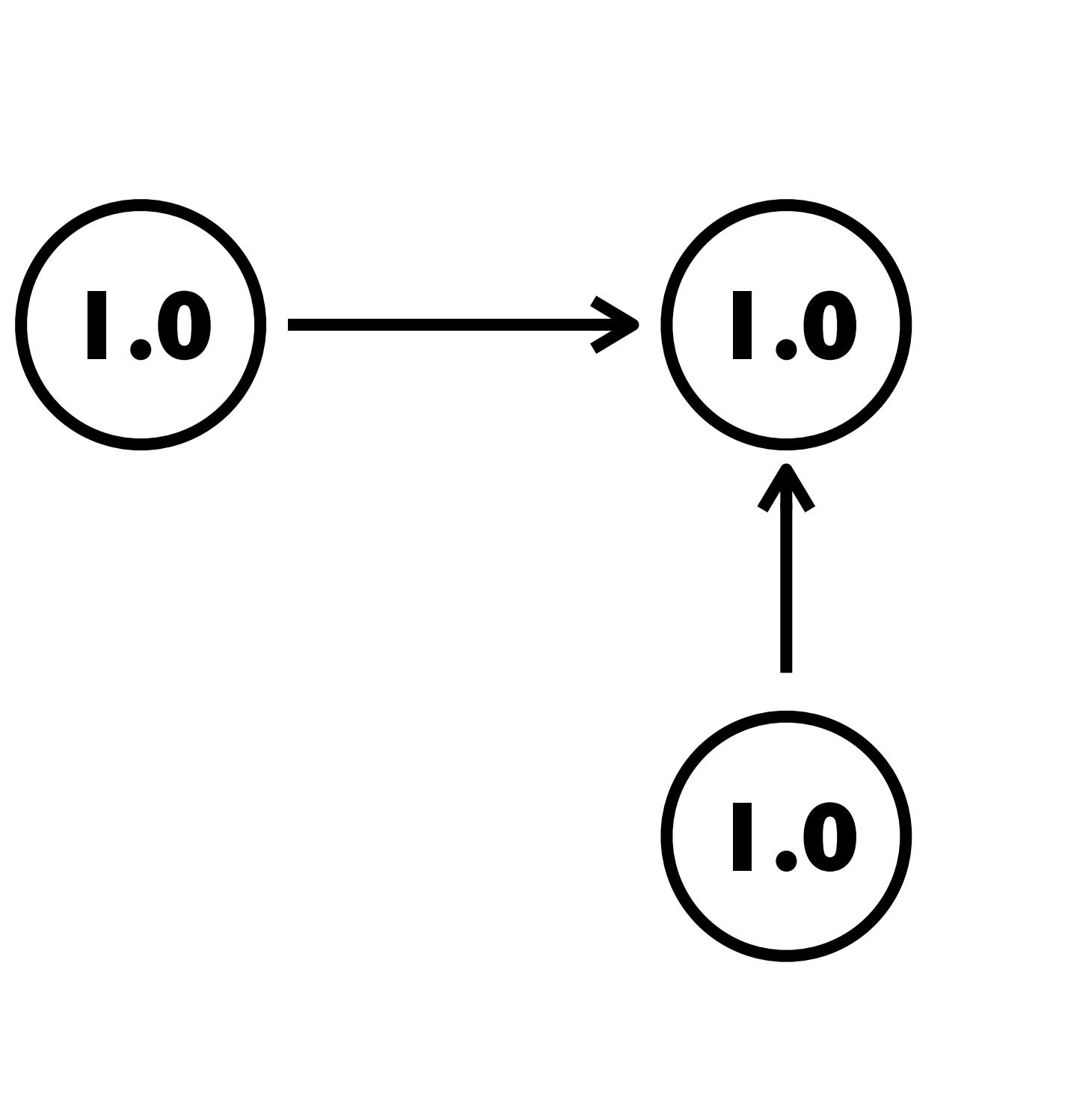
### 2. GNNExplainer Overview

#### Subgraph

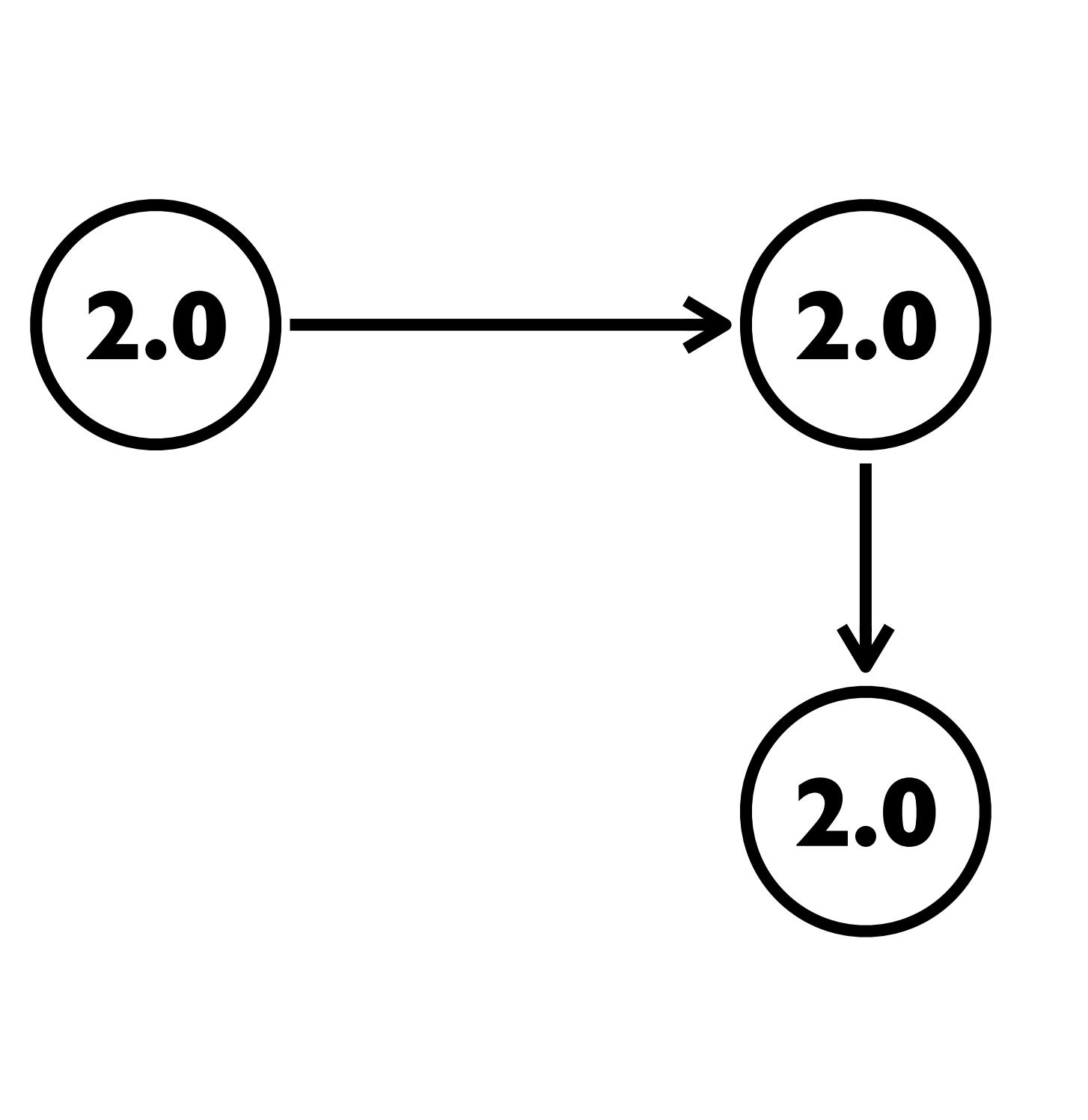


# 서브그래프의 표현력 한계

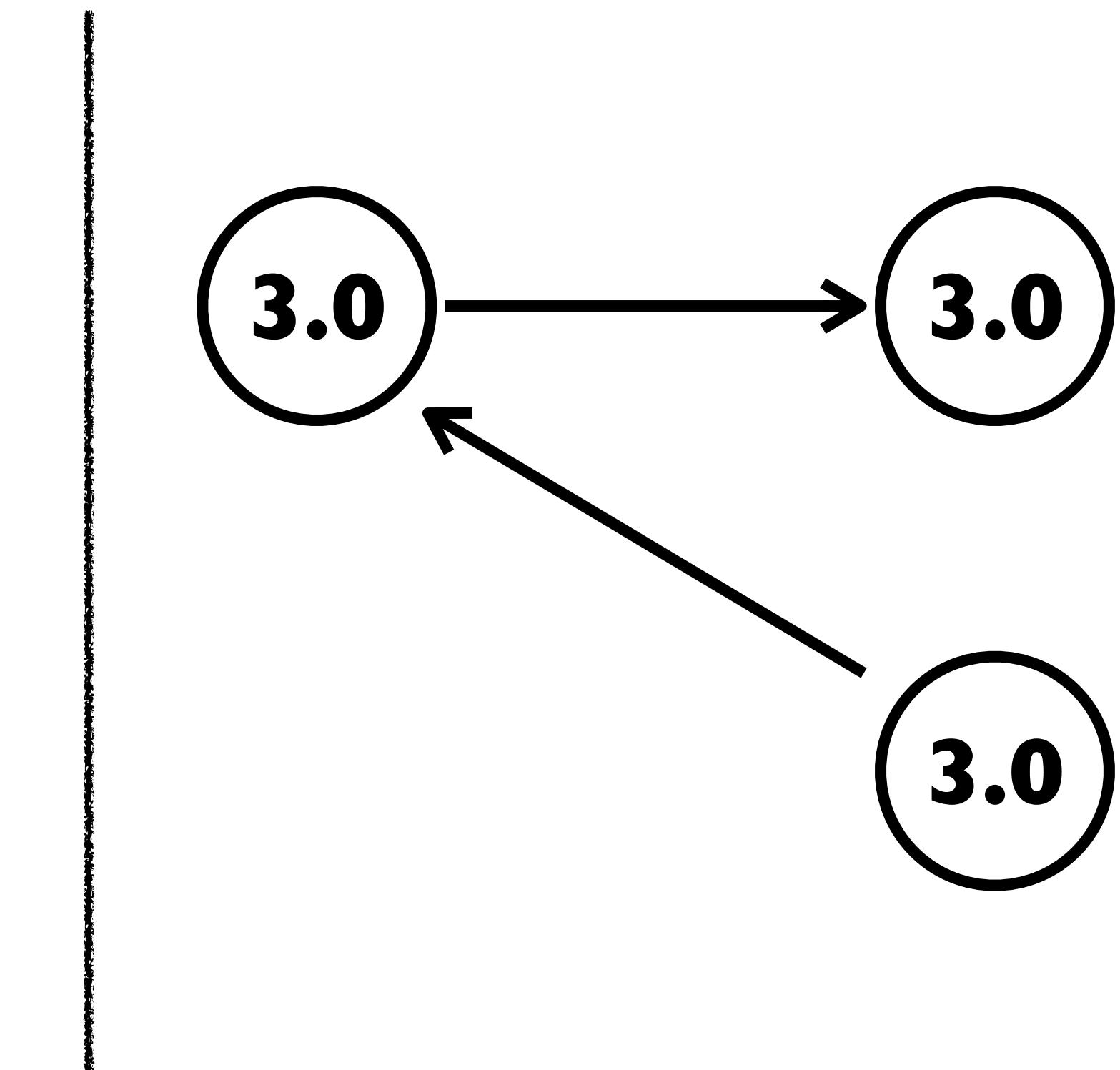
- 세 그래프 데이터의 공통된 패턴은?



그래프 1



그래프 2

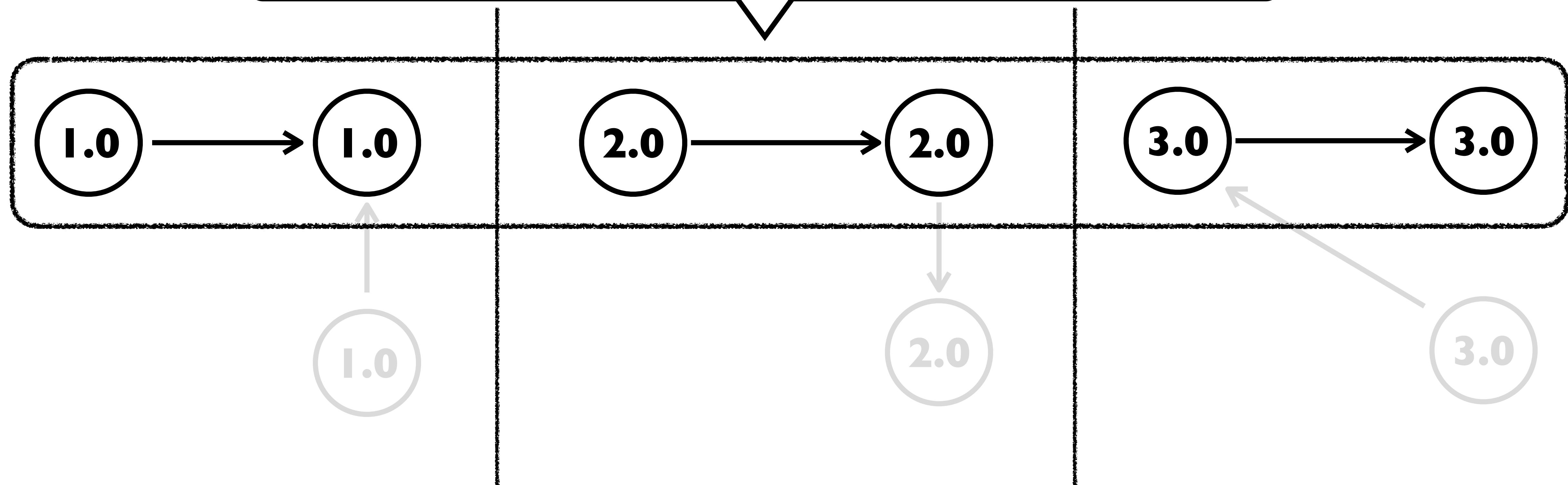


그래프 3

연결된 두 노드의 feature 값이 같다.

$$[-\infty, \infty] \equiv [-\infty, \infty]$$

- 세 그래프



그래프 1

그래프 2

그래프 3

# 그래프 패턴 프로그래밍 언어 (GDL)

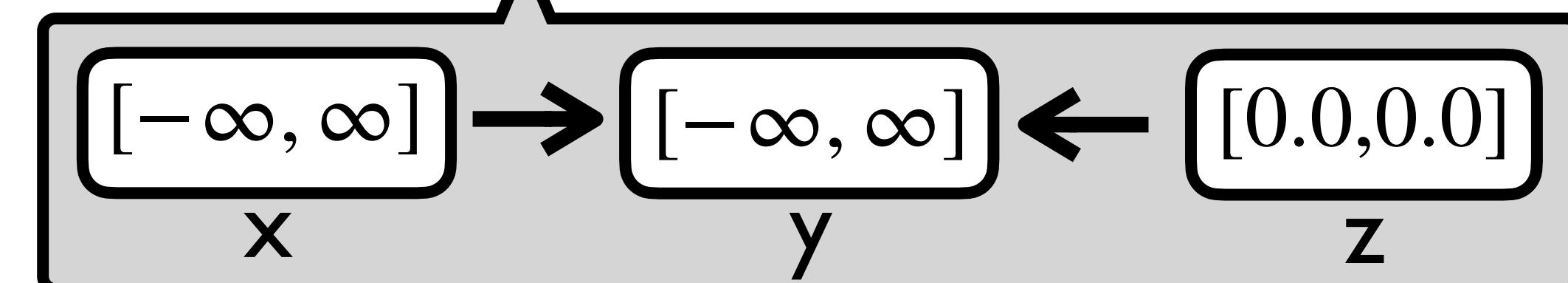
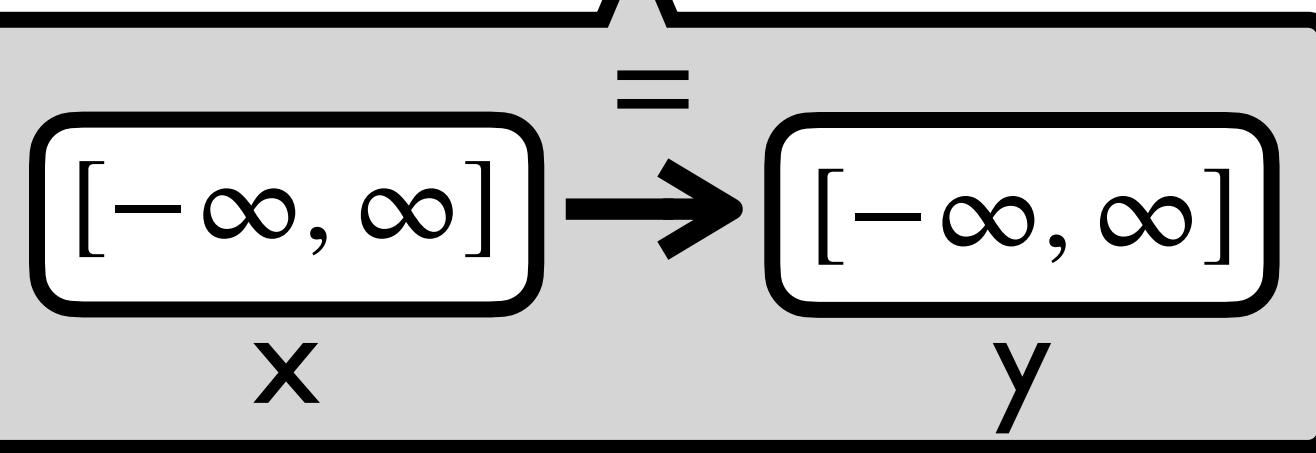
Programs	$P_4 ::= \bar{\delta} \text{ target } t$	$\in \mathbb{P} = \mathbb{D}^* \times \mathbb{T}$
Descriptions	$\delta ::= \delta_V \mid \delta_E$	$\in \mathbb{D} = \mathbb{D}_V \uplus \mathbb{D}_E$
Node Descriptions	$\delta_V ::= \text{node } x <\!\!\phi\!\!>?$	$\in \mathbb{D}_V = \mathbb{X} \times \Phi^d$
Edge Descriptions	$\delta_E ::= \text{edge } (x,x) <\!\!\phi\!\!>?$	$\in \mathbb{D}_E = \mathbb{X} \times \mathbb{X} \times \Phi^e$
Target Symbols	$t ::= \text{node } x \mid \text{edge } (x,x) \mid \text{graph}$	$\in \mathbb{T} = \mathbb{X} \uplus (\mathbb{X} \times \mathbb{X}) \uplus \{\epsilon\}$
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	$x ::= x \mid y \mid z \mid \dots$	$\in \mathbb{X}$

**GDL program 1**  
 node x  $[-\infty, \infty]$   
 node y  $[-\infty, \infty]$   
 edge (x, y) “=”  
 target graph

**GDL program 2**  
 node x  $[-\infty, \infty]$   
 node y  $[-\infty, \infty]$   
 node z  $[0.0, 0.0]$   
 edge (x, y)  
 edge (z, y)  
 target graph

**GDL program 3**

[0.0,0.0]  
 x



# 그래프 패턴 프로그래밍 언어 (GDL)

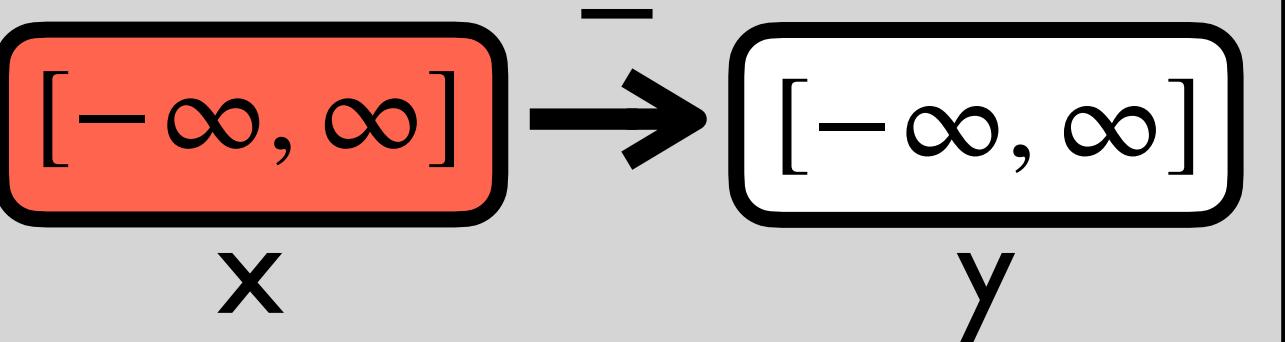
Programs	$P_4 ::= \bar{\delta} \text{ target } t$	$\in \mathbb{P} = \mathbb{D}^* \times \mathbb{T}$
Descriptions	$\delta ::= \delta_V \mid \delta_E$	$\in \mathbb{D} = \mathbb{D}_V \uplus \mathbb{D}_E$
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Edge Descriptions	$\delta_E ::= \text{edge } (x,x) <\!\!\phi\!\!>?$	$\in \mathbb{D}_E = \mathbb{X} \times \mathbb{X} \times \Phi^e$
Target Symbols	$t ::= \text{node } x \mid \text{edge } (x,x) \mid \text{graph}$	$\in \mathbb{T} = \mathbb{X} \uplus (\mathbb{X} \times \mathbb{X}) \uplus \{\epsilon\}$
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	$x ::= x \mid y \mid z \mid \dots$	$\in \mathbb{X}$

**node**  $x \times [-\infty, \infty]$   
**node**  $y \times [-\infty, \infty]$   
**edge**  $(x,y) \text{ ``=``}$   
**target** **node**  $x$

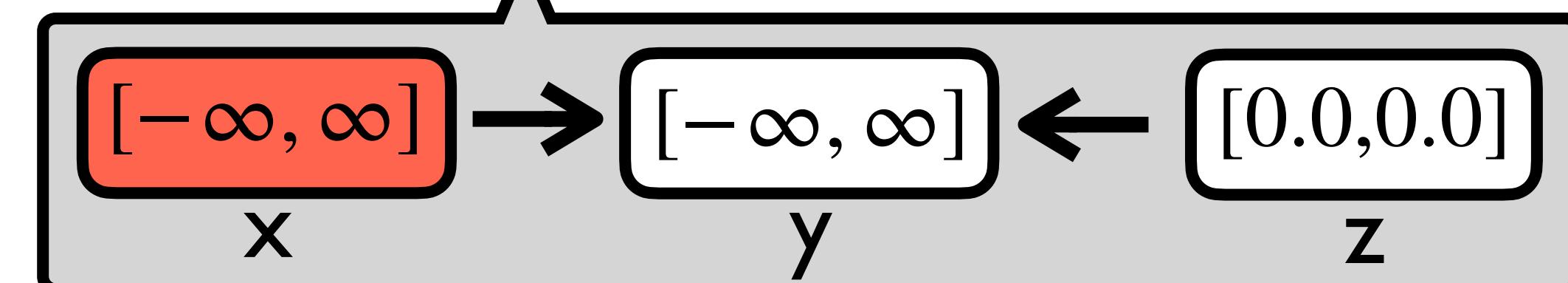
GDL program 1

**node**  $x \times [-\infty, \infty]$   
**node**  $y \times [-\infty, \infty]$   
**node**  $z \times [0.0, 0.0]$   
**edge**  $(x,y)$   
**edge**  $(z,y)$   
**target** **node**  $x$

GDL program 2



GDL program 3

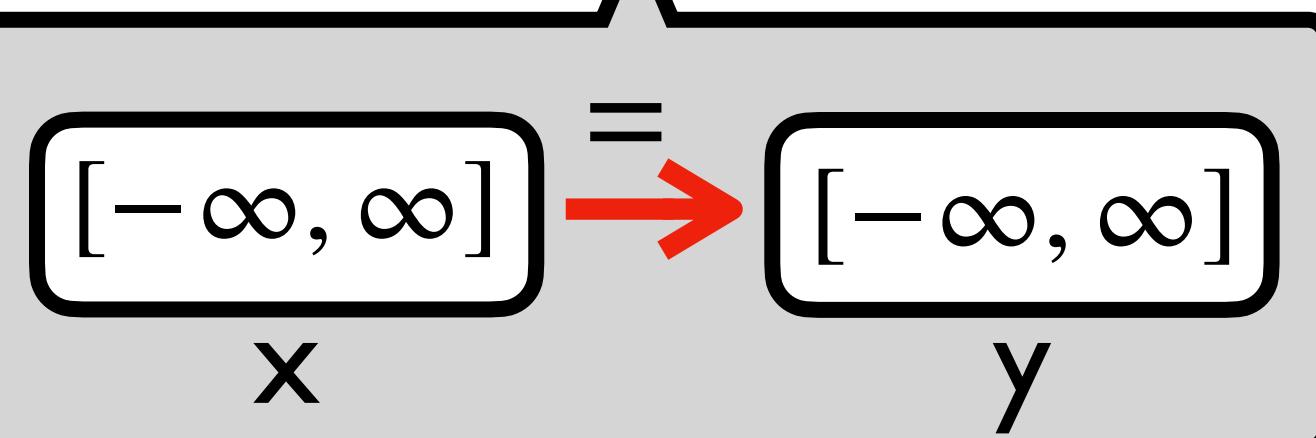


# 그래프 패턴 프로그래밍 언어 (GDL)

Programs	$P_4 ::= \bar{\delta} \text{ target } t$	$\in \mathbb{P} = \mathbb{D}^* \times \mathbb{T}$
Descriptions	$\delta ::= \delta_V \mid \delta_E$	$\in \mathbb{D} = \mathbb{D}_V \uplus \mathbb{D}_E$
Node Descriptions	$\delta_V ::= \text{node } x <\overline{\phi}>?$	$\in \mathbb{D}_V = \mathbb{X} \times \Phi^d$
Edge Descriptions	$\delta_E ::= \text{edge } (x, x) <\overline{\phi}>?$	$\in \mathbb{D}_E = \mathbb{X} \times \mathbb{X} \times \Phi^c$
Target Symbols	$t ::= \text{node } x \mid \text{edge } (x, x) \mid \text{graph}$	$\in \mathbb{T} = \mathbb{X} \uplus (\mathbb{X} \times \mathbb{X}) \uplus \{\epsilon\}$
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	$x ::= x \mid y \mid z \mid \dots$	$\in \mathbb{X}$

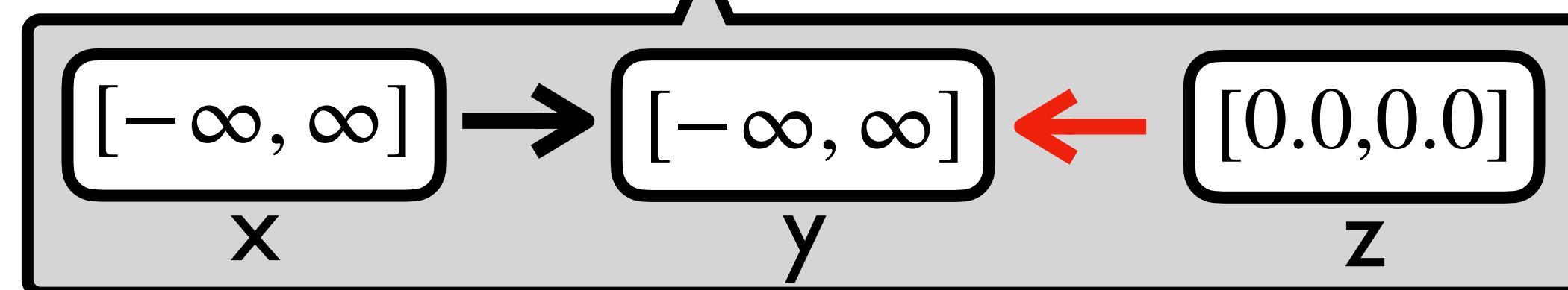
**node**  $x [-\infty, \infty]$   
**node**  $y [-\infty, \infty]$   
**edge**  $(x, y) “=”$   
**target edge**  $(x, y)$

GDL program 1



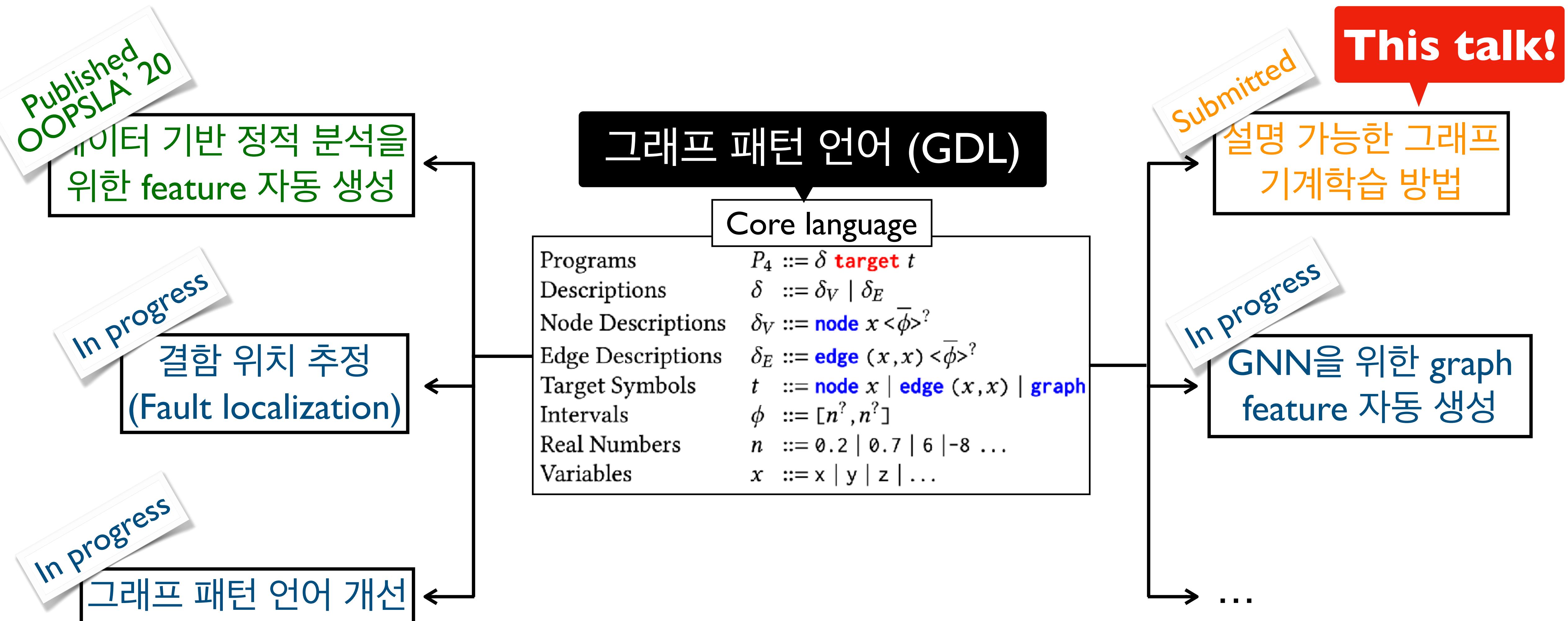
**node**  $x [-\infty, \infty]$   
**node**  $y [-\infty, \infty]$   
**node**  $z [0.0, 0.0]$   
**edge**  $(x, y)$   
**edge**  $(z, y)$   
**target edge**  $(z, y)$

GDL program 2



# Graph Description Language (GDL) Project

- 목표: 그래프 표현 언어를 확장 및 사용하여 각 분야의 핵심 문제 해결하기



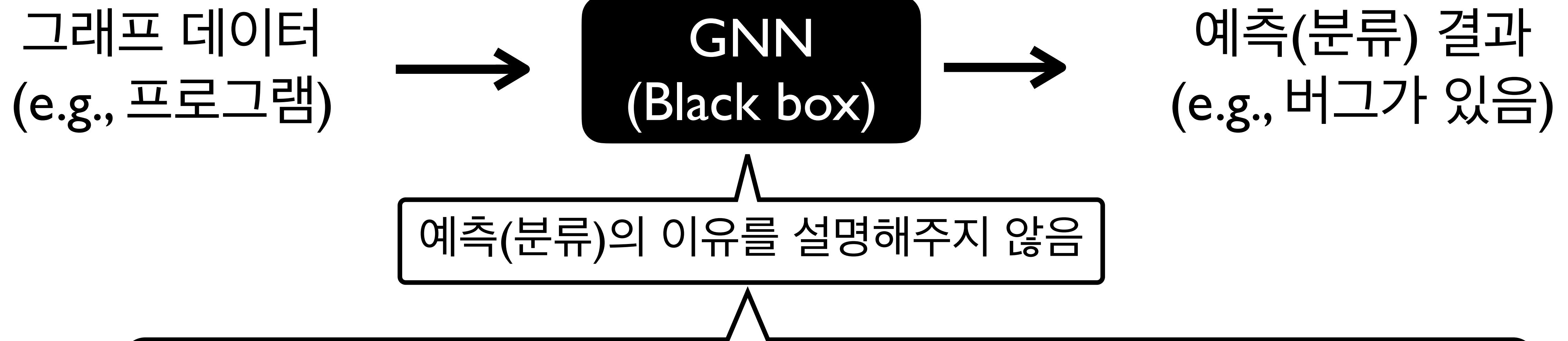
# 그래프 패턴 언어를 활용한 설명 가능한 기계학습 방법

전민석

ERC Workshop @ KAIST, Korea



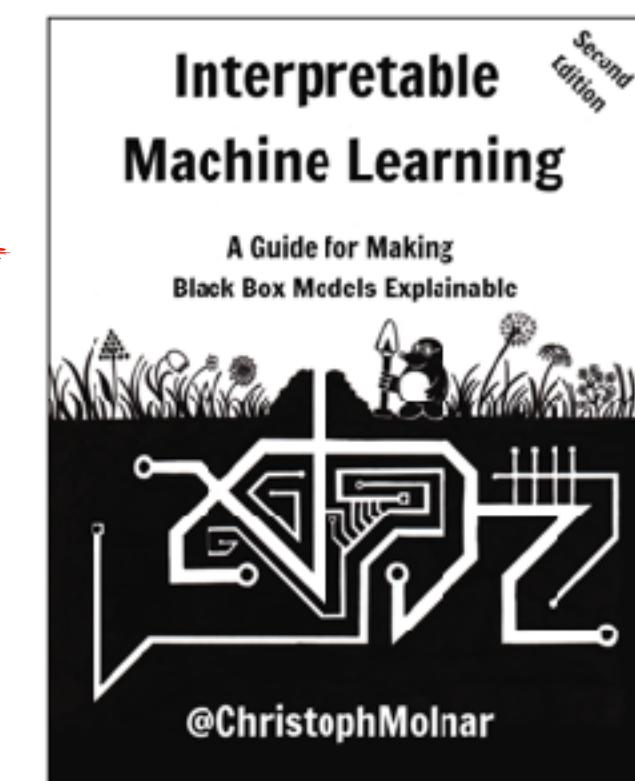
- 기존: 설명 불가능한 기계학습 방법 (Graph Neural Network)



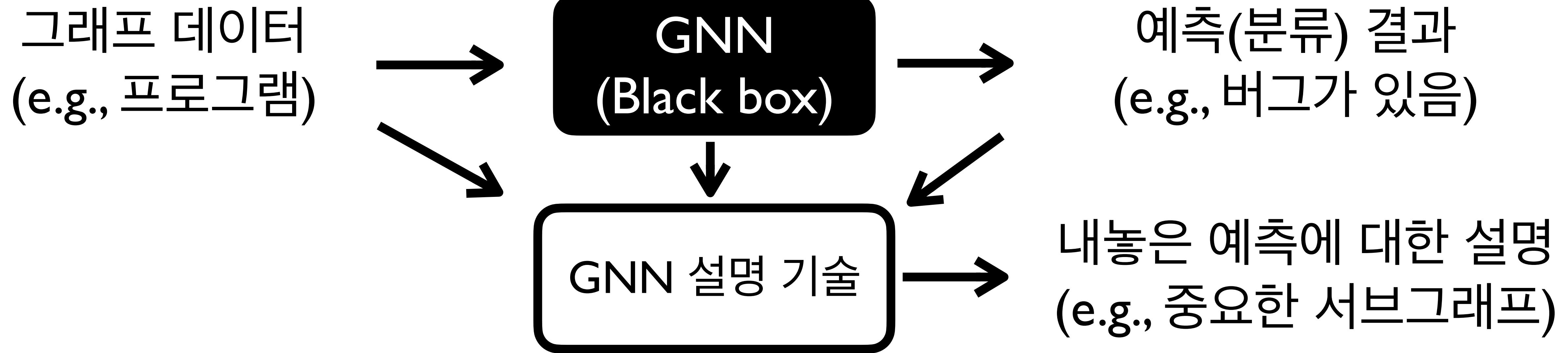
Value of explainability is growing fast

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

- Molnar [2022]

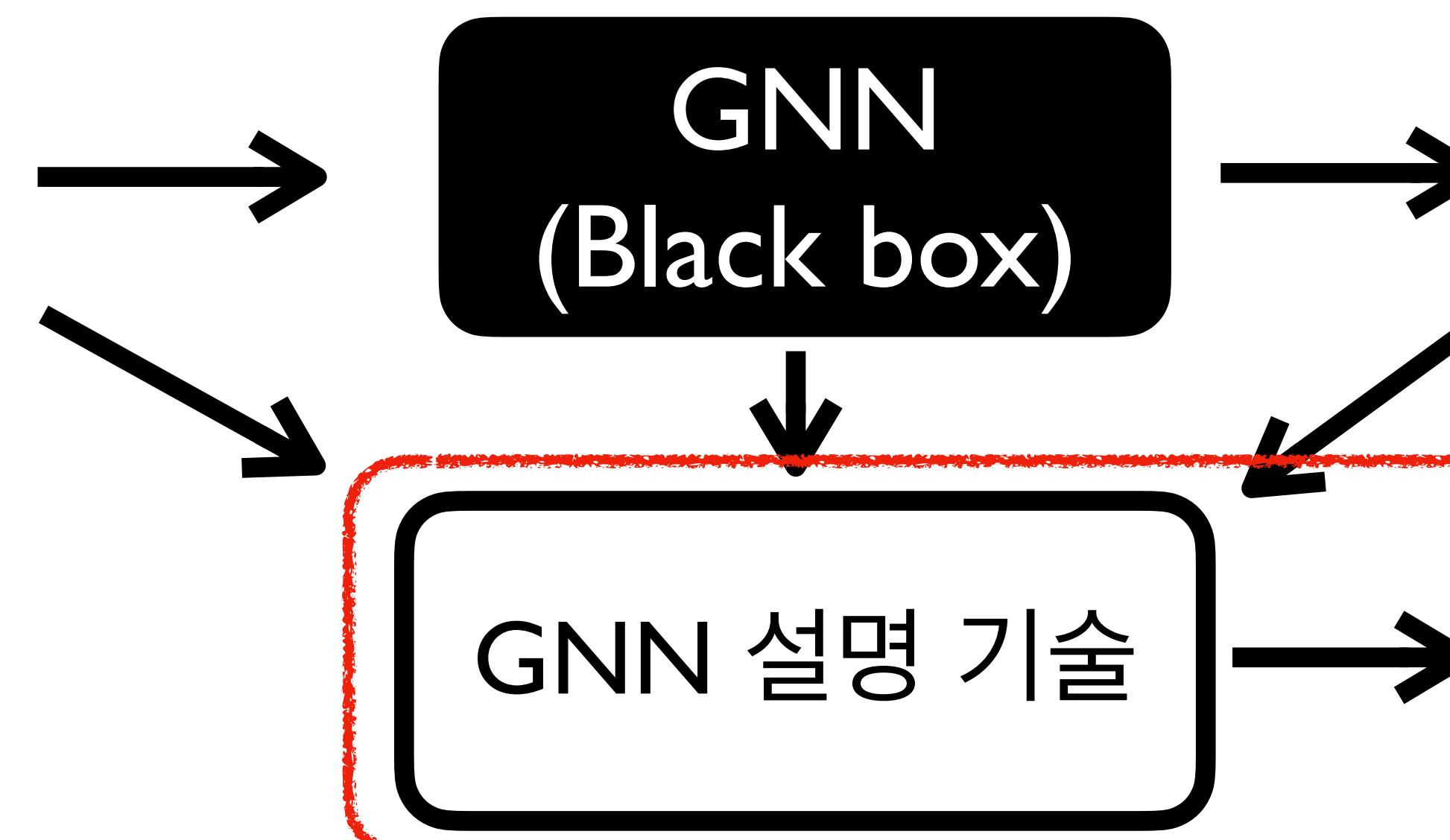


- 기존: 설명 불가능한 기계학습 방법 (Graph Neural Network)



- 기존: 설명 불가능한 기계학습 방법 (Graph Neural Network)

그래프 데이터  
(e.g., 프로그램)



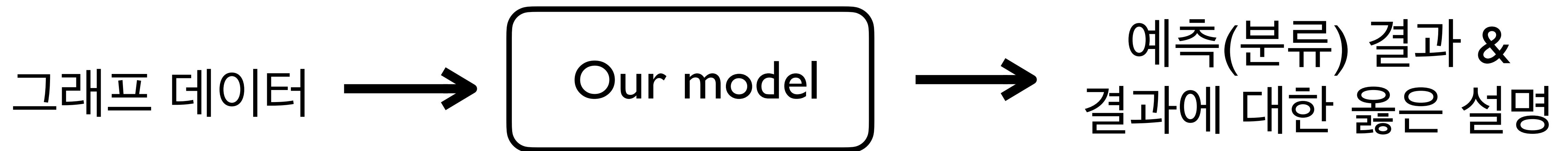
예측(분류) 결과  
(e.g., 버그가 있음)

내놓은 예측에 대한 설명  
(e.g., 중요한 서브그래프)

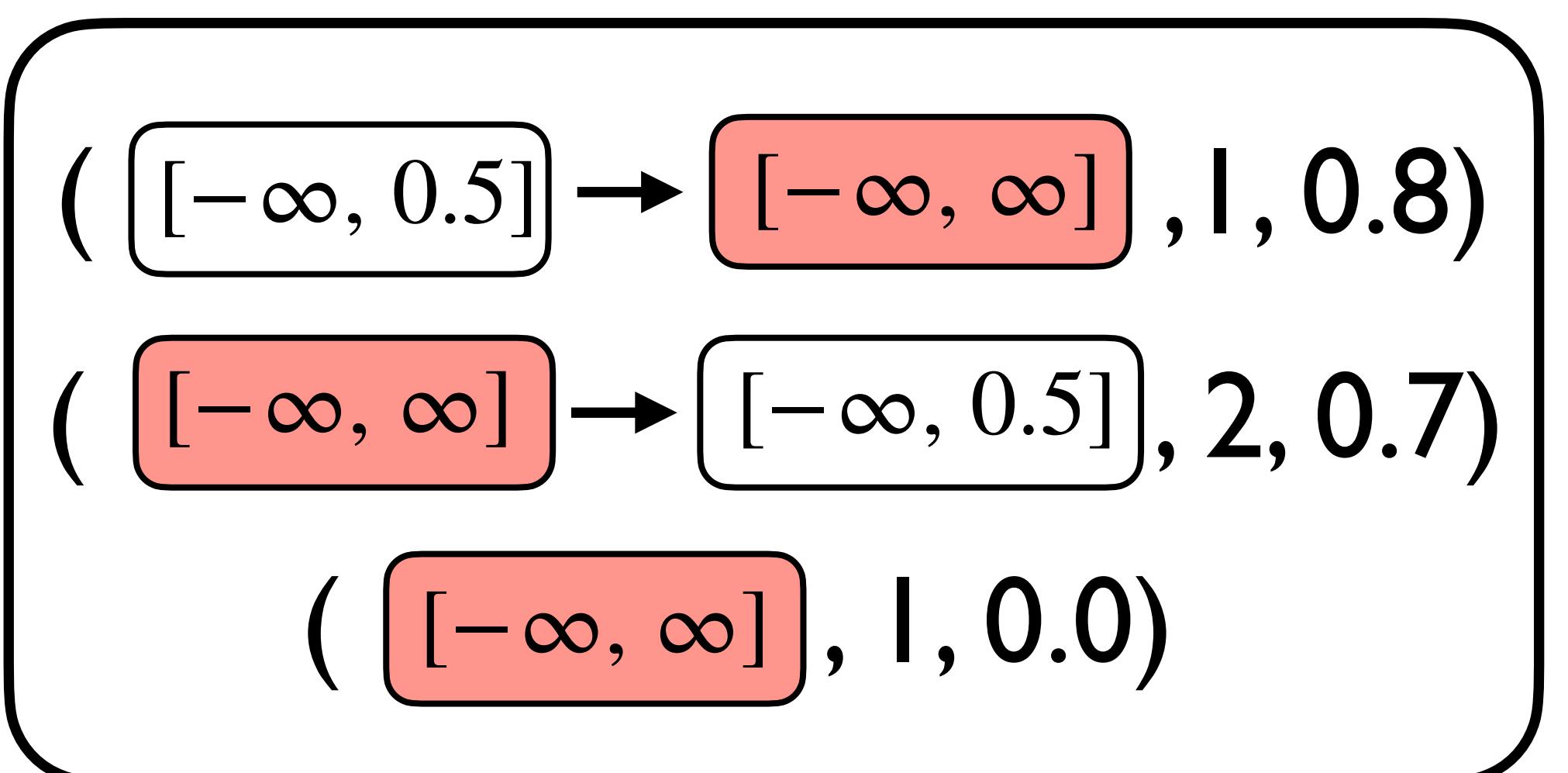
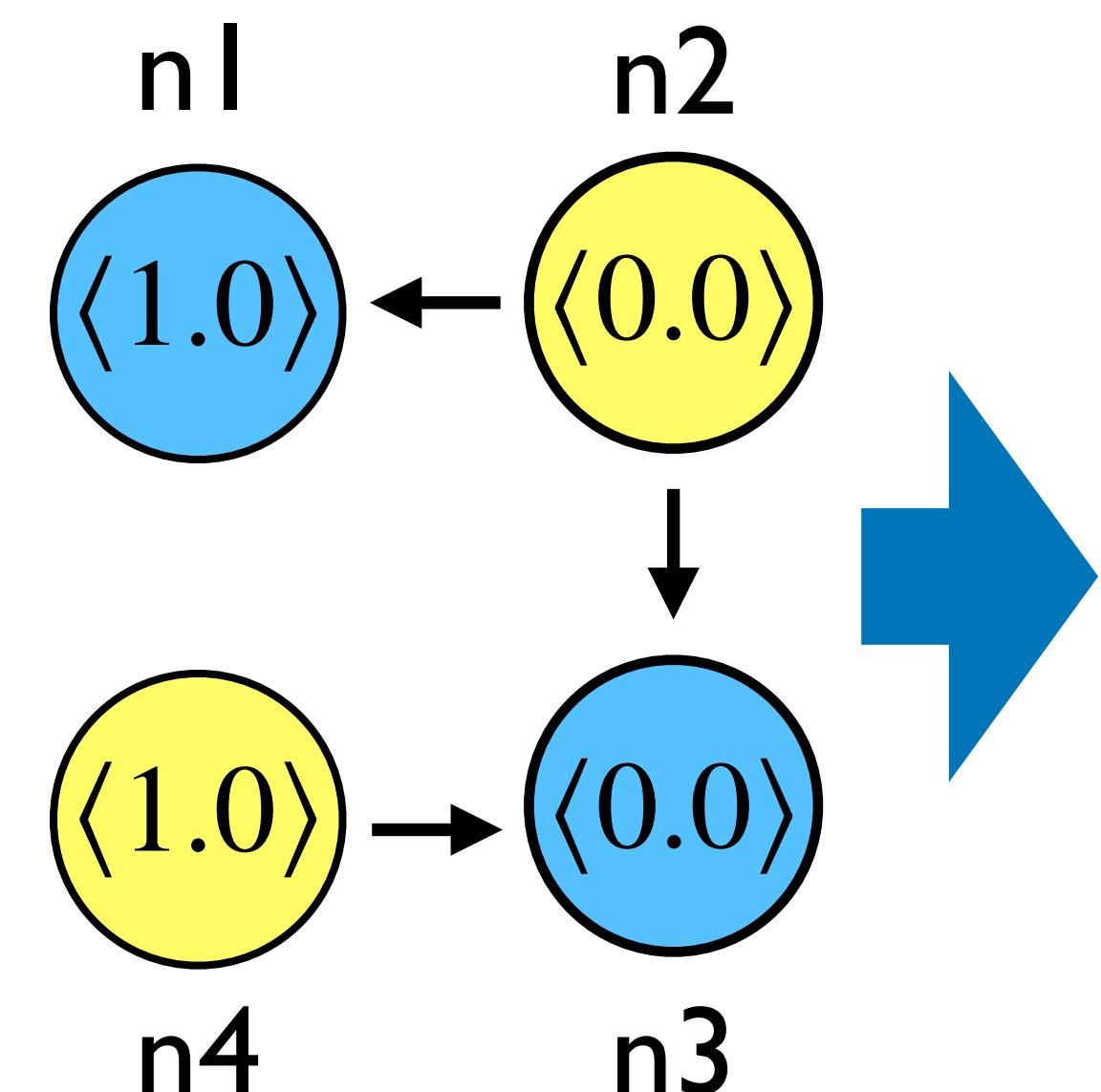
### 근본적인 문제 두가지

- 설명을 생성하기 위해 (비싼) 추가비용을 지불해야함
- 제공된 설명이 옳은 설명임을 보장해주지 않음

- PL4XGL: 그래프 패턴 언어(GDL) 기반 설명 가능한 그래프 기계학습 방법



- 추가적인 설명 비용 필요없음
- 제공된 설명은 옳은 설명임을 보장함

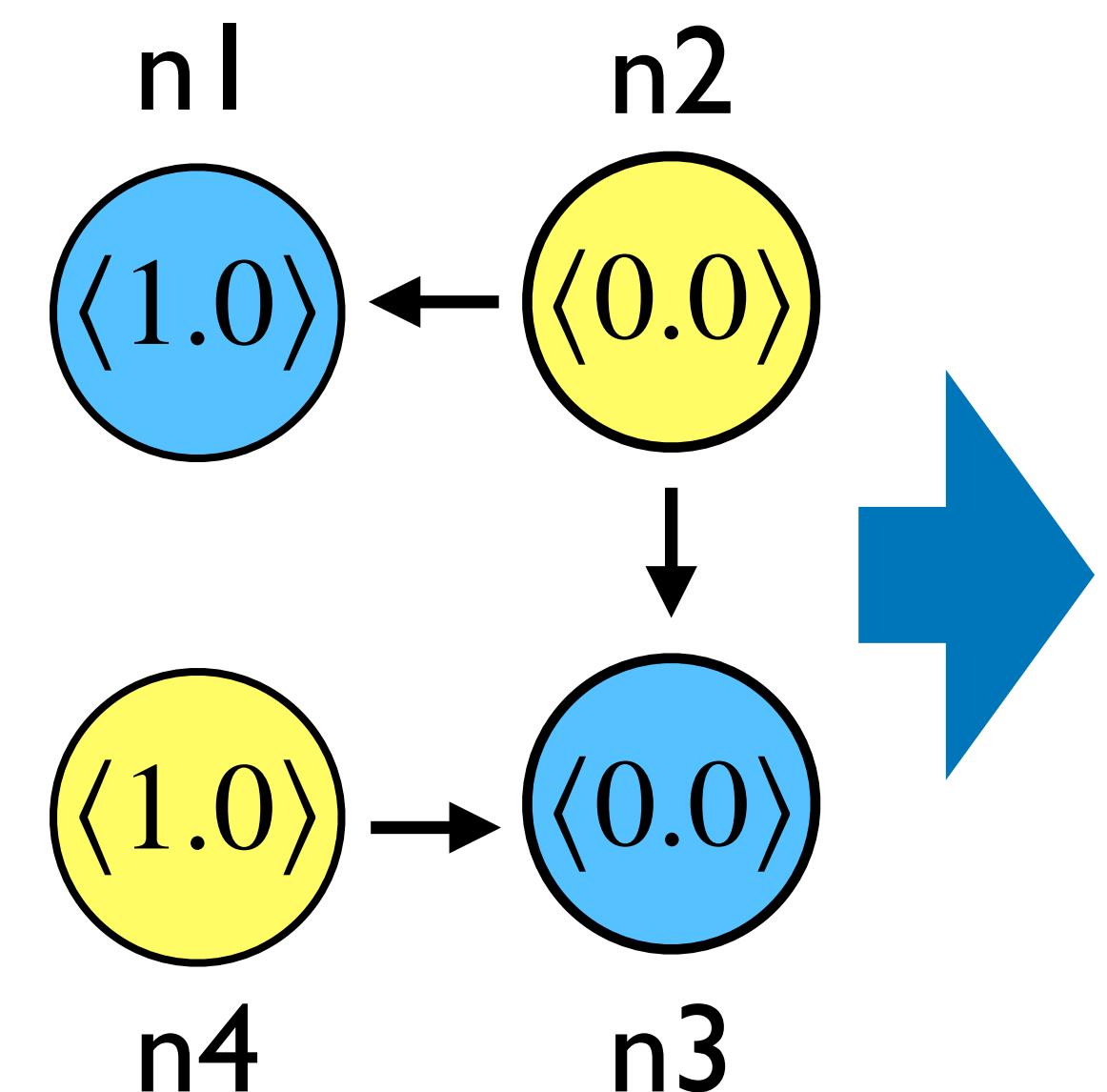


분류 모델

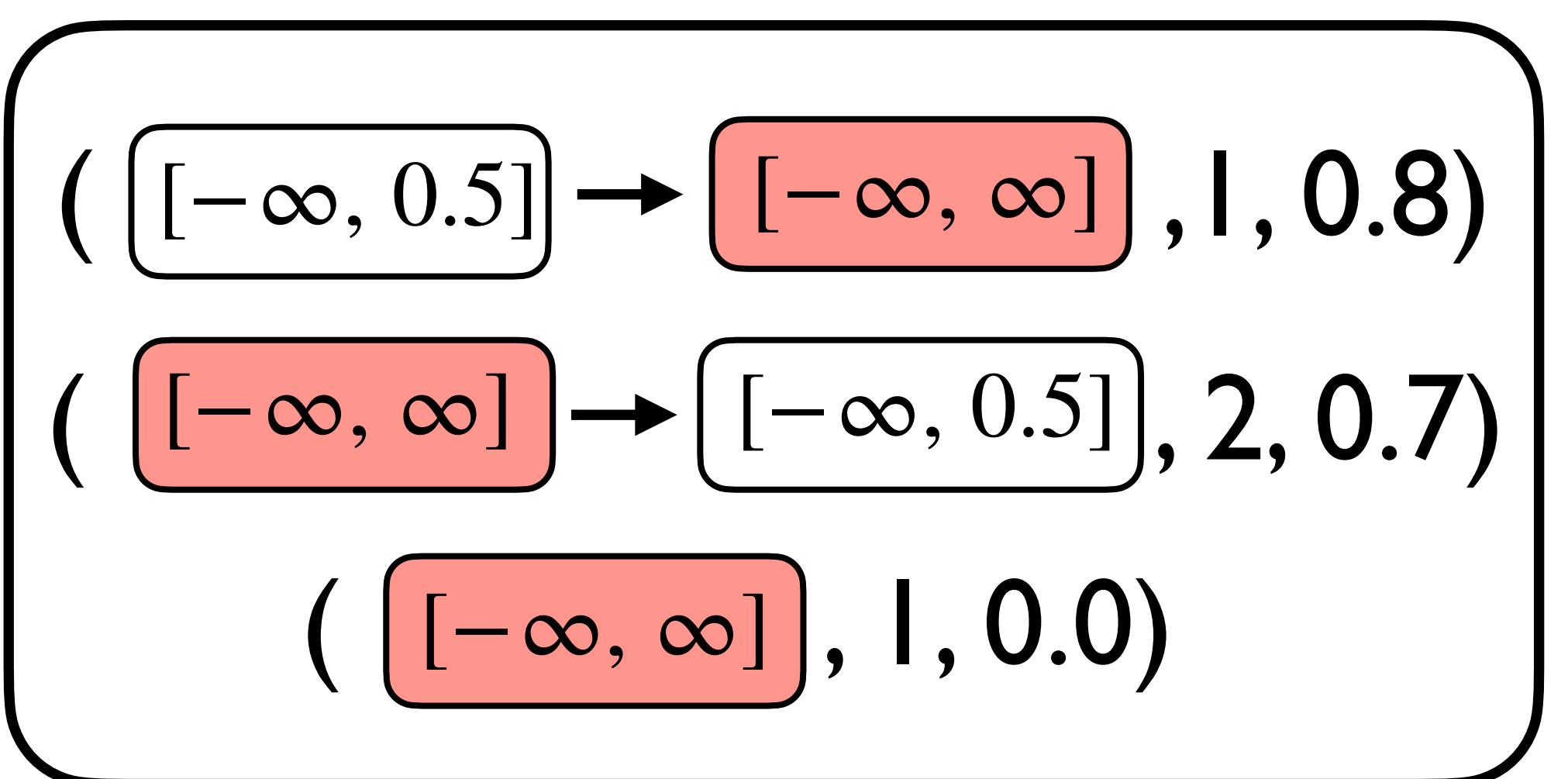
예측 결과	설명
$n1: (1, [-\infty, 0.5] \rightarrow [-\infty, \infty])$	
$n2: (2, [-\infty, \infty] \rightarrow [-\infty, 0.5])$	
$n3: (1, [-\infty, 0.5] \rightarrow [-\infty, \infty])$	
$n4: (2, [-\infty, \infty] \rightarrow [-\infty, 0.5])$	

그래프 데이터

분류 결과



그래프 데이터

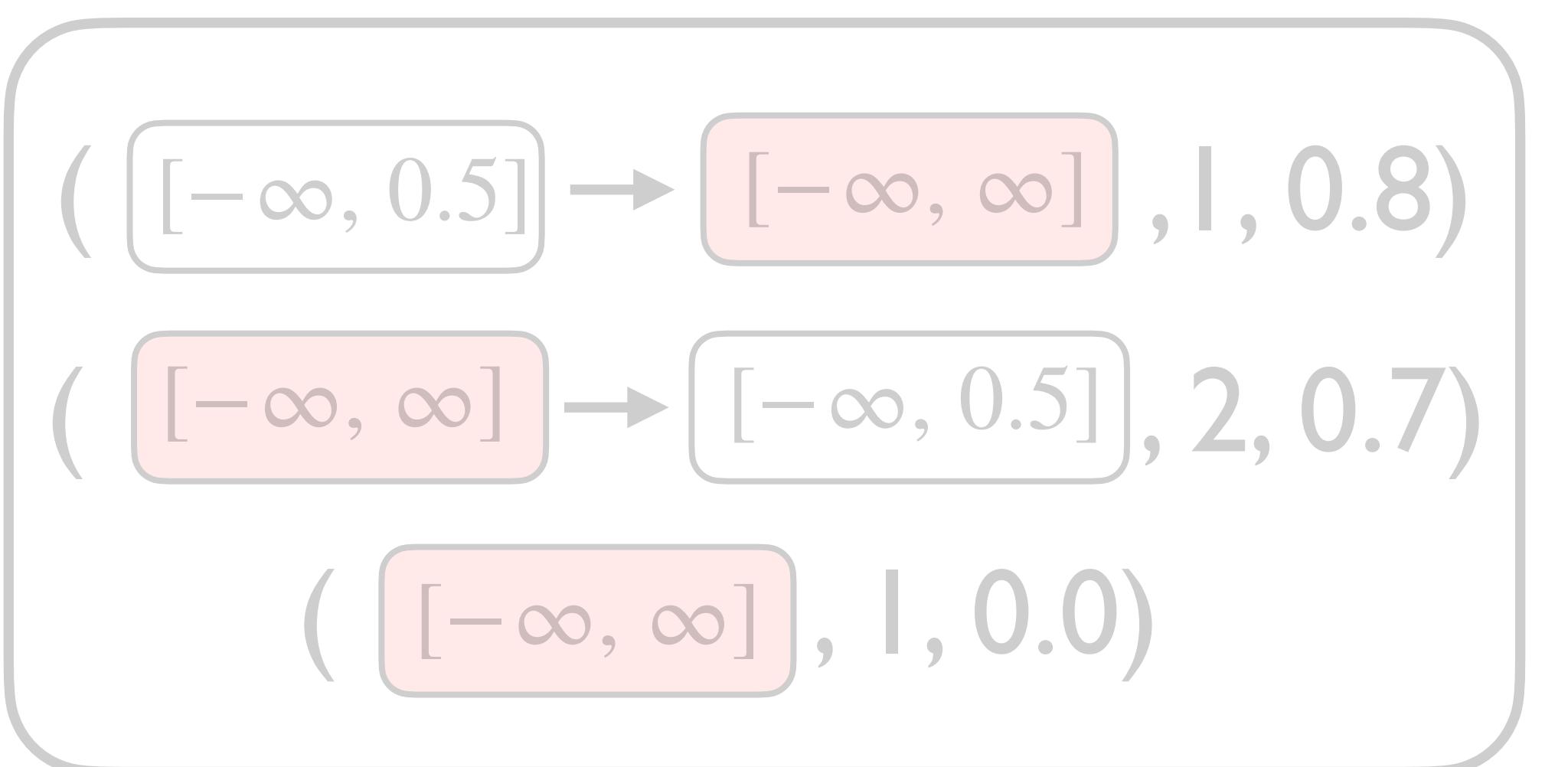
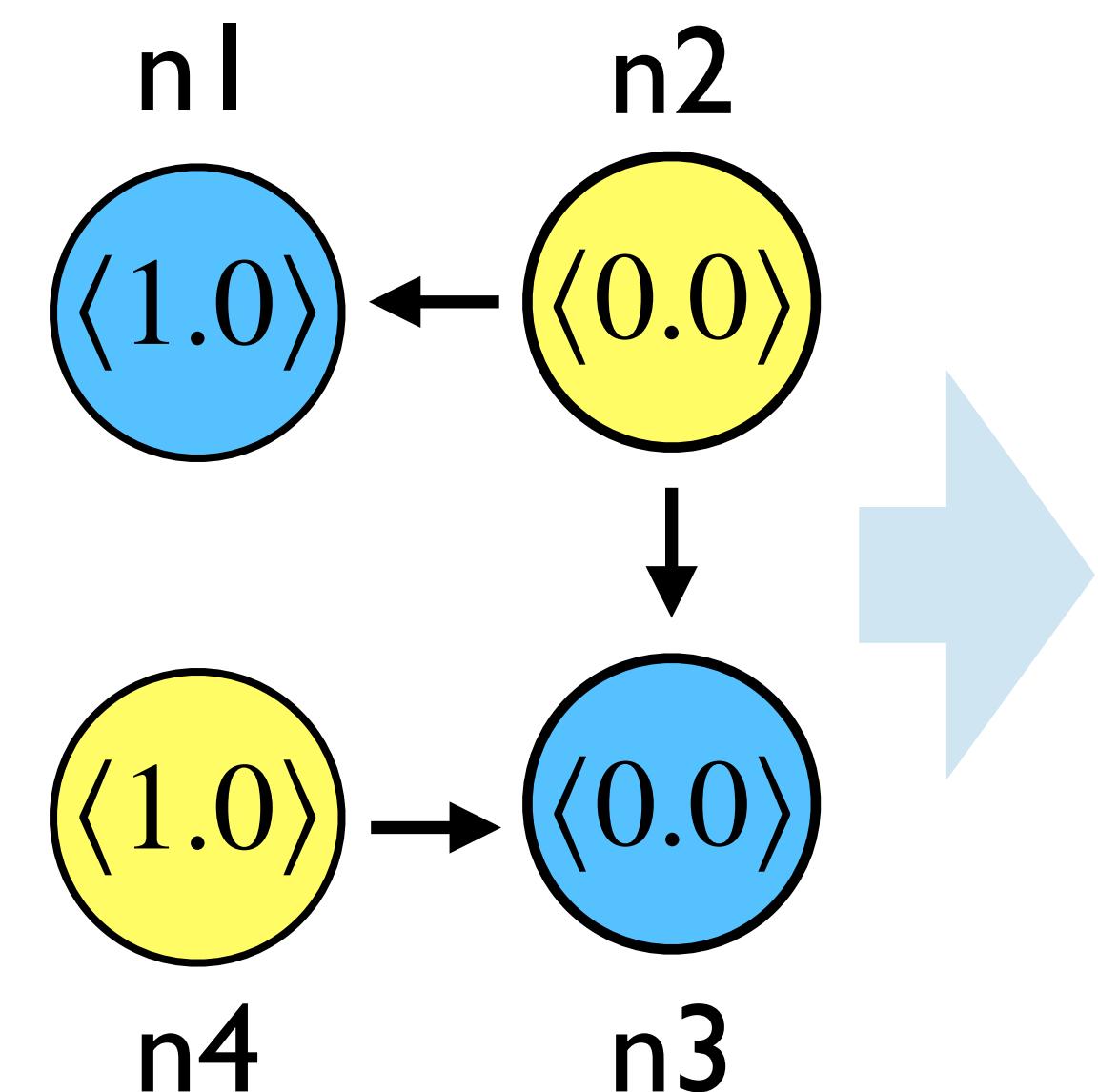
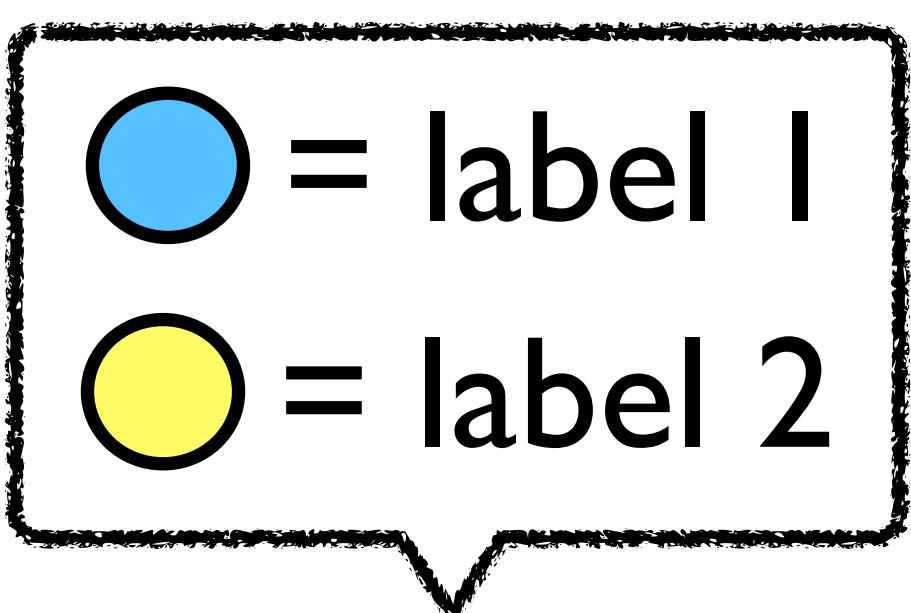


분류 모델

예측 결과      설명

$n1: (l, [-\infty, 0.5] \rightarrow [-\infty, \infty])$	$\downarrow$
$n2: (2, [-\infty, \infty] \rightarrow [-\infty, 0.5])$	$\downarrow$
$n3: (l, [-\infty, 0.5] \rightarrow [-\infty, \infty])$	$\downarrow$
$n4: (2, [-\infty, \infty] \rightarrow [-\infty, 0.5])$	$\downarrow$

분류 결과



분류 모델

그래프 데이터

예측 결과

설명

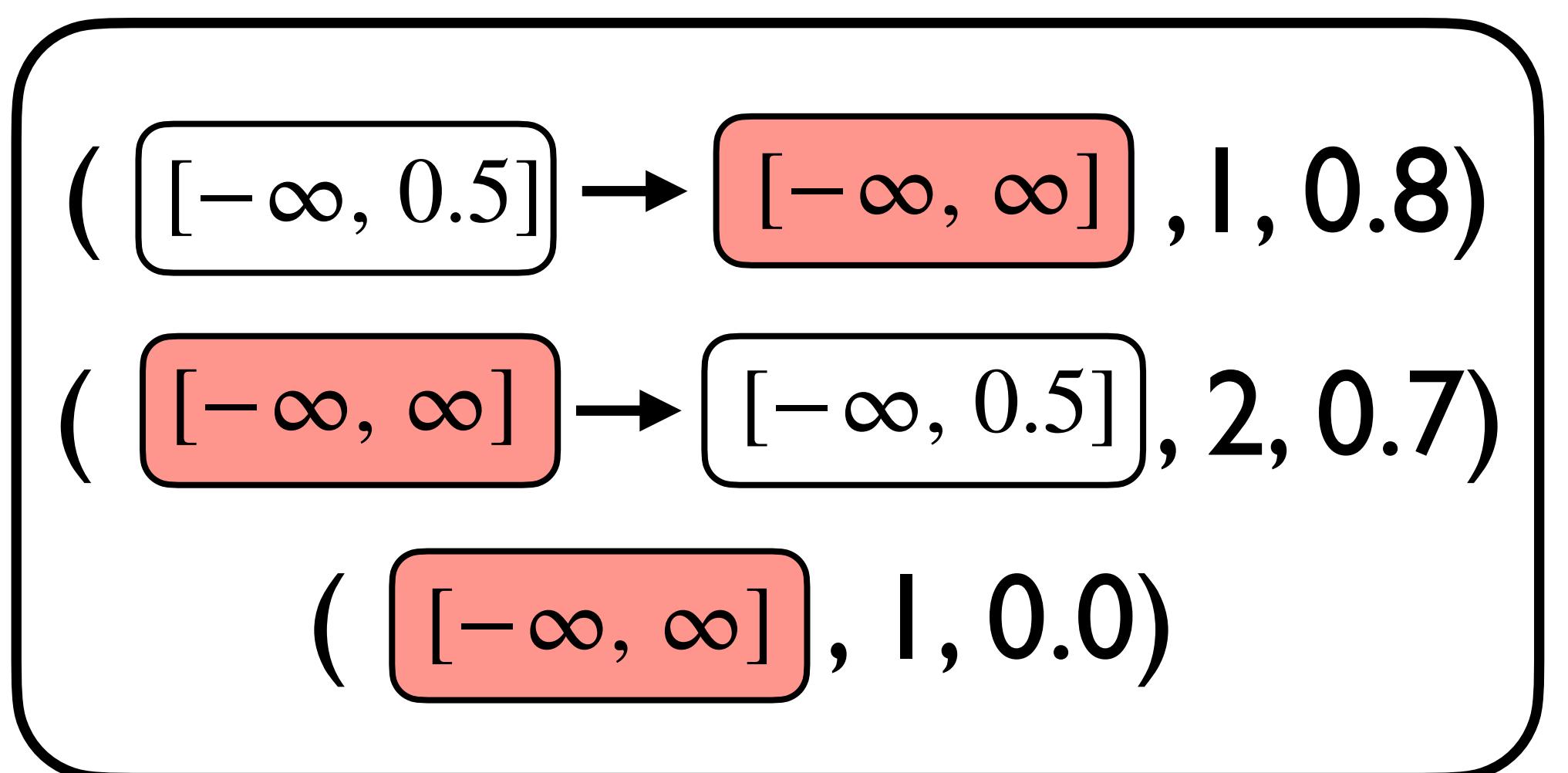
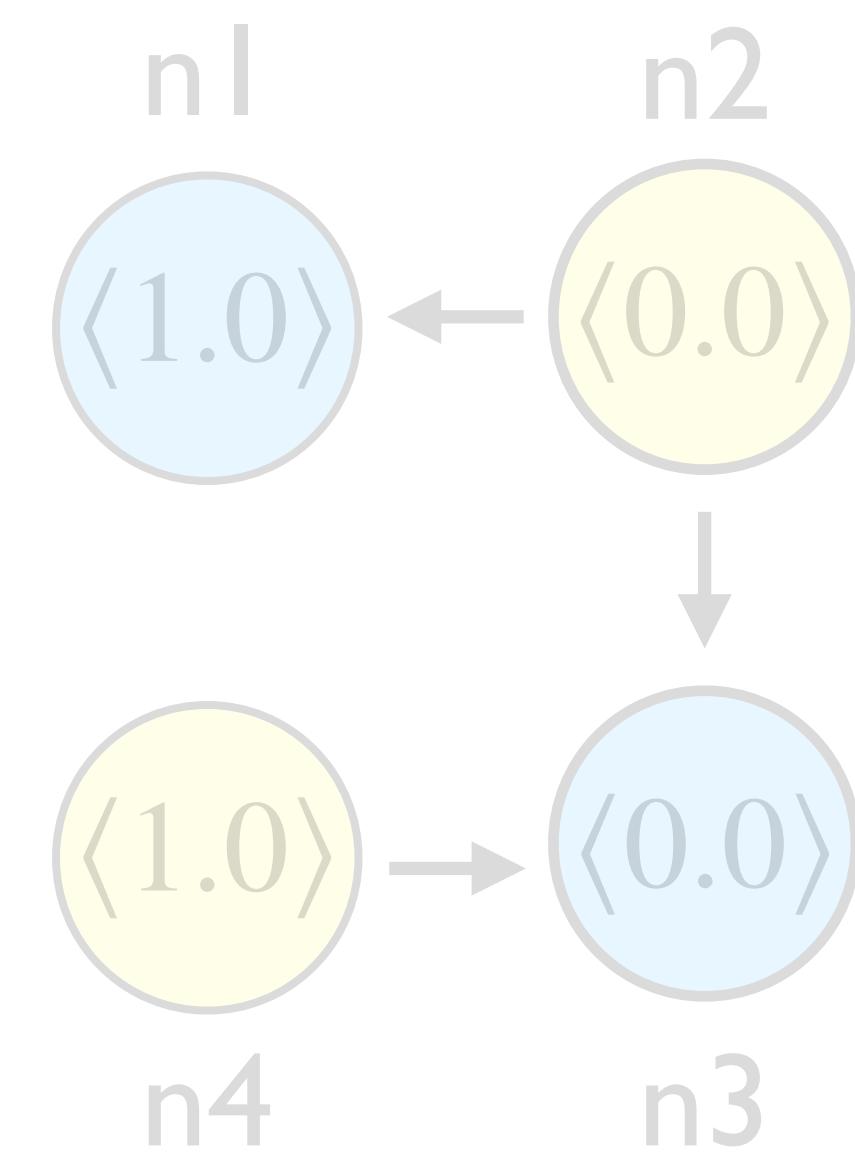
$n1: (1, [-\infty, 0.5] \rightarrow [-\infty, \infty])$

$n2: (2, [-\infty, \infty] \rightarrow [-\infty, 0.5])$

$n3: (1, [-\infty, 0.5] \rightarrow [-\infty, \infty])$

$n4: (2, [-\infty, \infty] \rightarrow [-\infty, 0.5])$

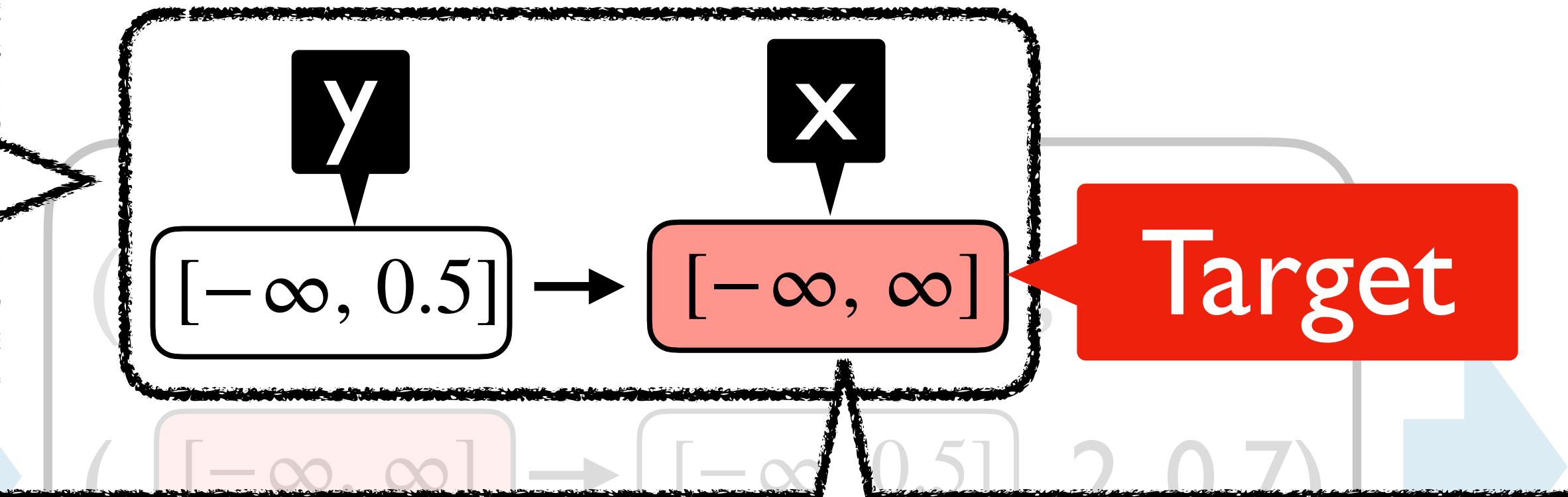
분류 결과



예측 결과      설명

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

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



표현하고 있는 노드 패턴:

“선행 노드(predecessor)중 feature값이 0.5 이하인 노드가 존재함”

그래프 데이터

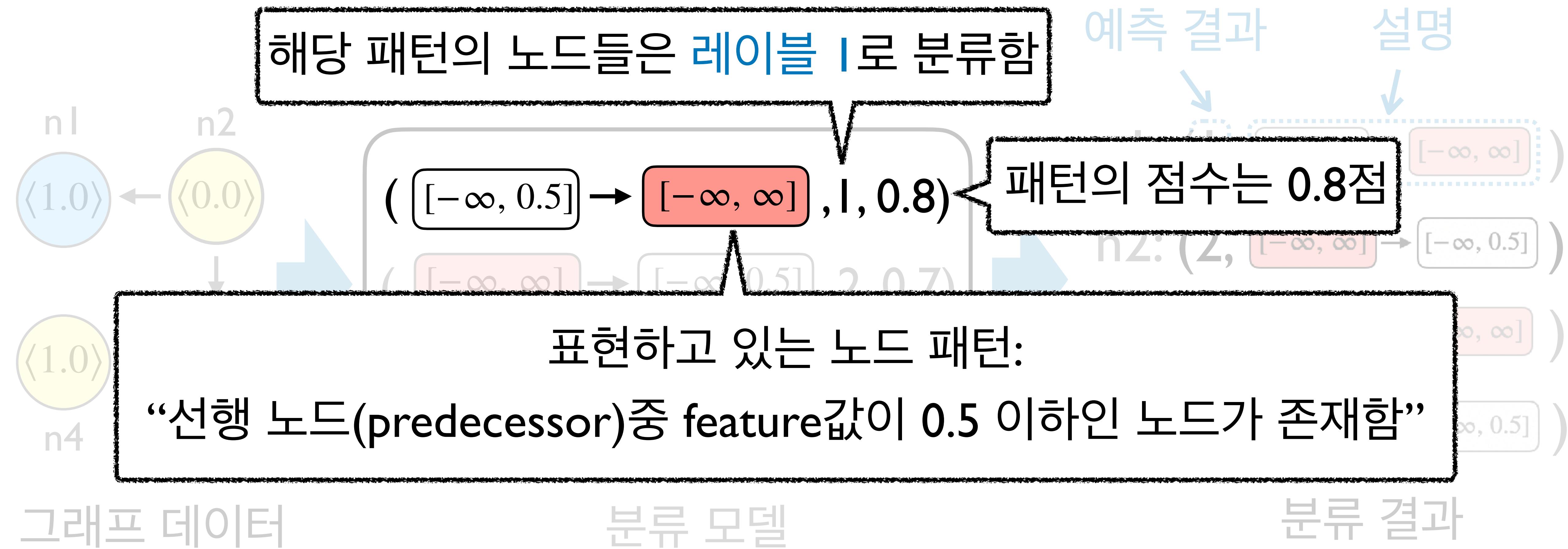
분류 모델

분류 결과

예측 결과  
설명

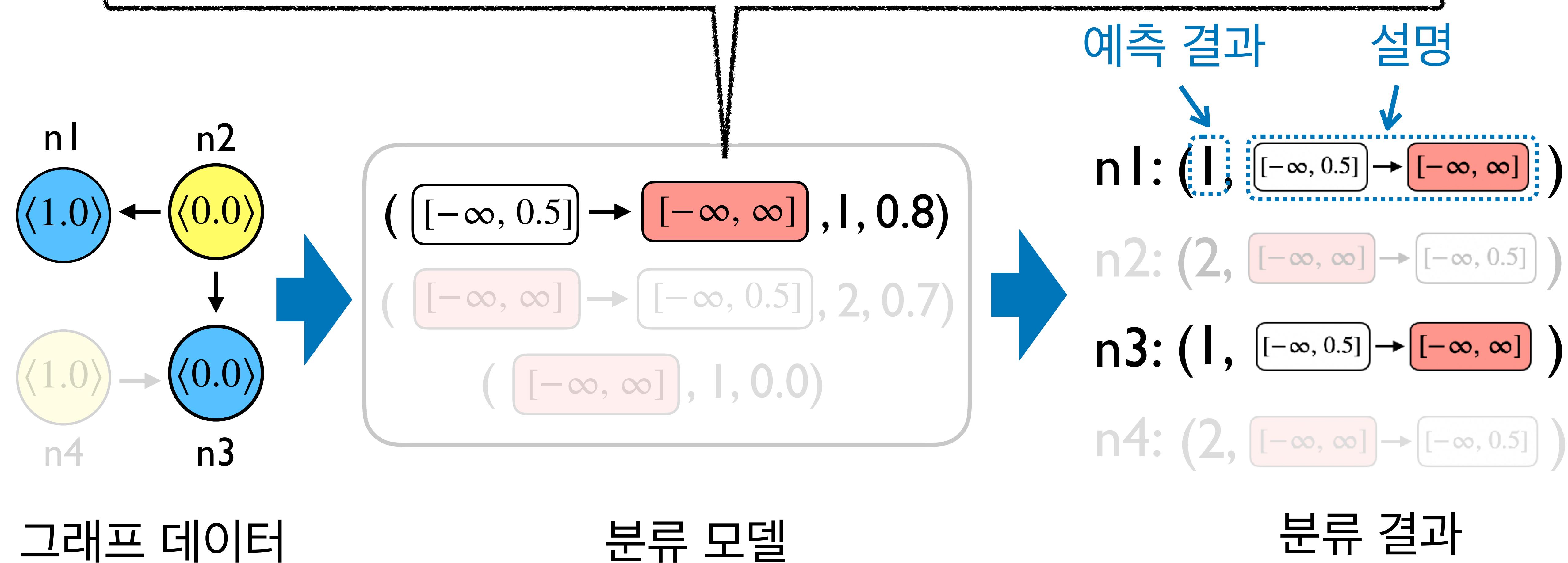
n1: (1,  $[-\infty, 0.5] \rightarrow [-\infty, \infty]$ )

n2: (2,  $[-\infty, \infty] \rightarrow [-\infty, 0.5]$ )



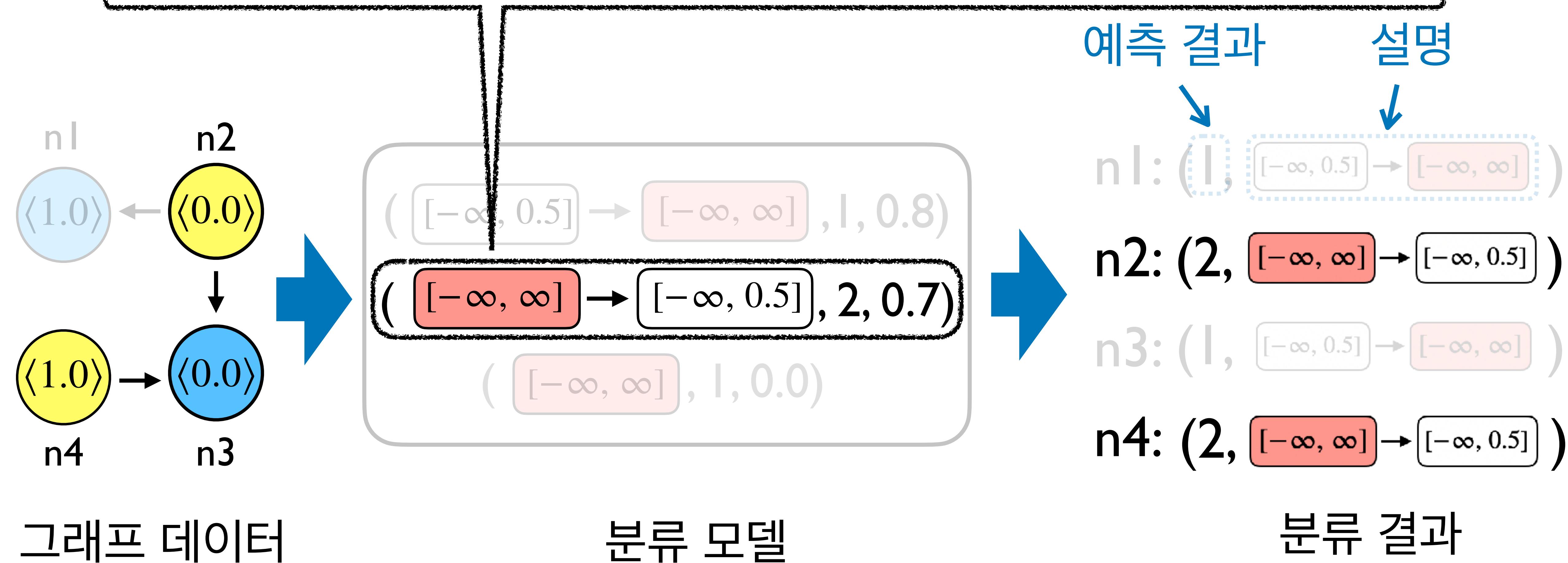
표현하고 있는 노드 패턴:

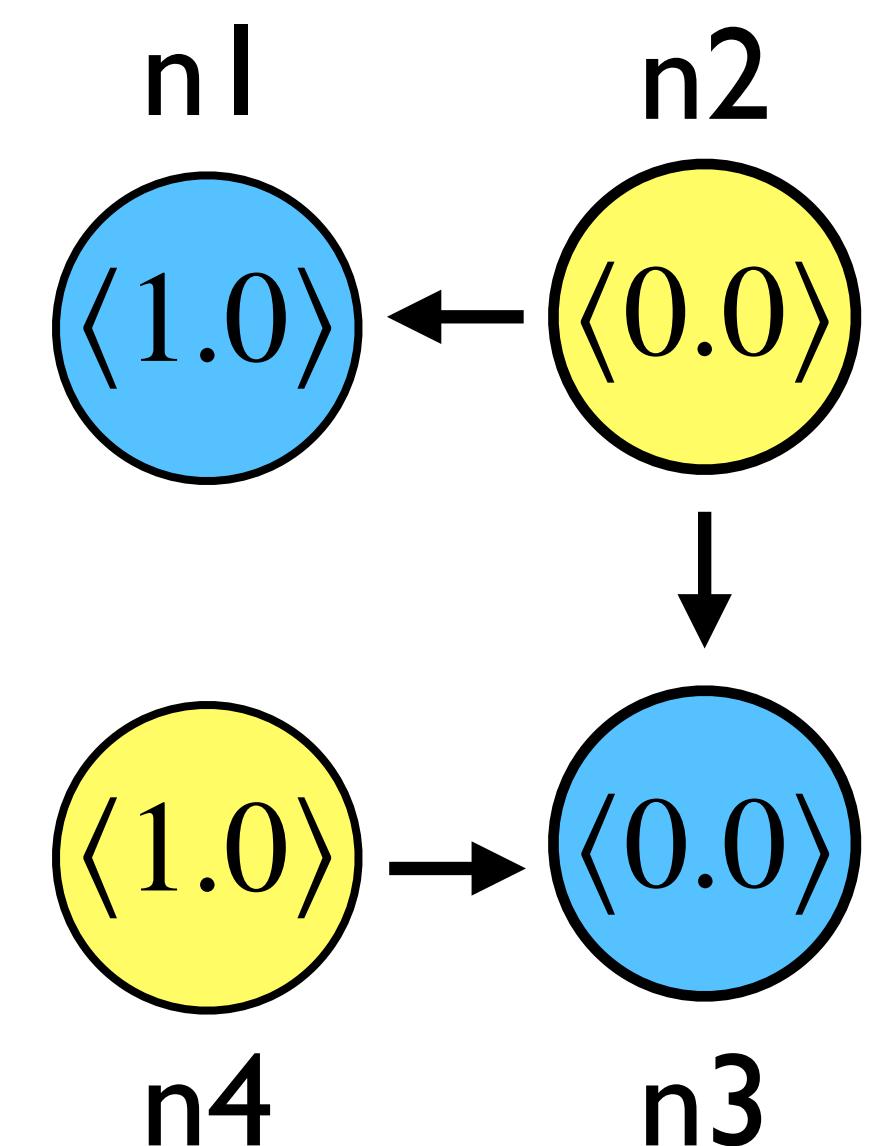
“선행 노드(predecessor)중 feature값이 0.5 이하인 노드가 존재함”



표현하고 있는 노드 패턴:

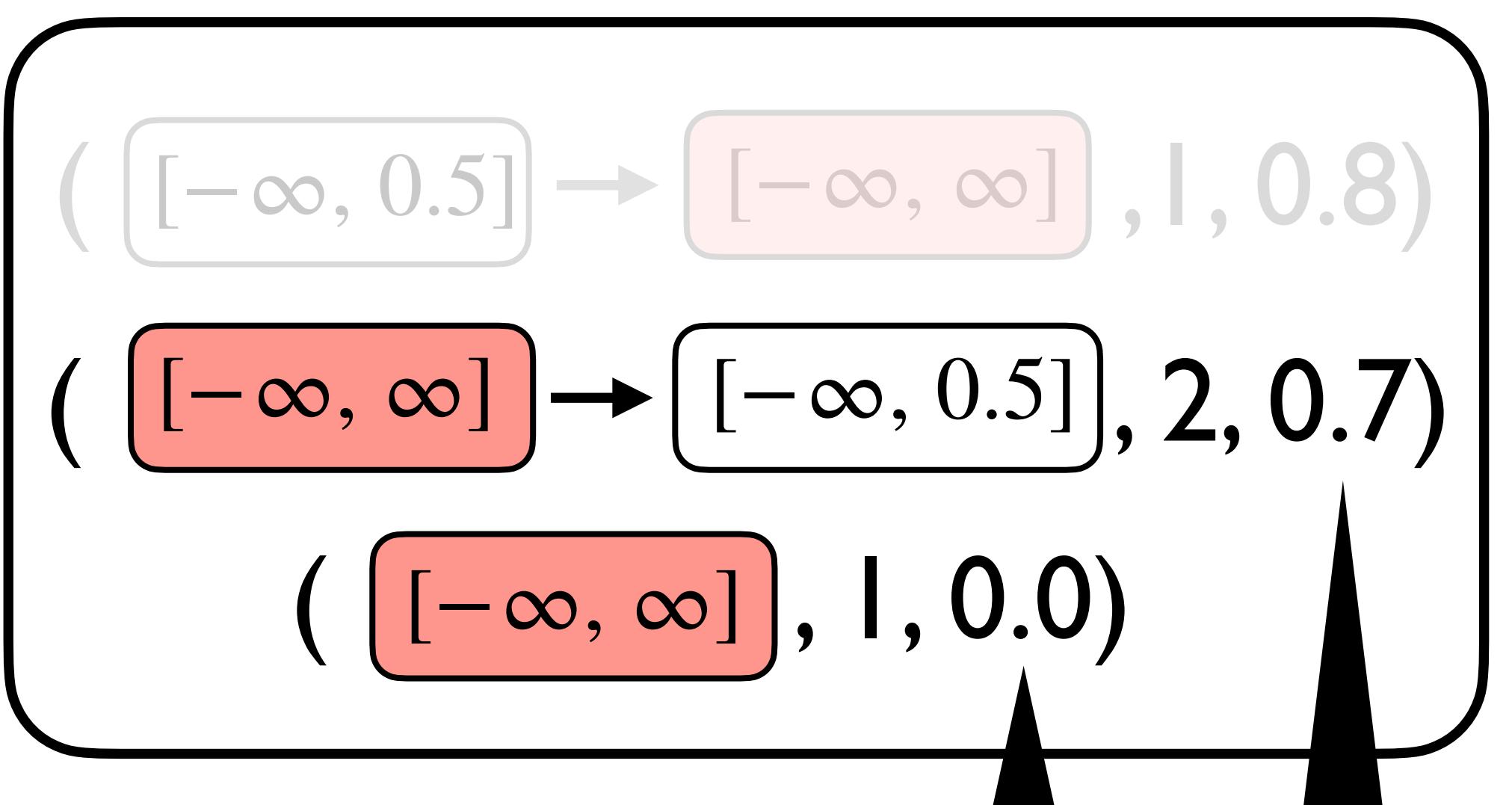
“후속 노드(successor)중 feature값이 0.5 이하인 노드가 존재함”





그래프 데이터

패턴이 겹칠 경우 더 높은 점수의 패턴으로 분류

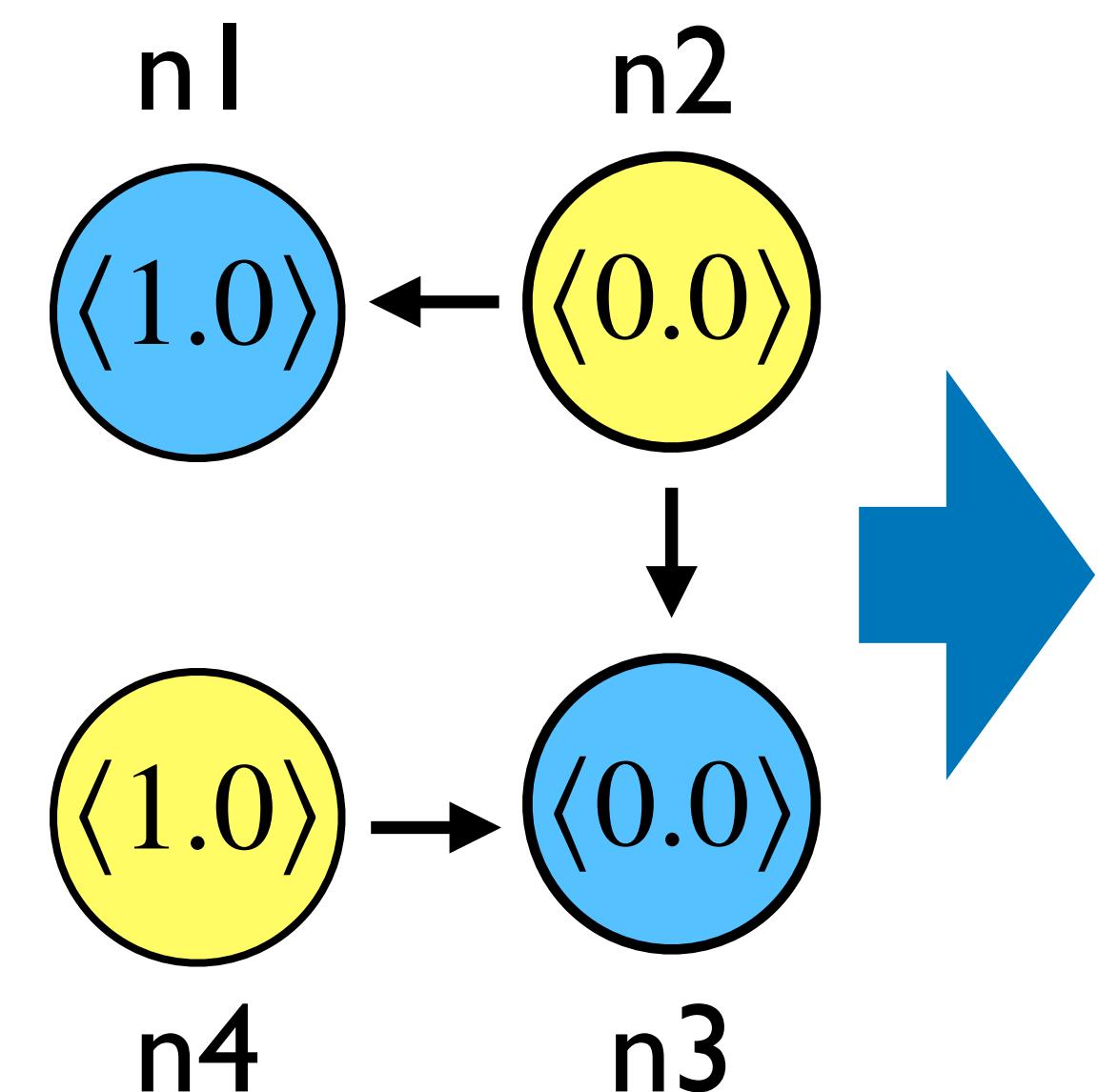


예측 결과      설명

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

분류 결과

- 추가적인 설명 비용 필요없음
  - 제공된 설명은 옳은 설명임을 보장함



# 분류 모델

# 분류 결과

# 예측 결과 설명

## 설명

$$n \mid : (|, [-\infty, 0.5] \rightarrow [-\infty, \infty])$$

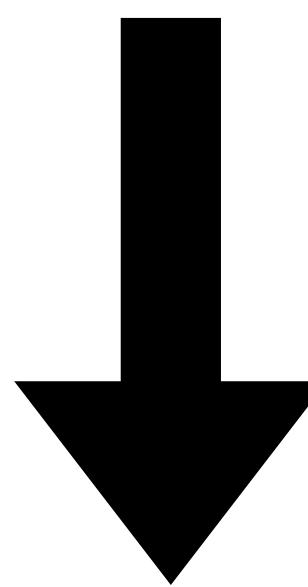
n2: (2, [-∞, ∞] → [-∞, 0.5])

n3: ( |, [-∞, 0.5] → [-∞, ∞] )

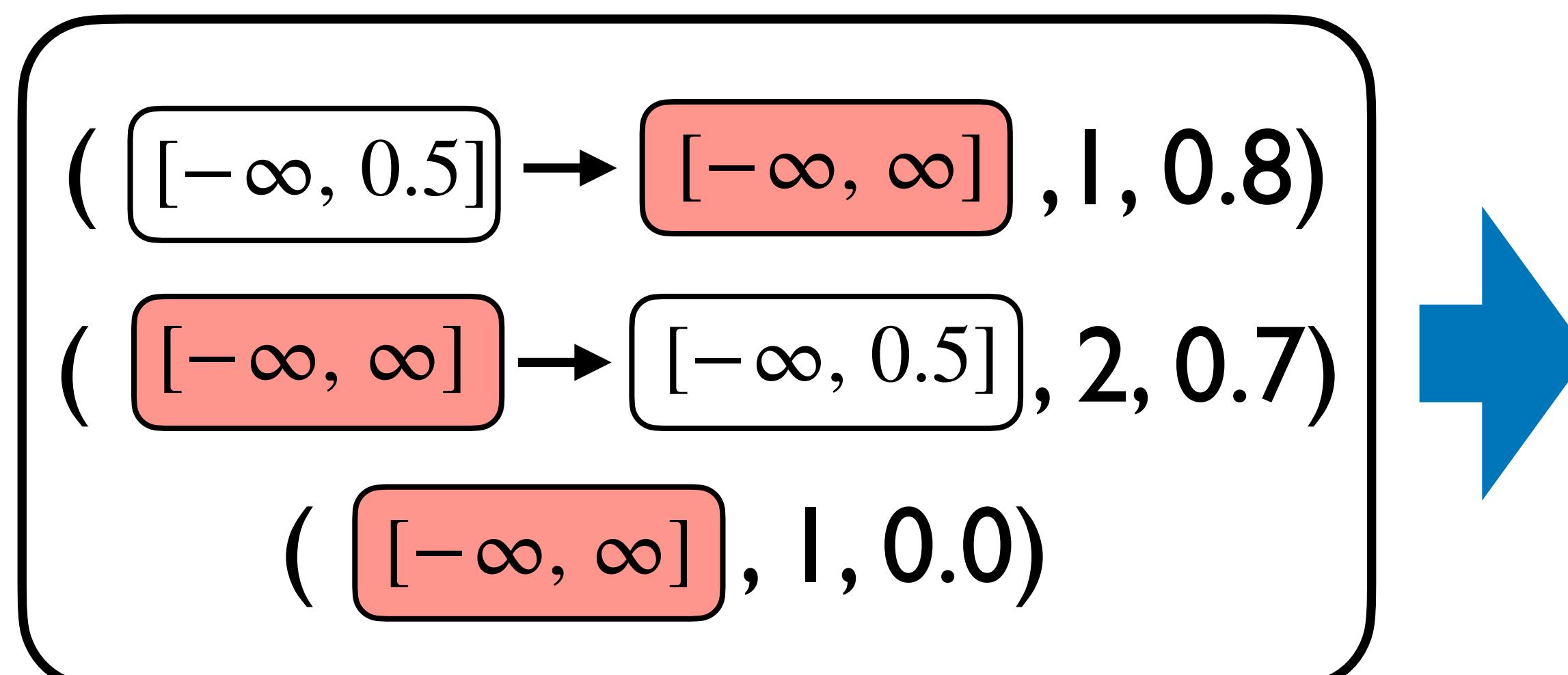
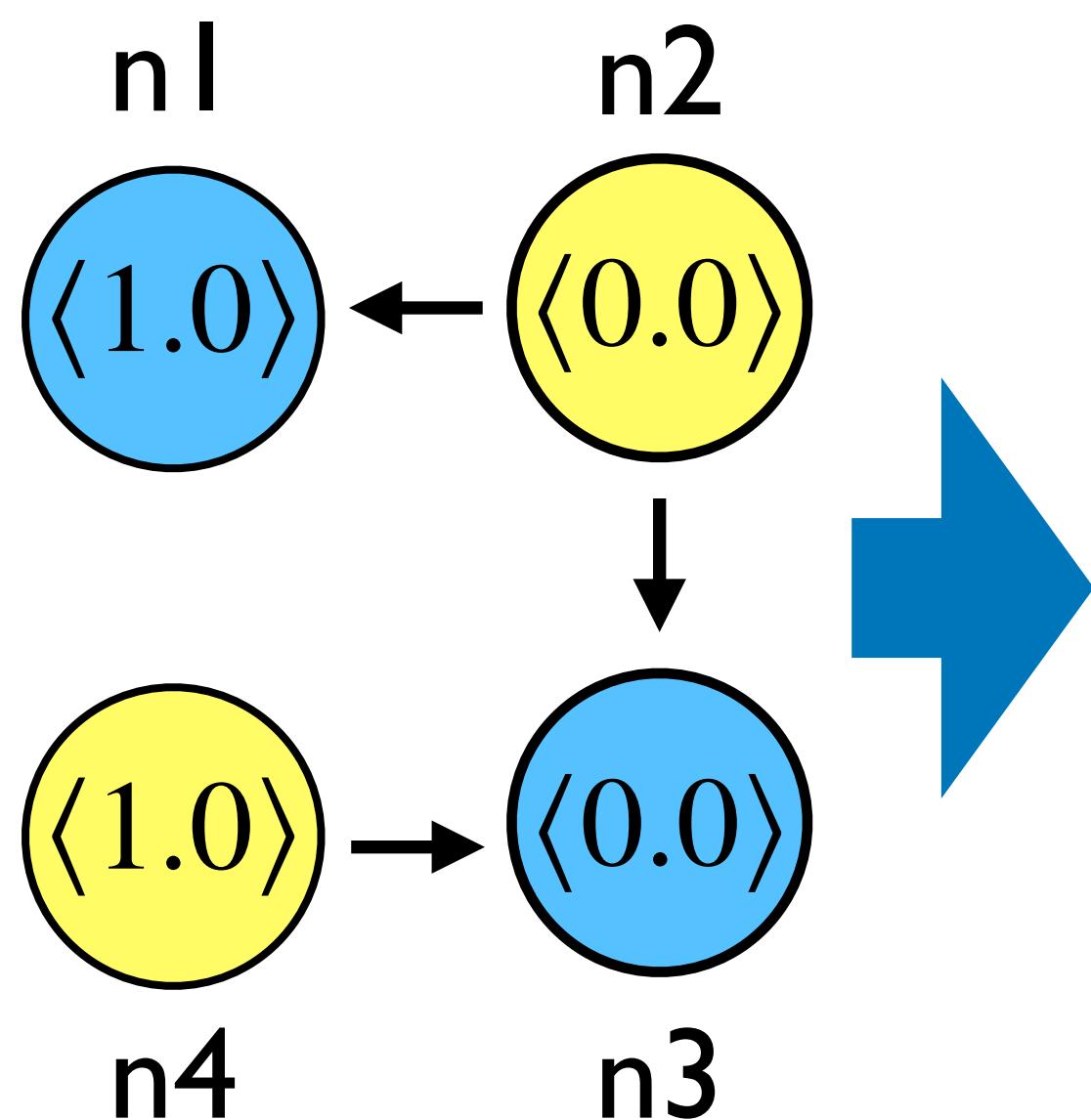
n4: (2.  $[-\infty, \infty]$   $\rightarrow$   $[-\infty, 0.5]$ )



학습 데이터



GDL 프로그램  
합성 알고리즘



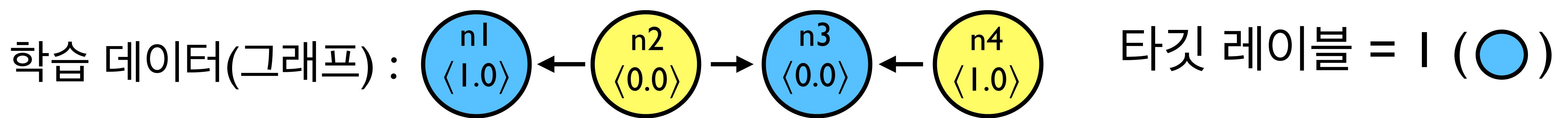
n1: (1,  $[-\infty, 0.5] \rightarrow [-\infty, \infty]$ )  
n2: (2,  $[-\infty, \infty] \rightarrow [-\infty, 0.5]$ )  
n3: (1,  $[-\infty, 0.5] \rightarrow [-\infty, \infty]$ )  
n4: (2,  $[-\infty, \infty] \rightarrow [-\infty, 0.5]$ )

그래프 데이터

분류 모델

분류 결과

# 하향식(Top-down) GDL 프로그램 합성 알고리즘



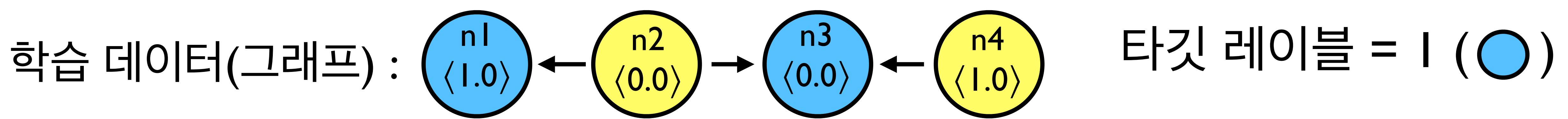
(I) 가장 일반적인 패턴(간단한 GDL 프로그램)에서 부터 시작

$$\frac{|\{n1, n3\}|}{|\{n1, n2, n3, n4\}|}$$

Score : 0.5

$[-\infty, \infty]$

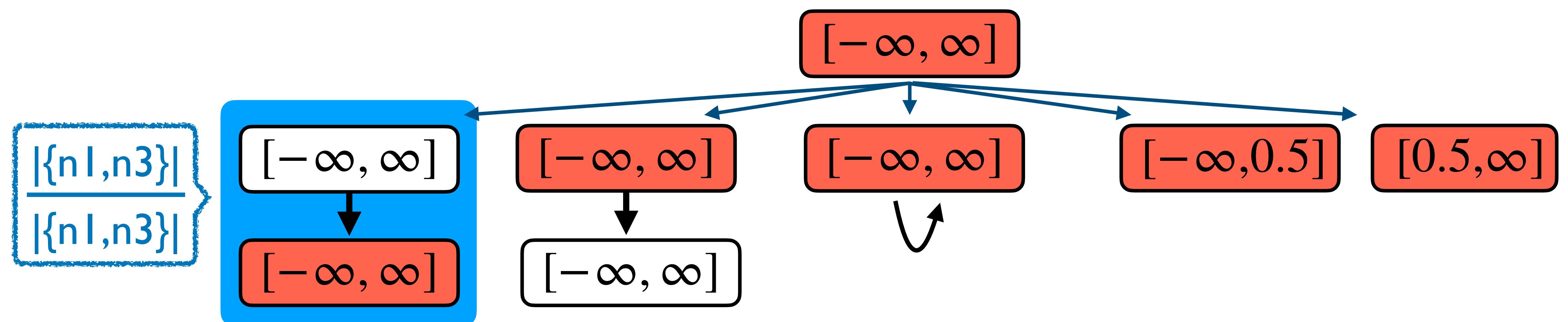
# 하향식(Top-down) GDL 프로그램 합성 알고리즘



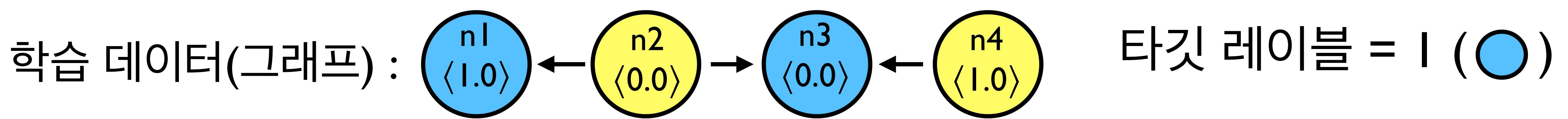
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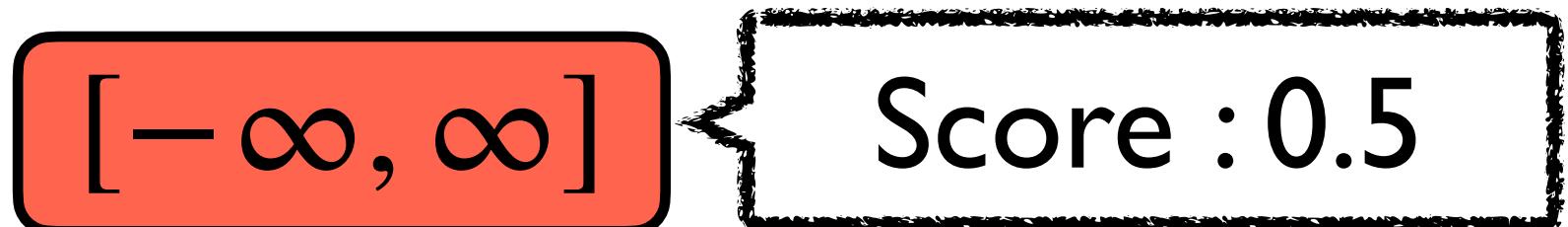
(2) 주어진 패턴을 다양하게 specify하여 나열 후 가장 높은 점수의 패턴을 선택 (나열 탐색)



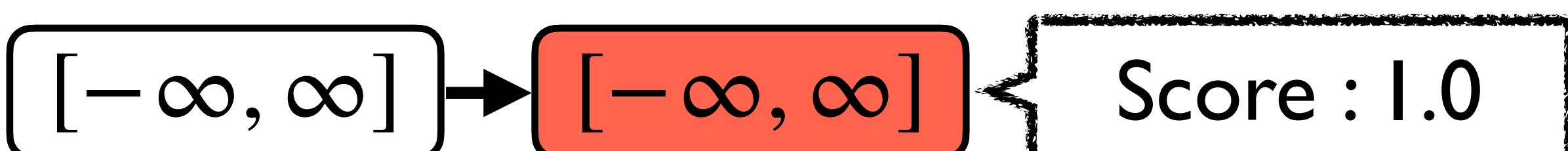
# 하향식(Top-down) GDL 프로그램 합성 알고리즘



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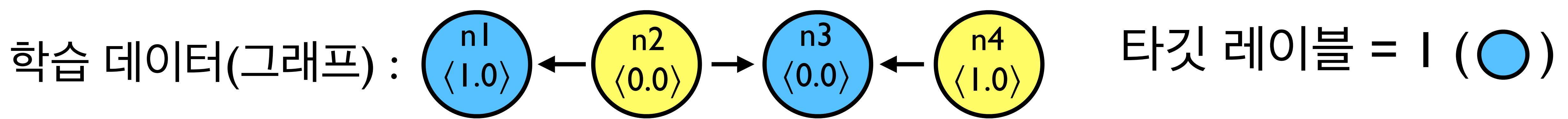


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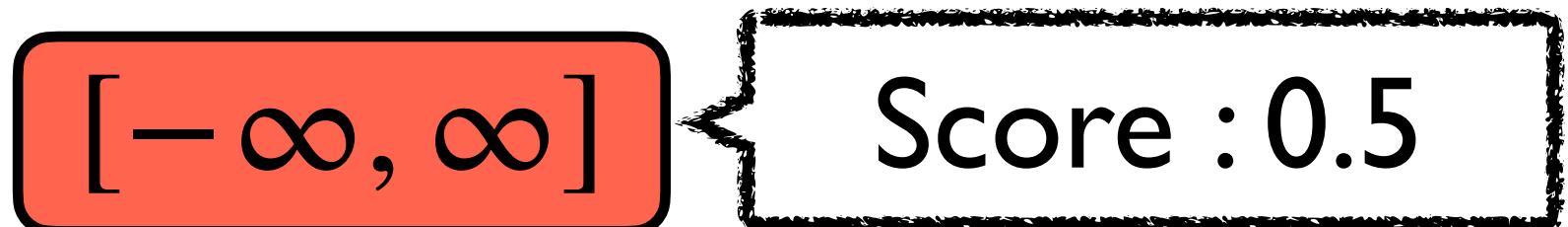


(3) 모든 나열된 패턴이 현재 패턴보다 같거나 낮은 점수를 가질 때 까지 (2)를 반복

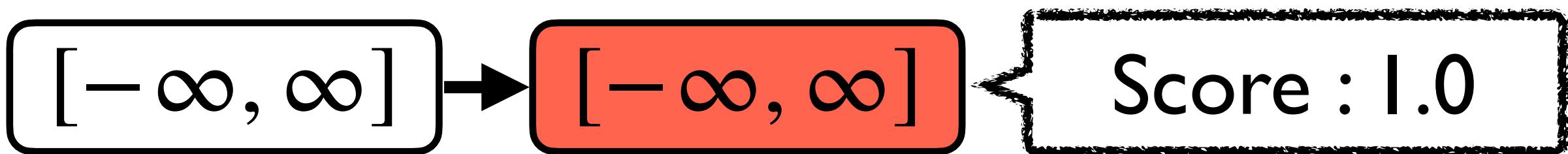
# 하향식(Top-down) GDL 프로그램 합성 알고리즘



(1) 가장 일반적인 패턴(간단한 GDL 프로그램)에서 부터 시작



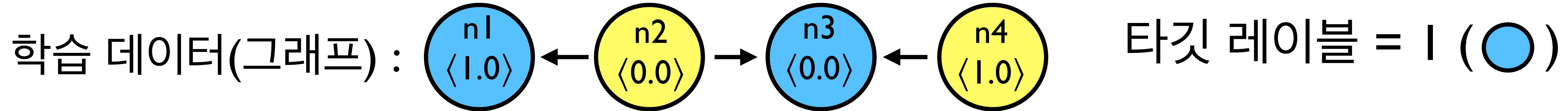
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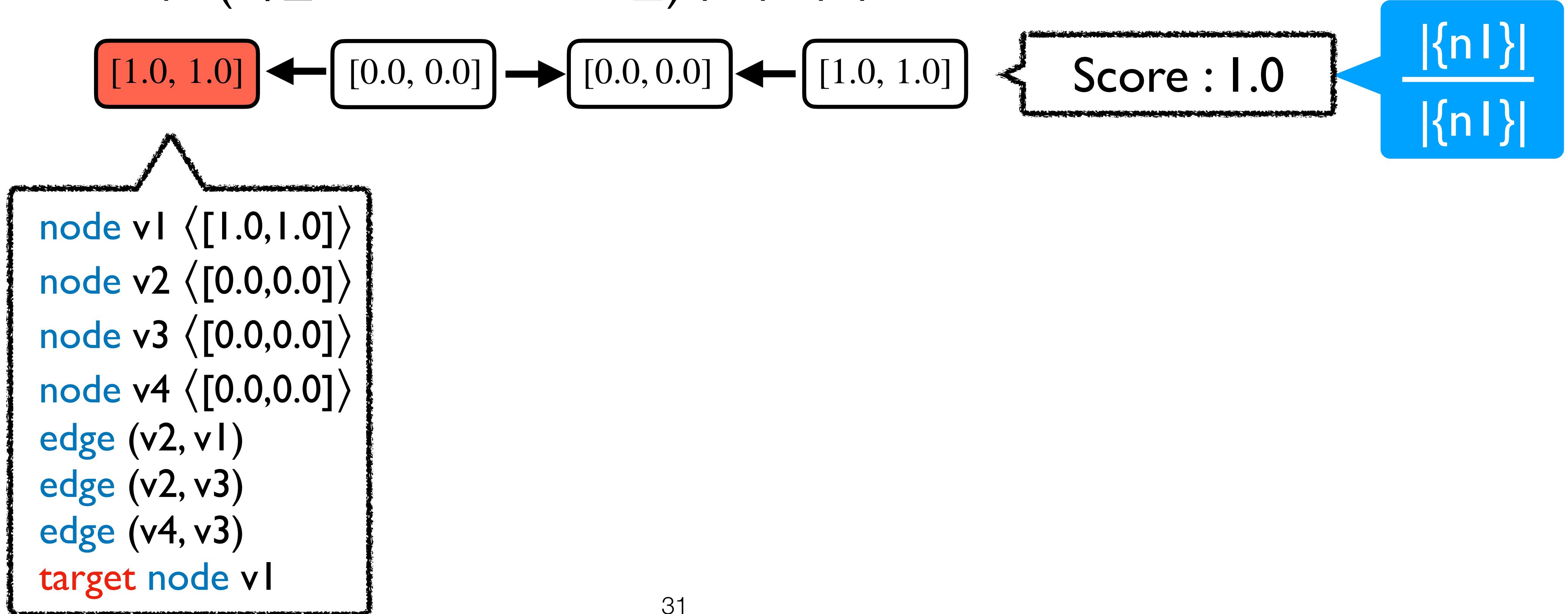
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(4) 현재 패턴을 반환 ( , label |, 1.0)

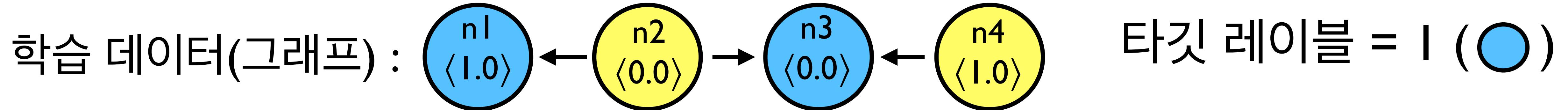
# 상향식(Bottom-up) GDL 프로그램 합성 알고리즘



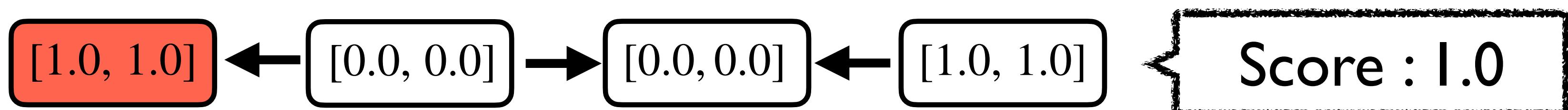
(I) 가장 specific한 패턴(복잡한 GDL 프로그램)부터 시작



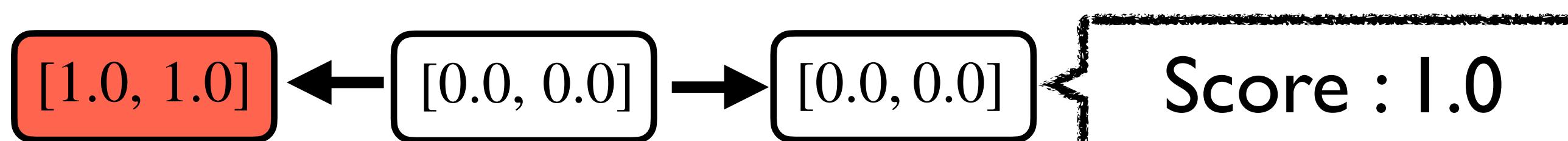
# 상향식(Bottom-up) GDL 프로그램 합성 알고리즘



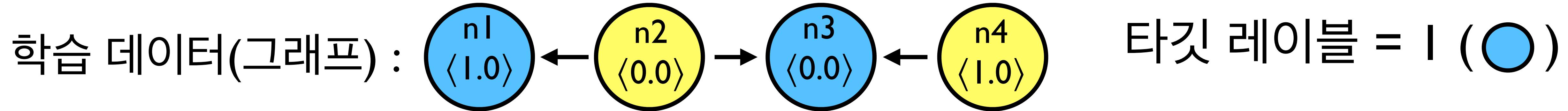
(1) 가장 specific한 패턴(복잡한 GDL 프로그램)부터 시작



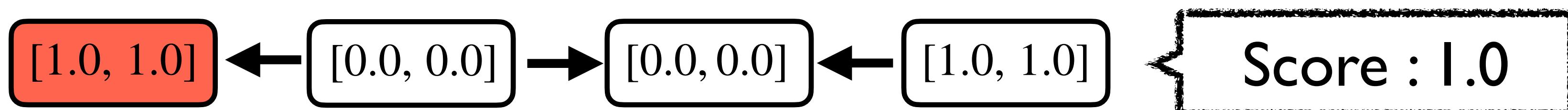
(2) 주어진 패턴을 다양하게 간단화하여 나열 후 가장 높은 점수의 패턴을 선택 (나열 탐색)



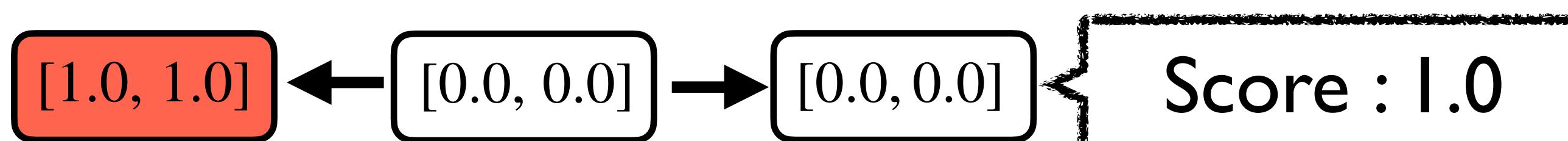
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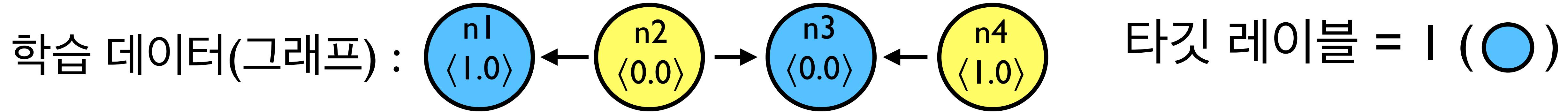


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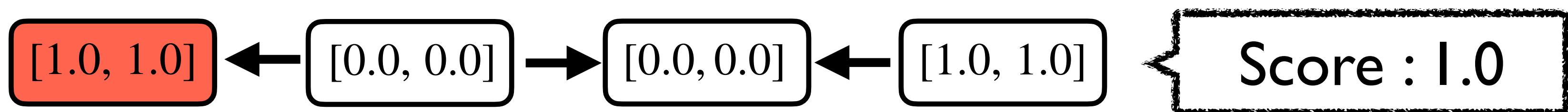


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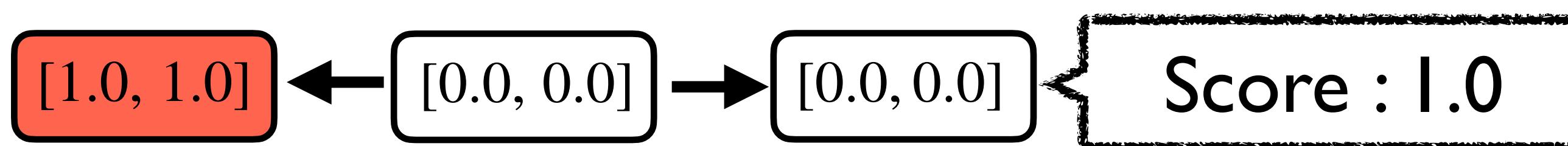
# 상향식(Bottom-up) GDL 프로그램 합성 알고리즘



(1) 가장 specific한 패턴(복잡한 GDL 프로그램)부터 시작



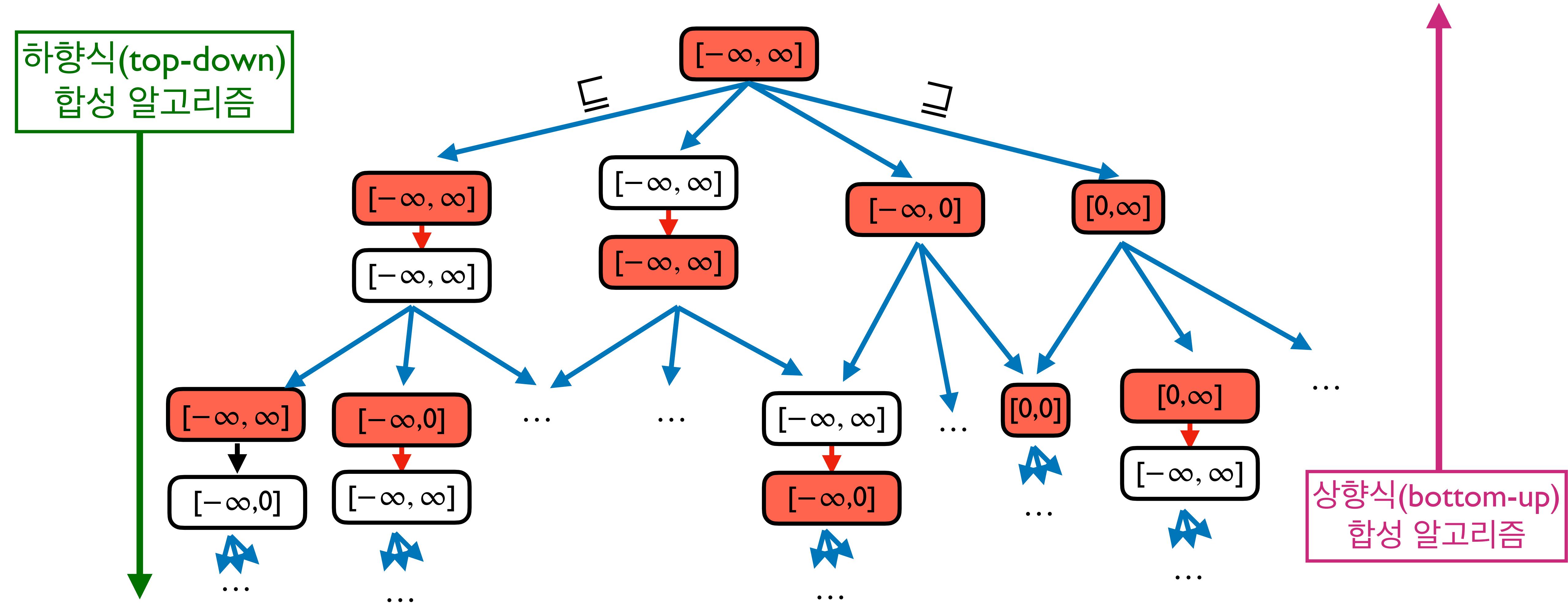
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(4) 현재 패턴을 반환 ( $[-\infty, \infty] \leftarrow [-\infty, \infty], |, 1.0$ )

# GDL 프로그램 합성 알고리즘



# 정확도 비교

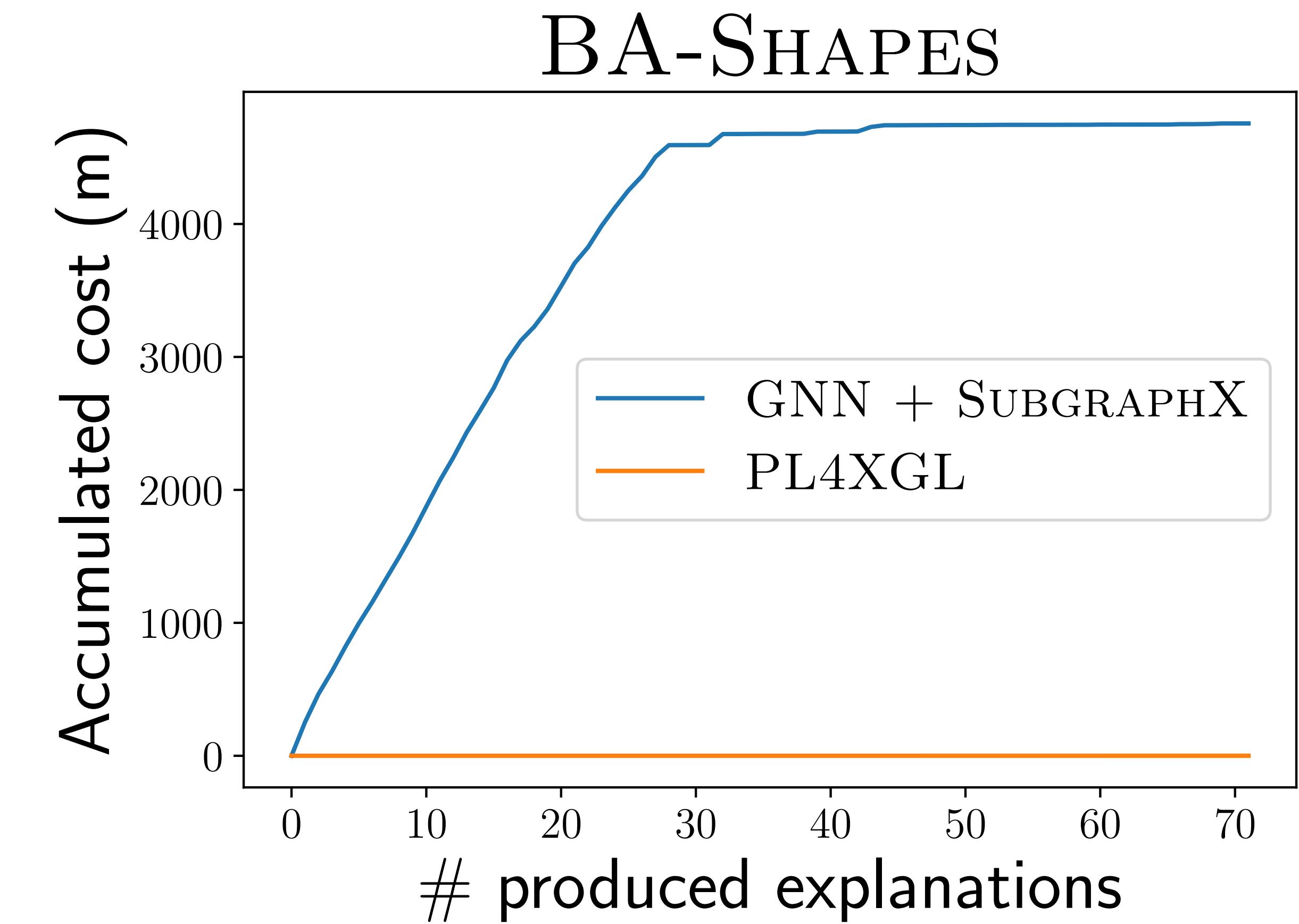
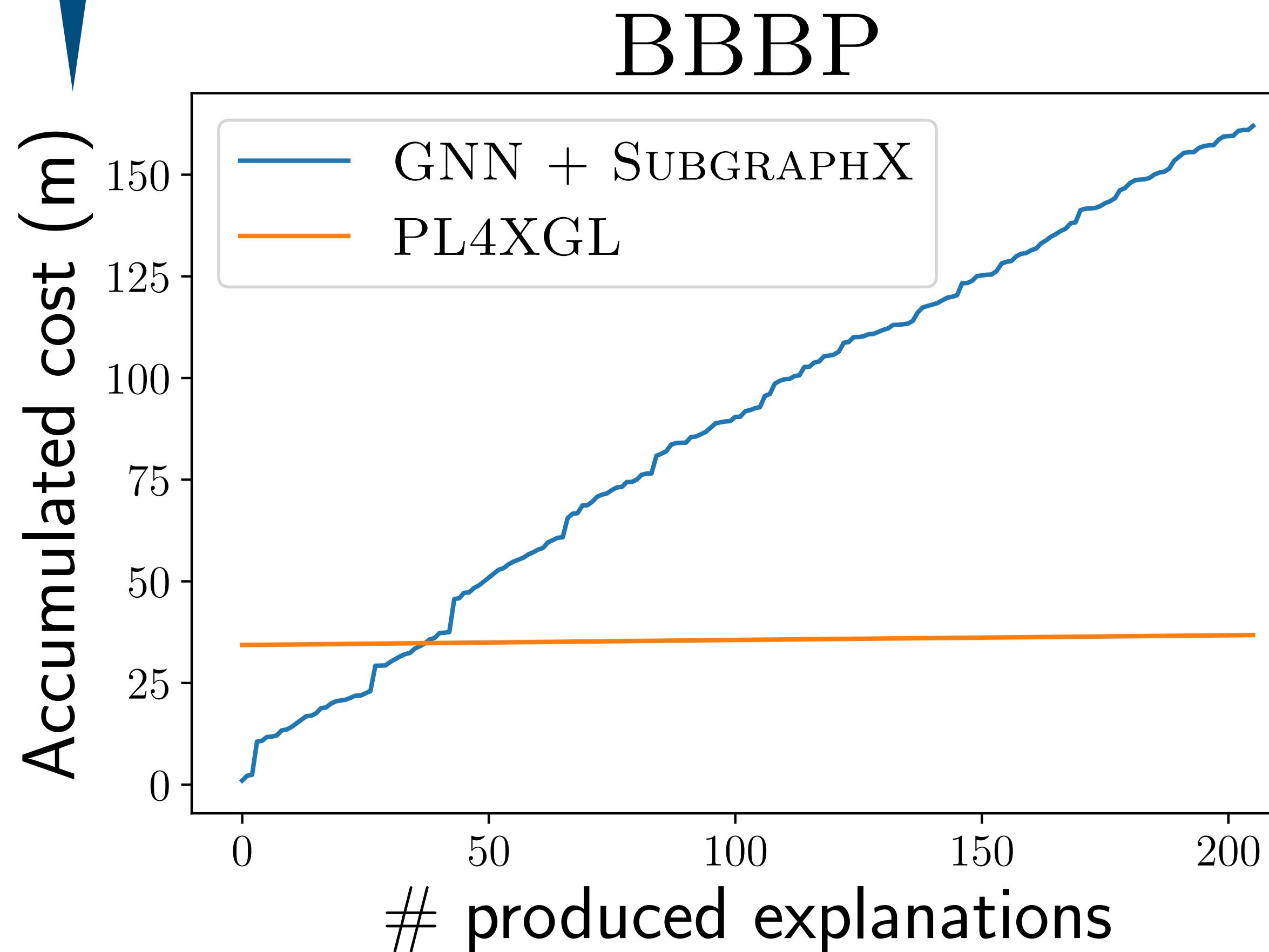
- We split the dataset into 8:1:1 for training, validation, and testing

Ours

	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	<b>100.0±0.0</b>
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	<b>86.8±0.0</b>
BACE	78.4±2.8	52.4±3.3	78.9±1.4	79.9±1.9	79.8±0.8	<b>80.9±0.4</b>	N/A	<b>80.9±0.0</b>
BA-SHAPES	95.1±0.6	76.8±2.3	<b>97.1±0.0</b>	94.3±0.0	<b>97.1±0.0</b>	92.0±1.1	95.1±0.7	95.7±0.0
TREE-CYCLES	97.7±0.0	90.9±0.0	<b>100.0±0.0</b>	98.9±0.0	<b>100.0±0.0</b>	93.2±0.0	99.2±0.5	<b>100.0±0.0</b>
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	<b>96.0±0.0</b>	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	<b>86.6±2.6</b>	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	<b>88.8±0.0</b>
CORA	85.6±0.3	86.4±1.8	86.5±5.2	84.9±3.5	86.3±3.2	<b>86.7±0.0</b>	83.2±5.9	80.0± 0.0
CITESEER	75.2±0.0	74.3±0.7	<b>79.1±0.9</b>	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	<b>88.7±1.0</b>	83.2±0.4	88.0±0.4	86.1±0.6	85.1±0.6	81.4±0.0

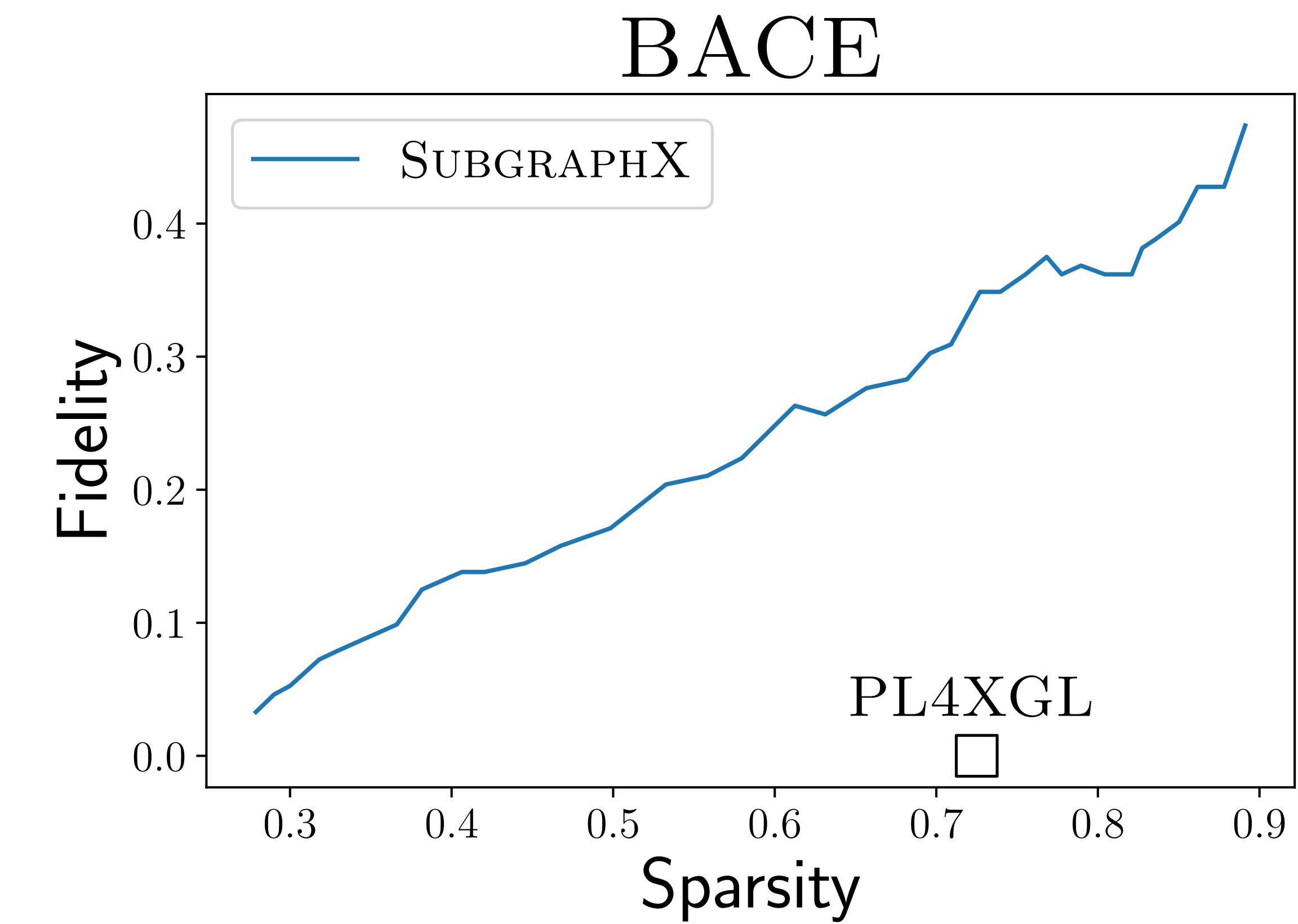
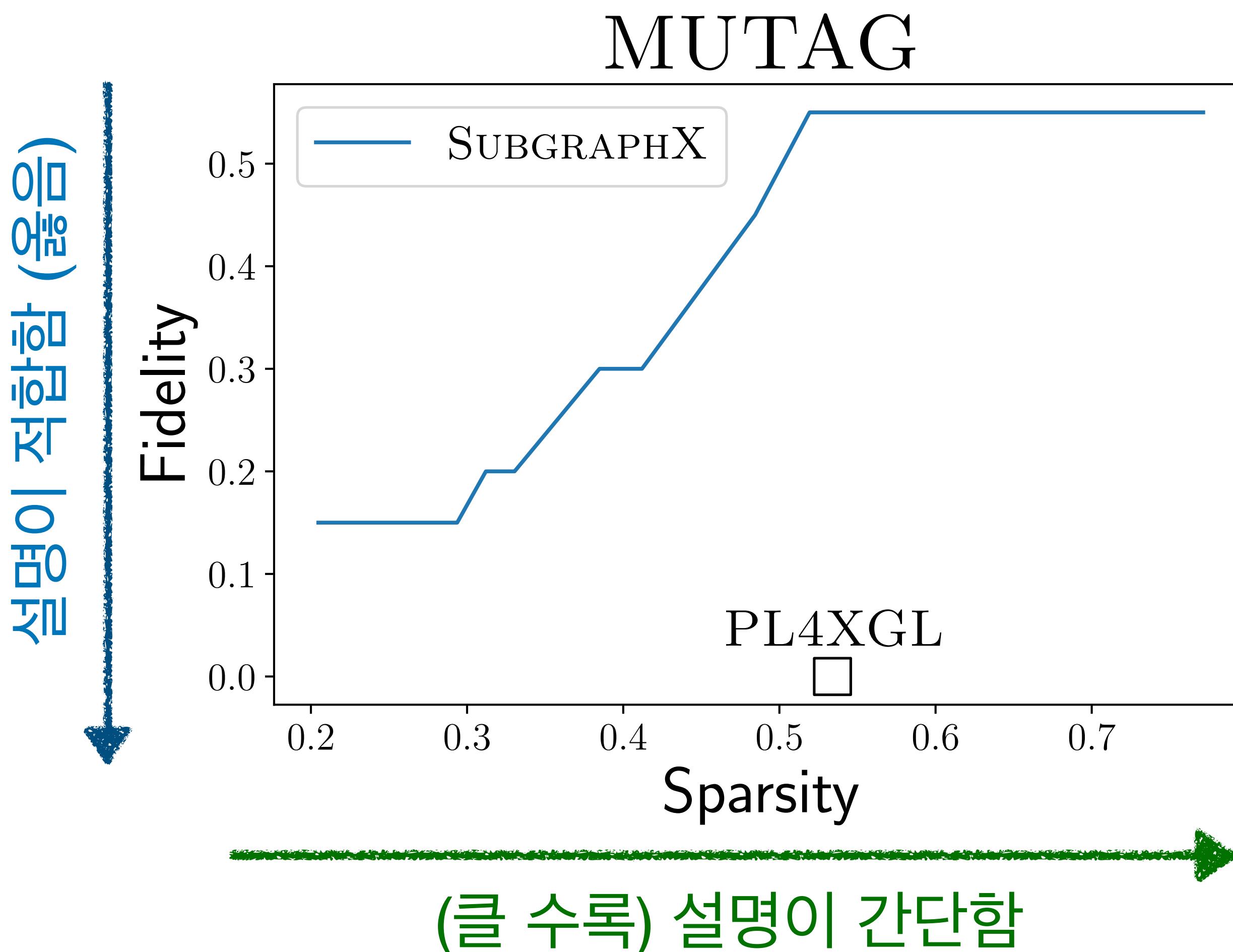
# 누적(학습+분류+설명)비용 비교

학습 비용 + 분류 비용 + 설명 비용



# 제공된 설명의 품질 비교

- 설명의 적합성(fidelity), 간단성(Sparsity) 비교



# Graph Description Language (GDL) Project

- 목표: 그래프 표현 언어를 확장 및 사용하여 각 분야의 핵심 문제 해결하기

