Learning Causally Invariant Representations for Out-of-Distribution Generalization on Graphs

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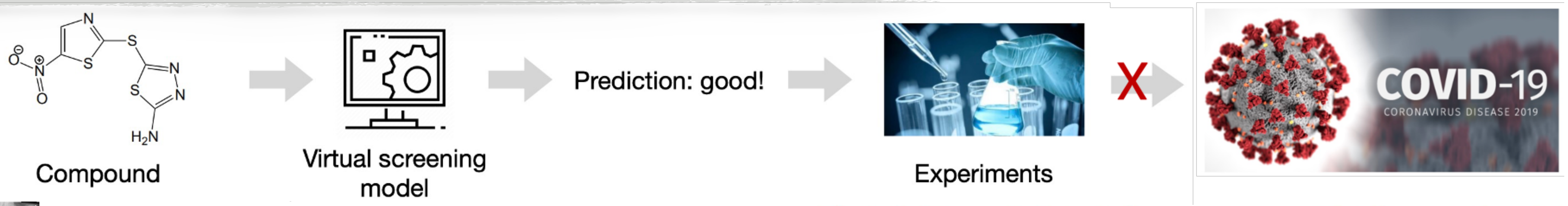
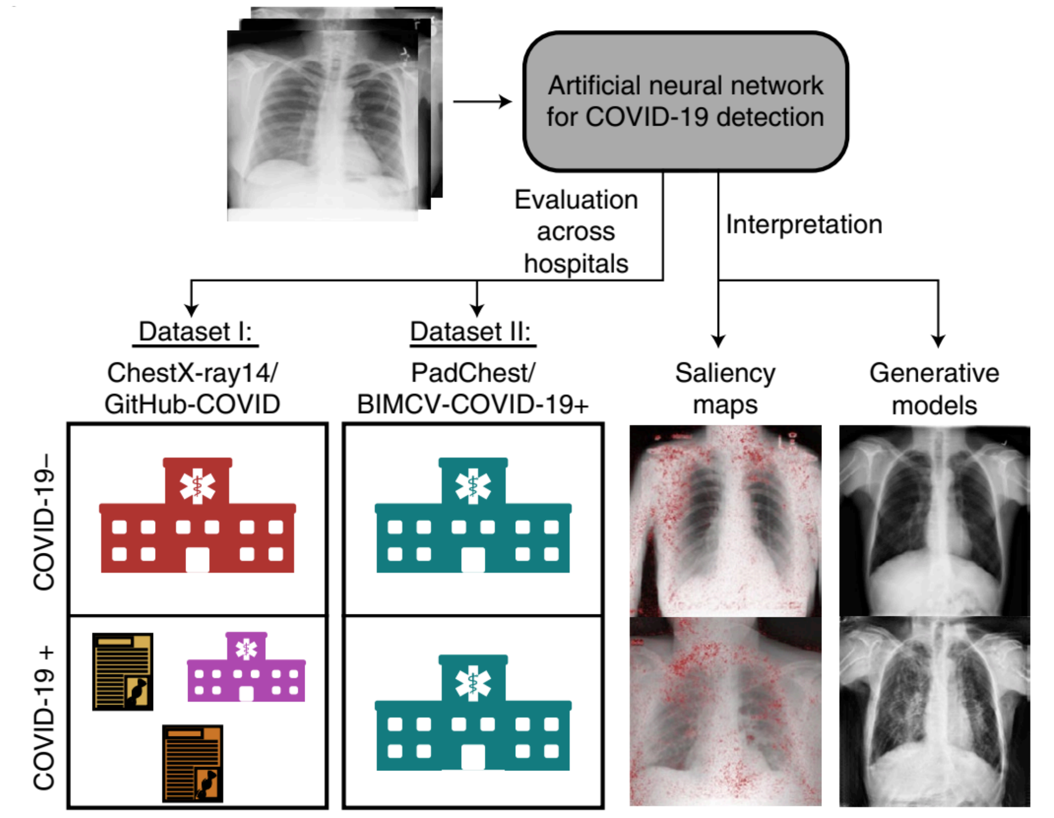
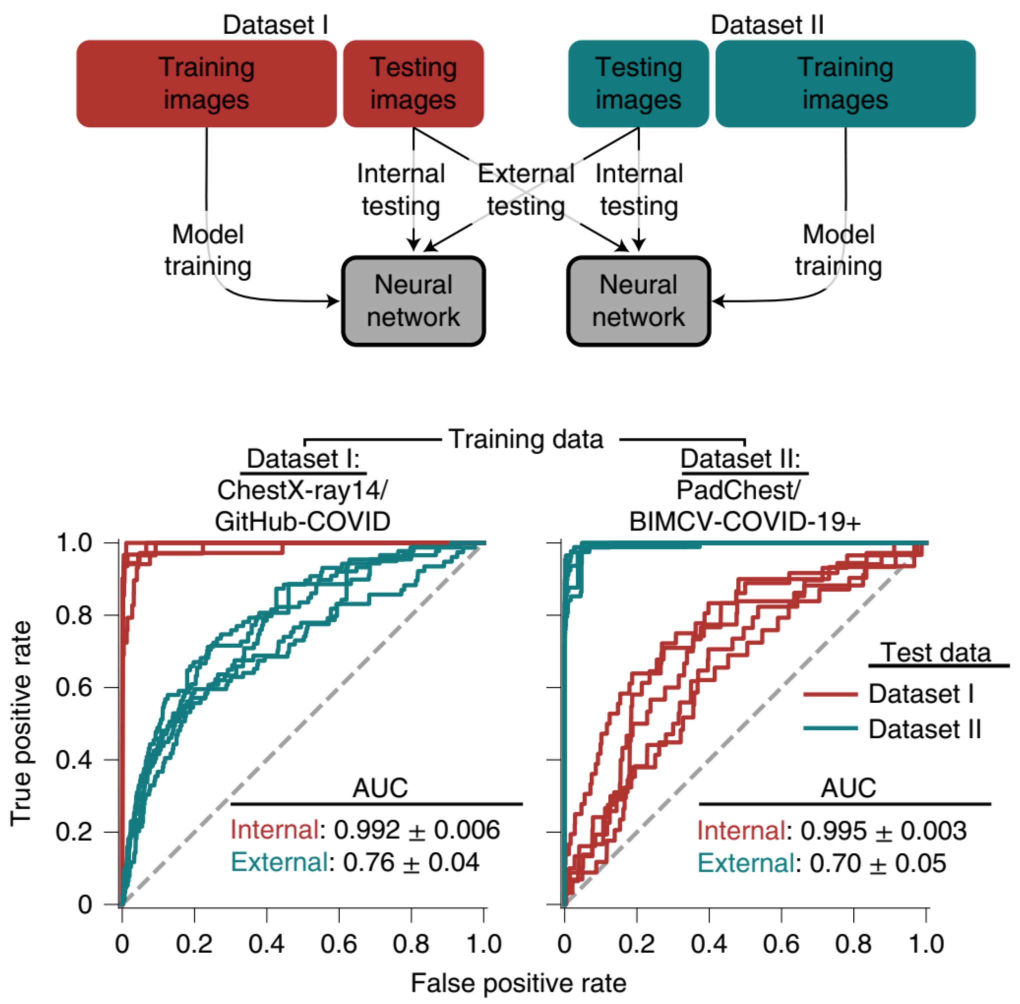
Out-of-Distribution (OOD) generalization

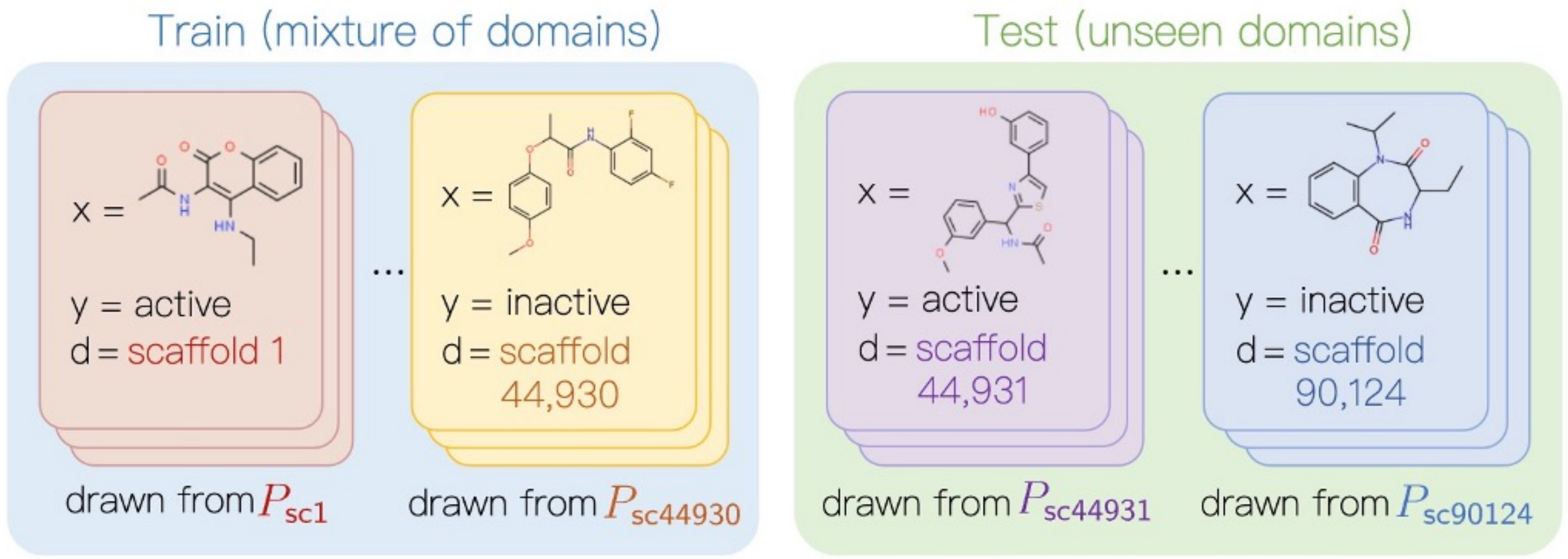




b

	Dataset I			Dataset II		
	Combined	Chest-X-ray14	GitHub-COVID	Combined	PadChest	BIMCV-COVID-19+
No. radiographs	112,528	112,120	408	97,866	96,270	1,596
No. patients	31,067	30,805	262	64,954	63,939	1,105
% COVID-19+	0.2	0	76.5	1.6	0	100
% AP images	39.9	40	26	5.6	4.7	58.1





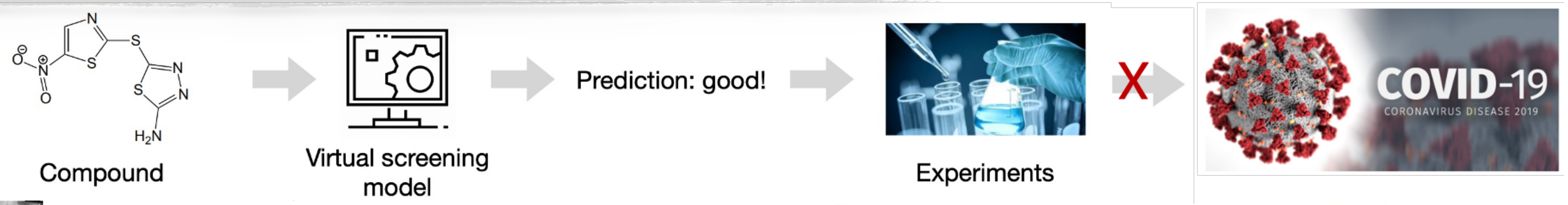
average precision = 27.2%

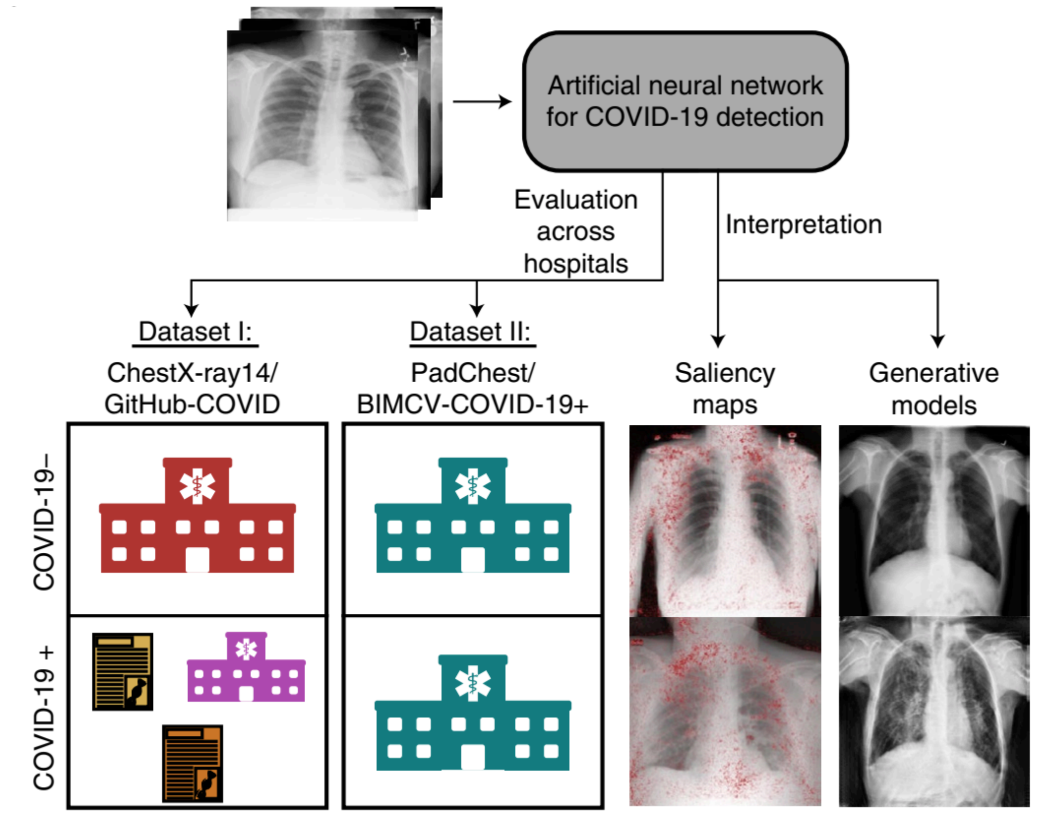
(Arjovsky et al., 2019; DeGrave et al. 2021; Wengong Jin, 2021; Koh et al., 2021;)

Models learned with Empirical Risk Minimization often:

- are prone to **spurious correlations**
- fail catastrophically in **OOD** data

Out-of-Distribution (OOD) generalization





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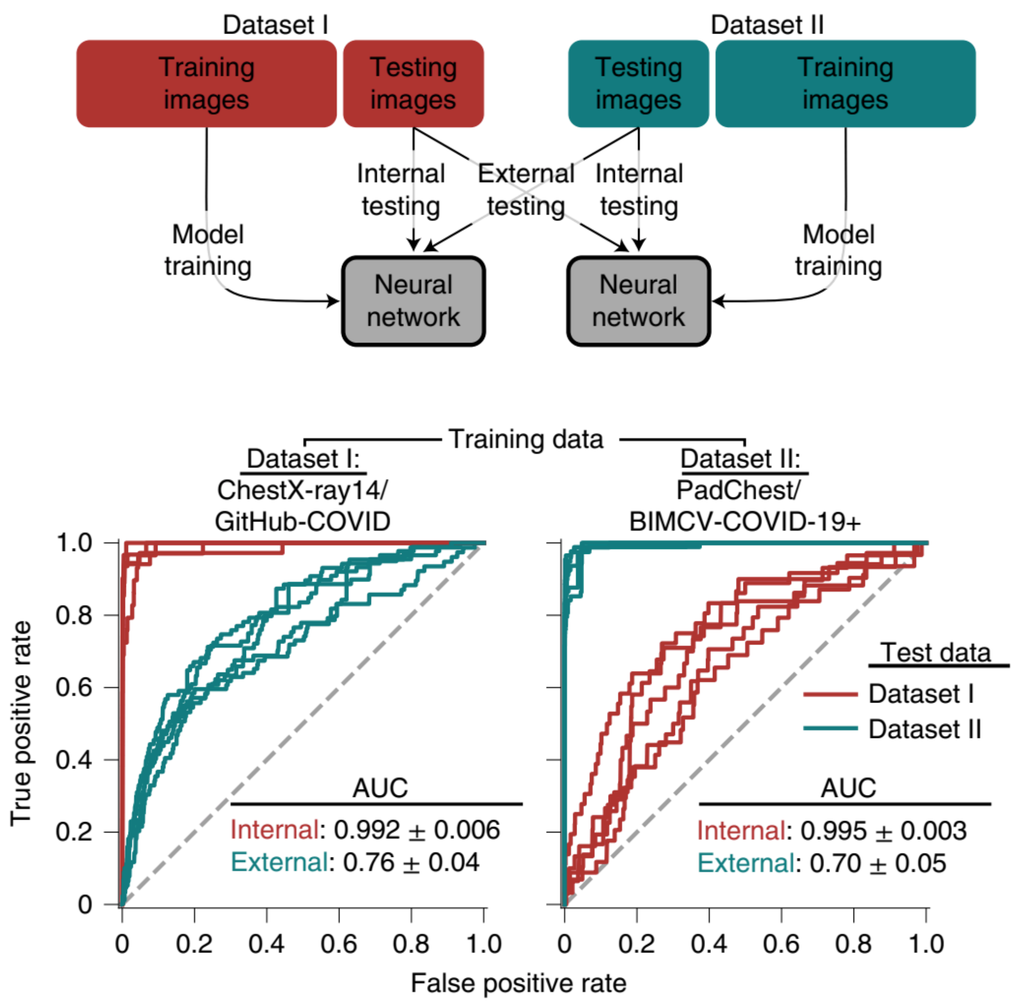
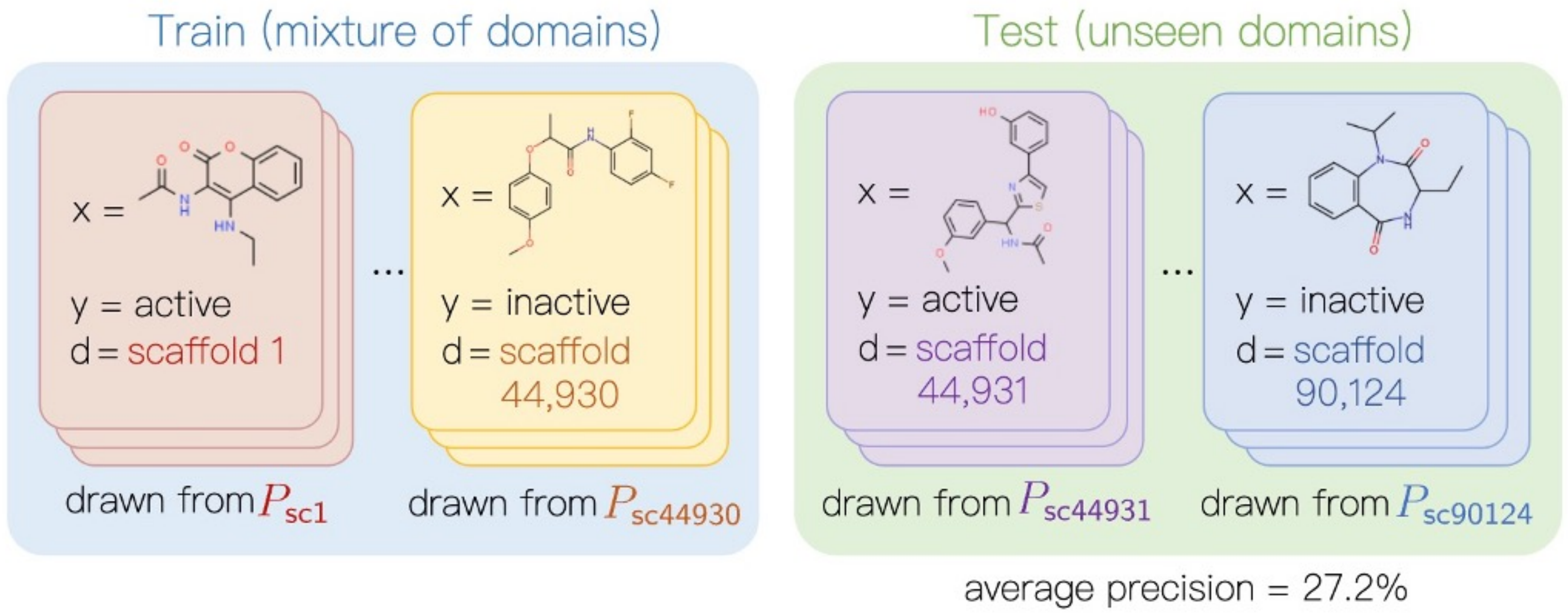




(*Arjovsky et al., 2019; DeGrave et al. 2021; Wengong Jin, 2021; Koh et al., 2021;*)

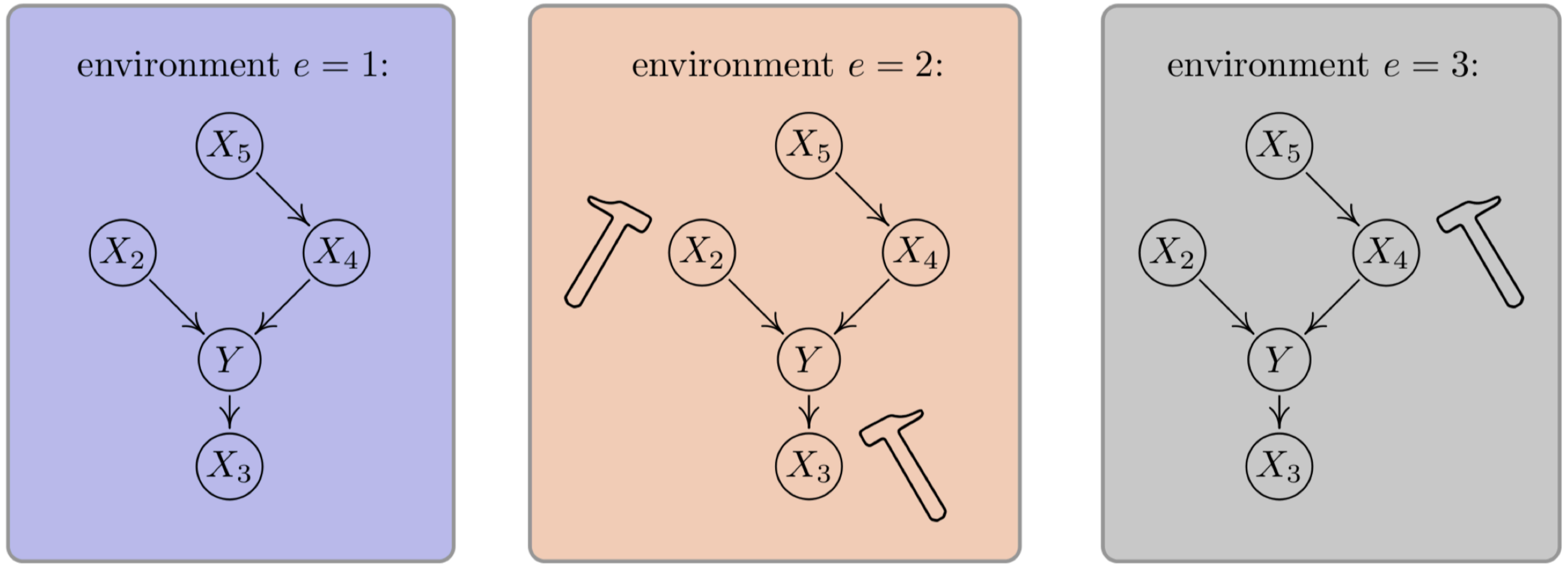
The goal of Out-of-Distribution (OOD) generalization:

$$\min_{f:\mathcal{X}\to\mathcal{Y}} \max_{e\in\mathcal{E}_{\text{all}}} \mathcal{L}_e(f)$$

given a subset of training **environments**/domains $\mathcal{E}_{\text{tr}} \subseteq \mathcal{E}_{\text{all}}$,

where each $e \in \mathcal{E}$ corresponds to a dataset $\mathcal{D}_e$ and a loss $\mathcal{L}_e$.

Out-of-Distribution (OOD) generalization



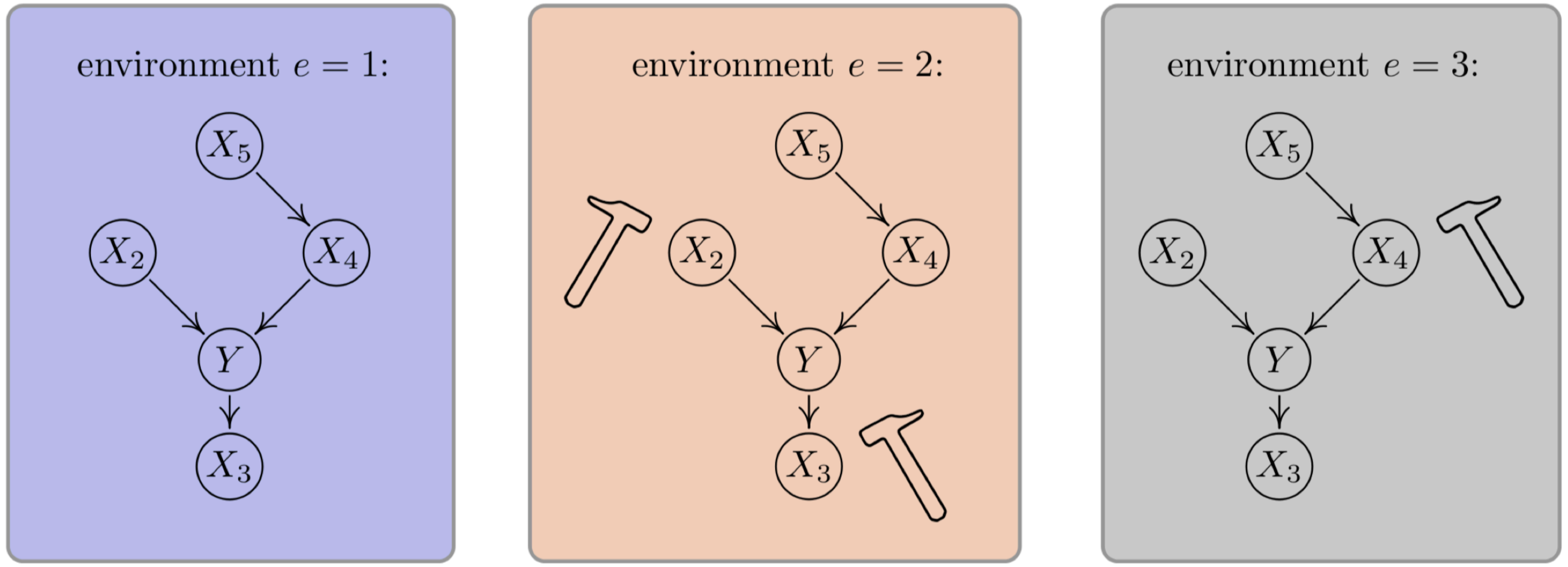
Leveraging the **Invariance Principle** from causality, previous approaches aim to learn an **invariant** predictor f,

$$\min_{f=w\circ\varphi} \sum_{e\in\mathscr{E}_{\text{tr}}} \mathscr{L}_e(w\circ\varphi),$$
$$\text{s.t. } w \in \arg\min_{\bar{w}} \mathscr{L}_e(\bar{w}\circ\varphi),\ \forall e \in \mathscr{E}_{\text{tr}},$$

that is **simultaneously optimal** across different environments/domains.

(Peters et al., 2015; Arjovsky et al., 2019; Bottou et al., 2021;)

Out-of-Distribution (OOD) generalization



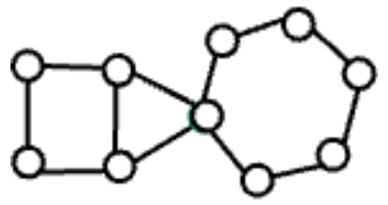
Previous approaches inspired by the **Invariance Principle** from causality can:

- help to learn the **invariant representations** 😋
- but only works on **linear** regime 🥲
- but only works on **single** distribution shifts 🥲
- but requires **environment**/domain label 🥲

(Peters et al., 2015; Arjovsky et al., 2019; Rosenfeld et al., 2021; Kamath et al., 2021; Ahuja et al., 2021;)

OOD generalization on graphs are more challenging

A Graph Neural Network (GNN) makes predictions taking both **structure-level** and node **attribute-level** features into account.

$f_{\text{GNN}}(\{$  $\}$, $\{$  $\})$ = **"House"**

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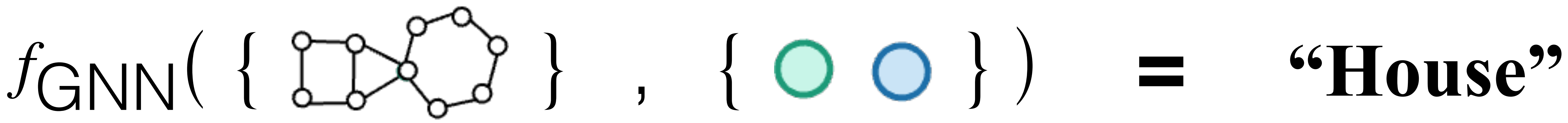

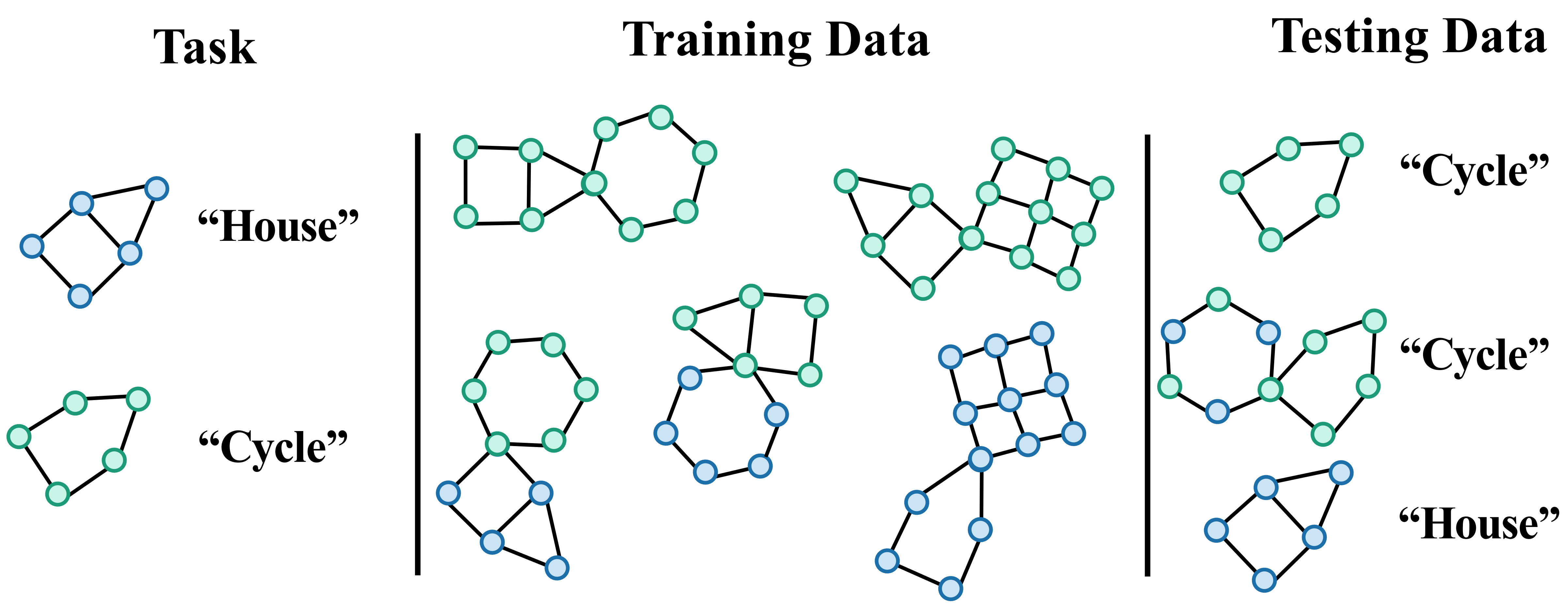

(Ying et al., 2019; Luo et al., 2020; Wu et al., 2022;)

OOD generalization on graphs are **much more challenging!**

- **Graphs are highly non-linear**

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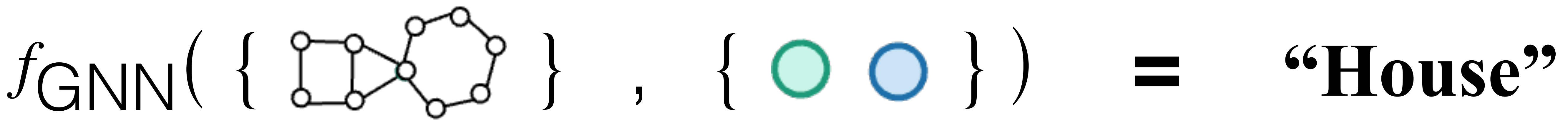

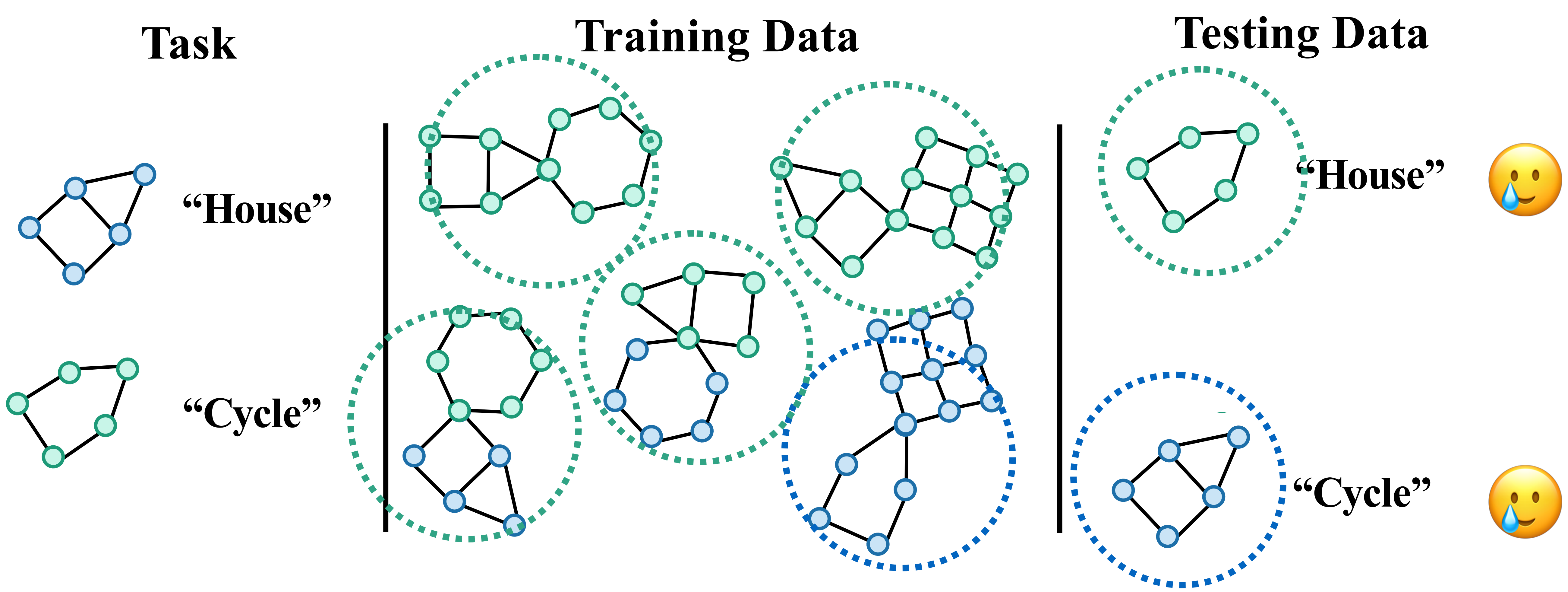

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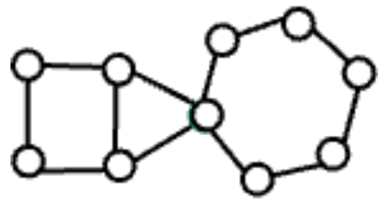
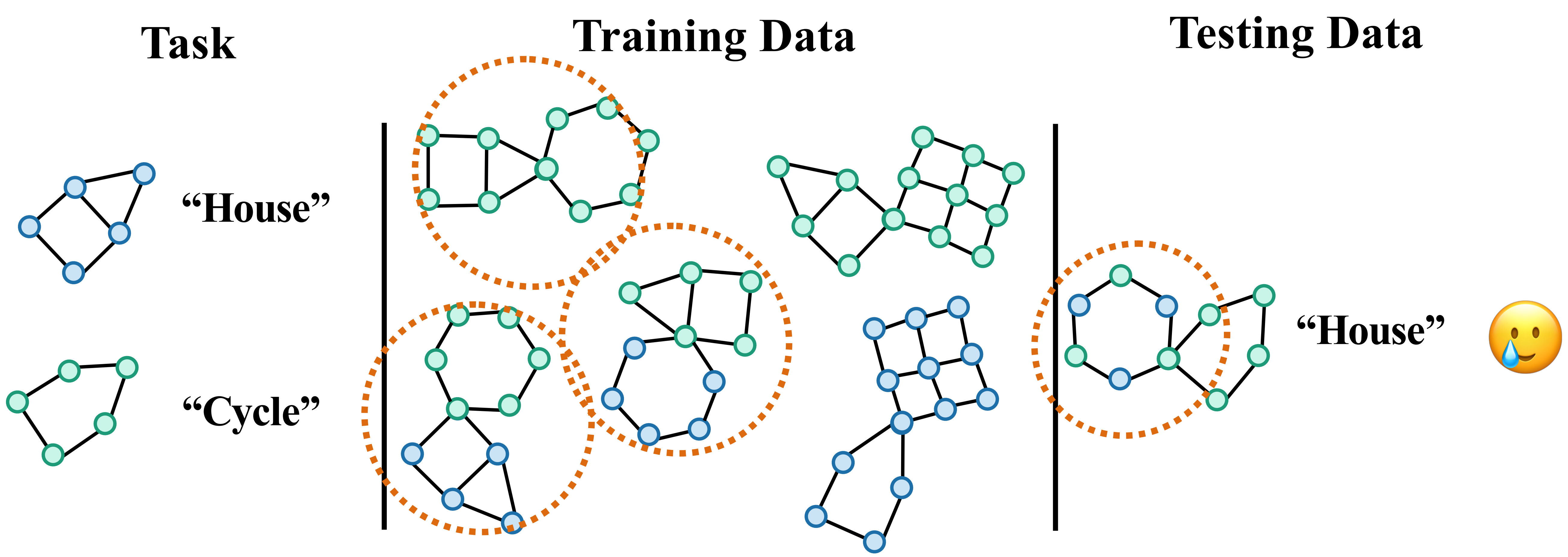
f_{GNN}({  } , {  }) = **"House"**



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OOD generalization on graphs are **much more challenging!**

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- Attribute-level shifts
- **Structure-level shifts**

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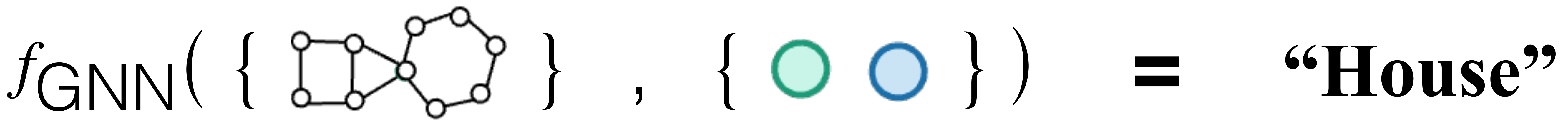

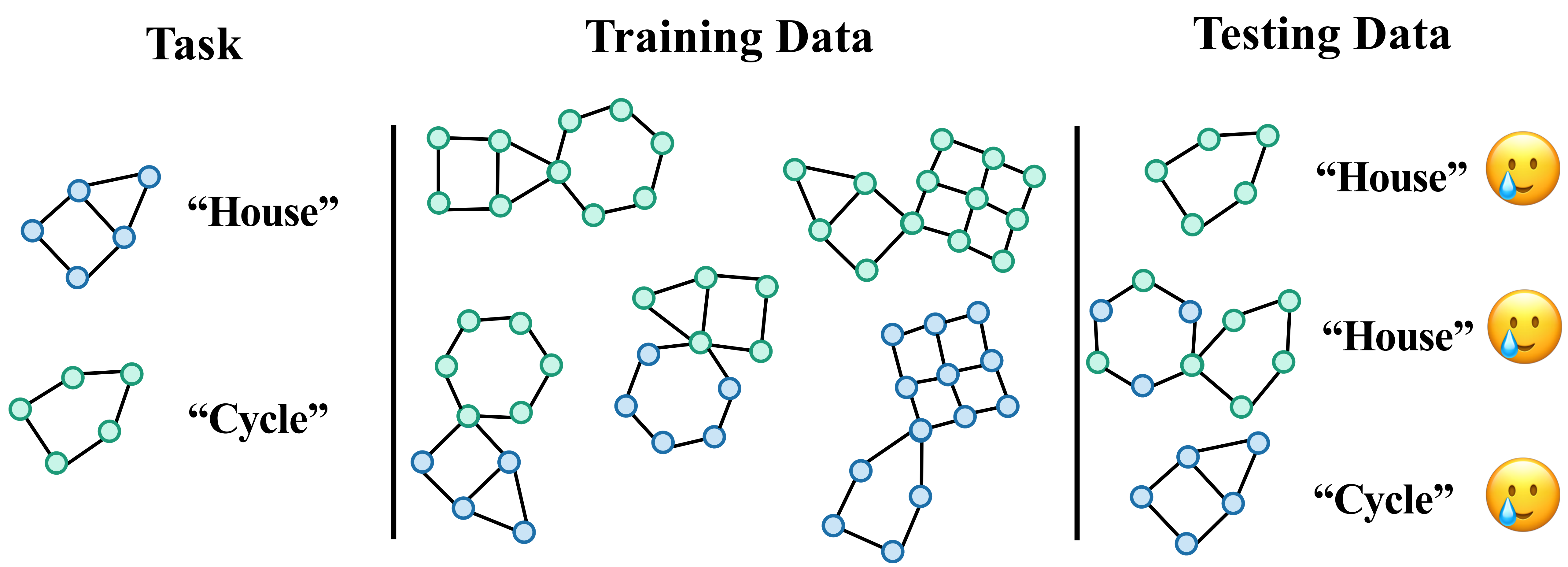

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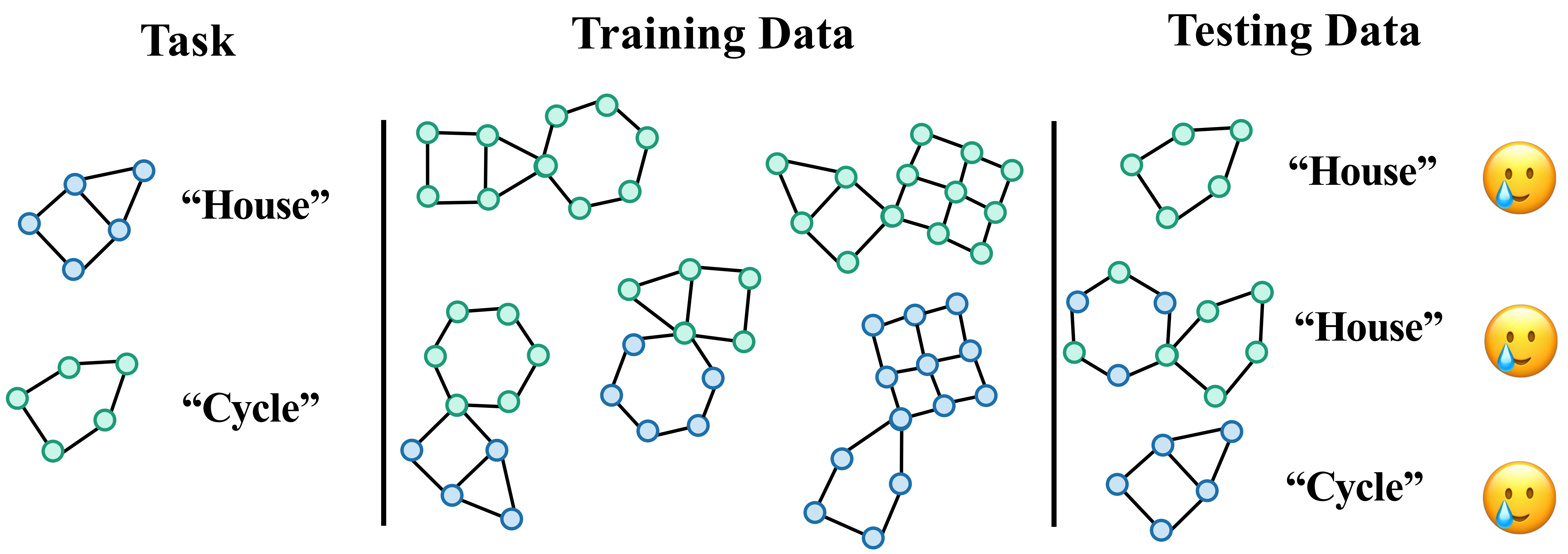
OOD generalization on graphs are **much more challenging!**

- Graphs are highly non-linear
- Attribute-level shifts
- Structure-level shifts
- Mixed shifts in different modes
- Expensive environment labels

OOD generalization on graphs are more challenging



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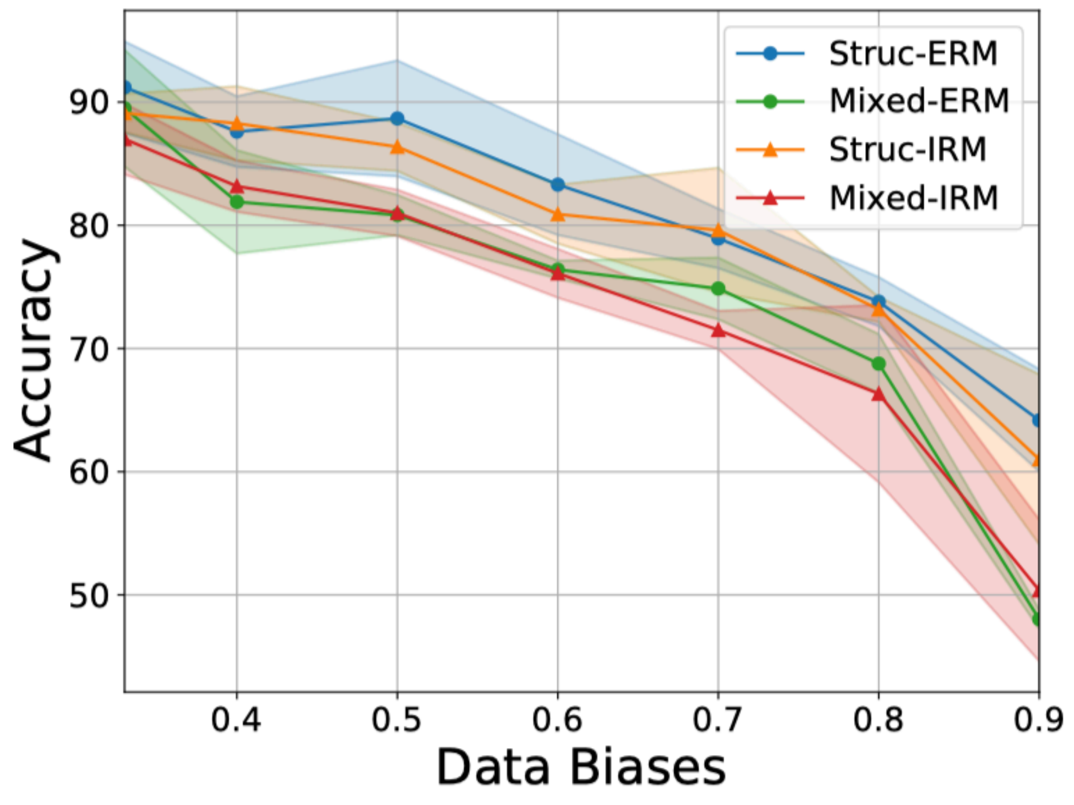
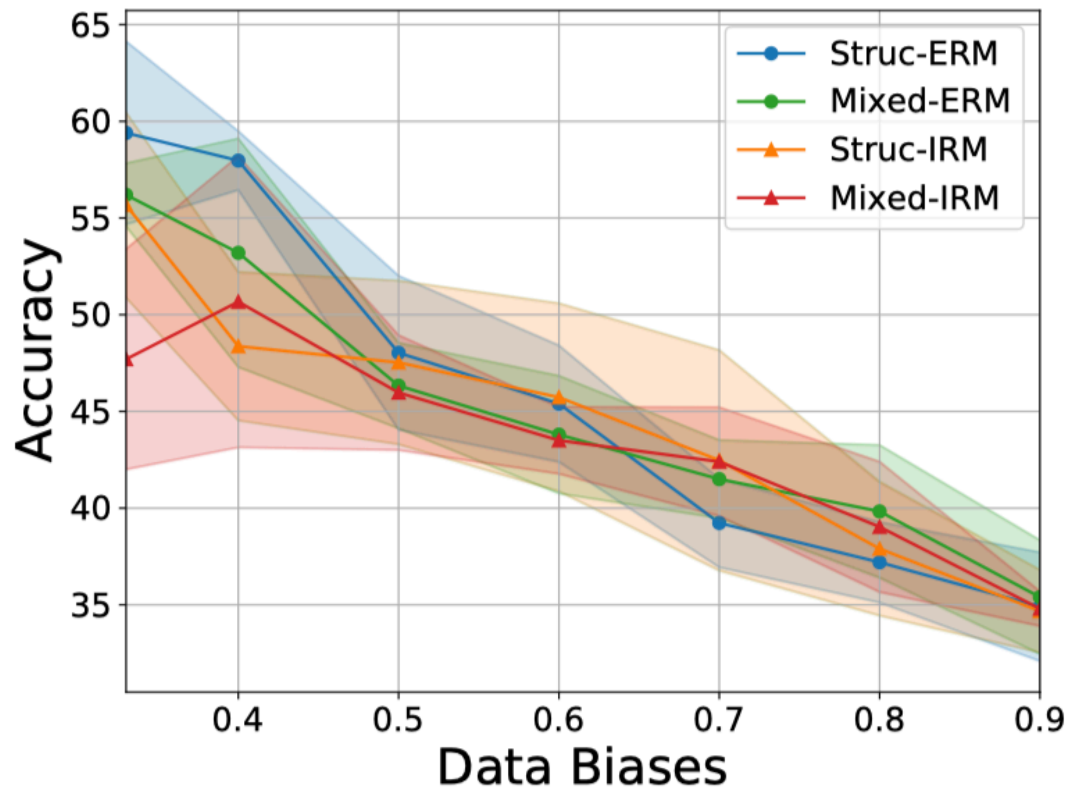
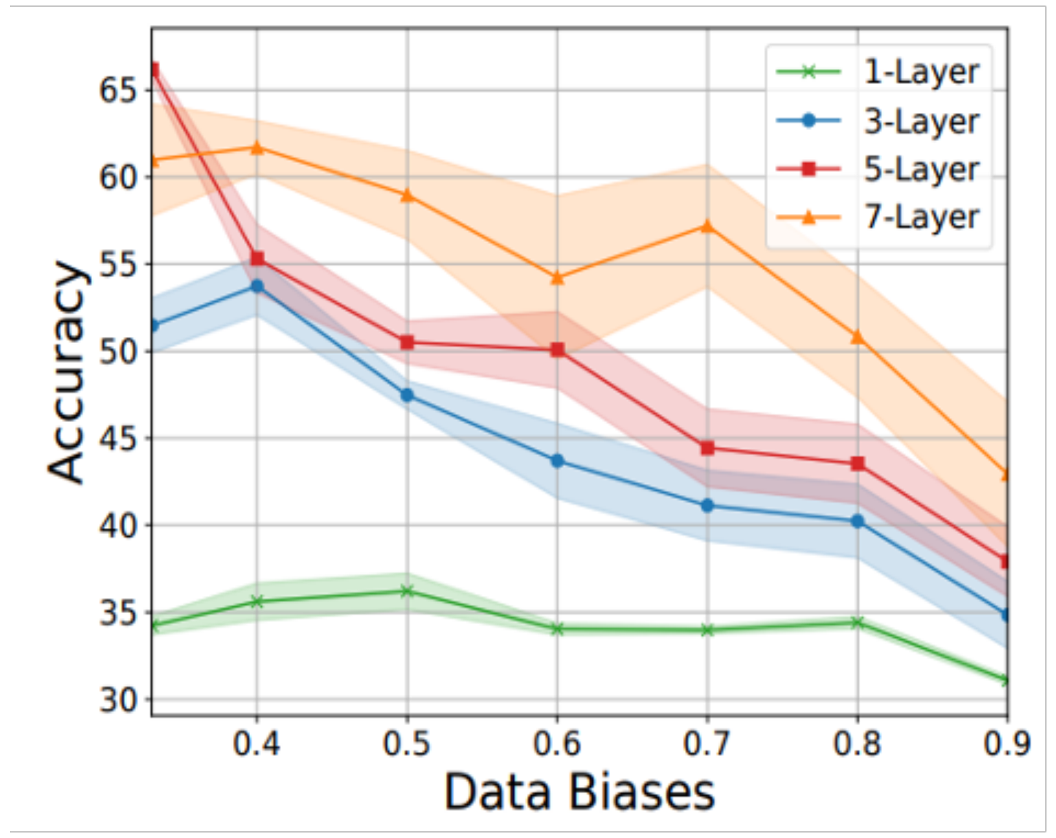


Structure and attribute shifts



Mixed with **graph size** shifts



Structure and attribute shifts

OOD failures of GNNs ***training objectives*** and ***architectures***

OOD generalization on graphs are more challenging

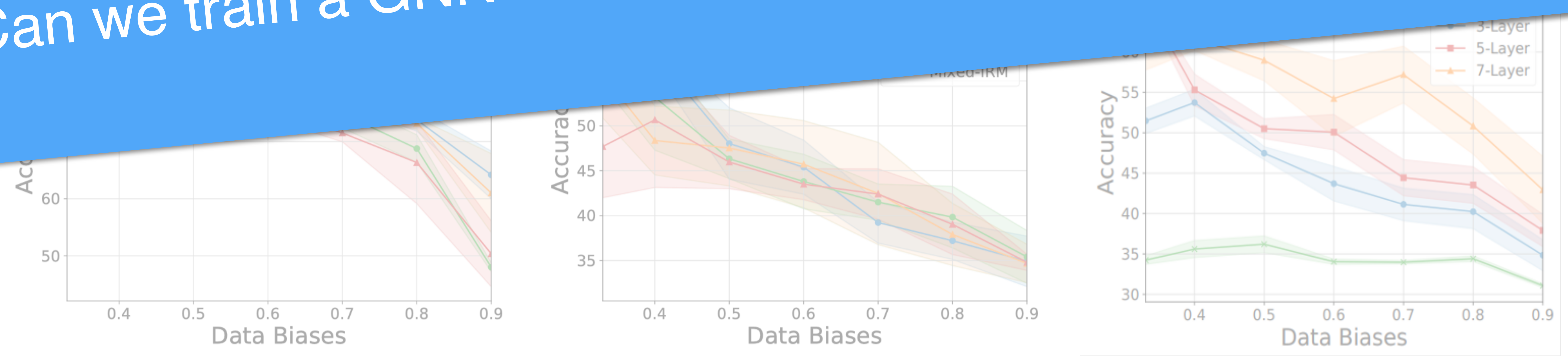
OOD generalization on graphs are **much more challenging!**

- Graphs are highly non-linear

As existing approaches are down…

How can we define and capture the invariance on graphs?

Can we train a GNN that is generalizable to OOD graphs?

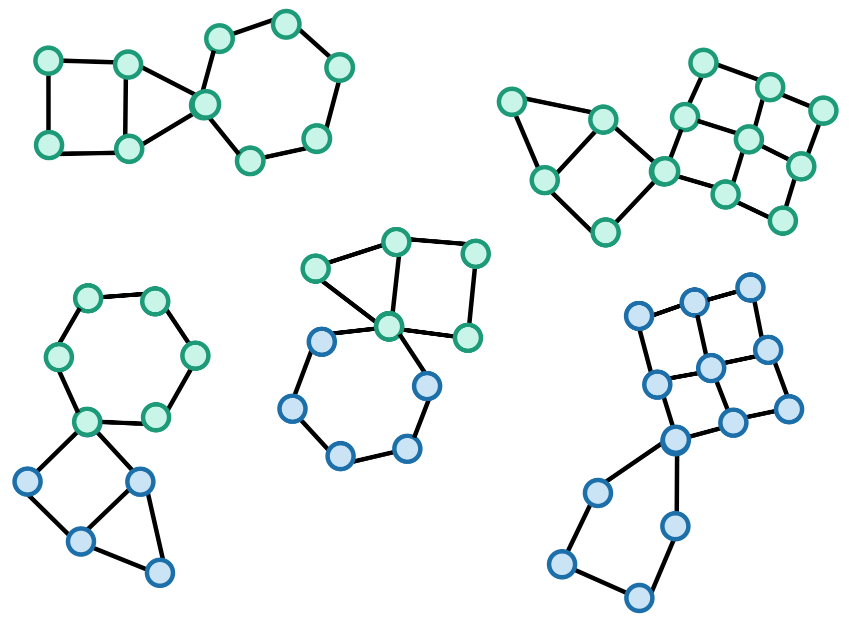


Structure and attribute shifts | Mixed with **graph size** shifts | Structure and attribute shifts

OOD failures of GNNs ***training objectives*** and ***architectures***

Invariance Principle Meets Graph Neural Networks

for generalizing to out-of-distribution graph data



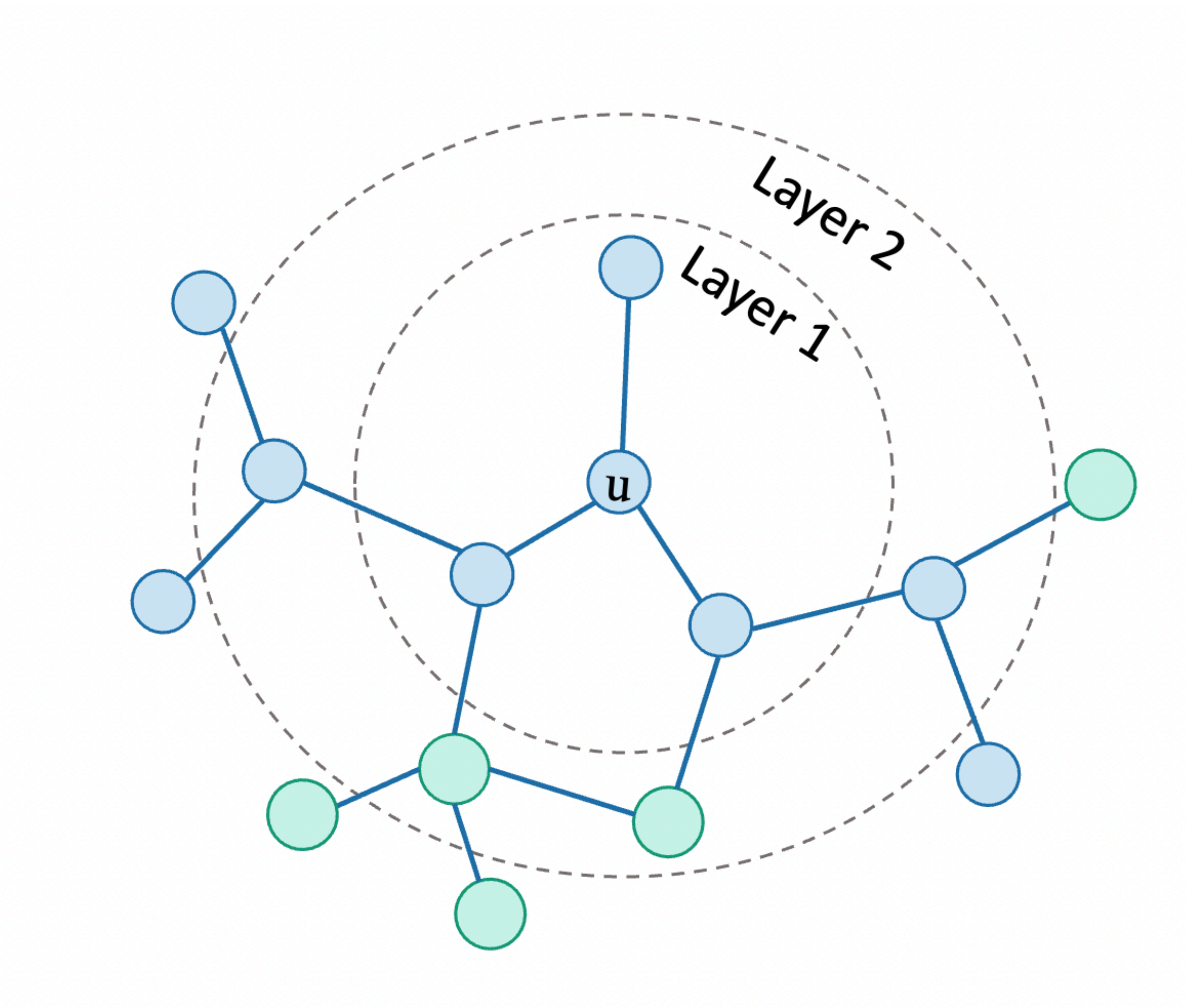


Figure source: Léon Bottou

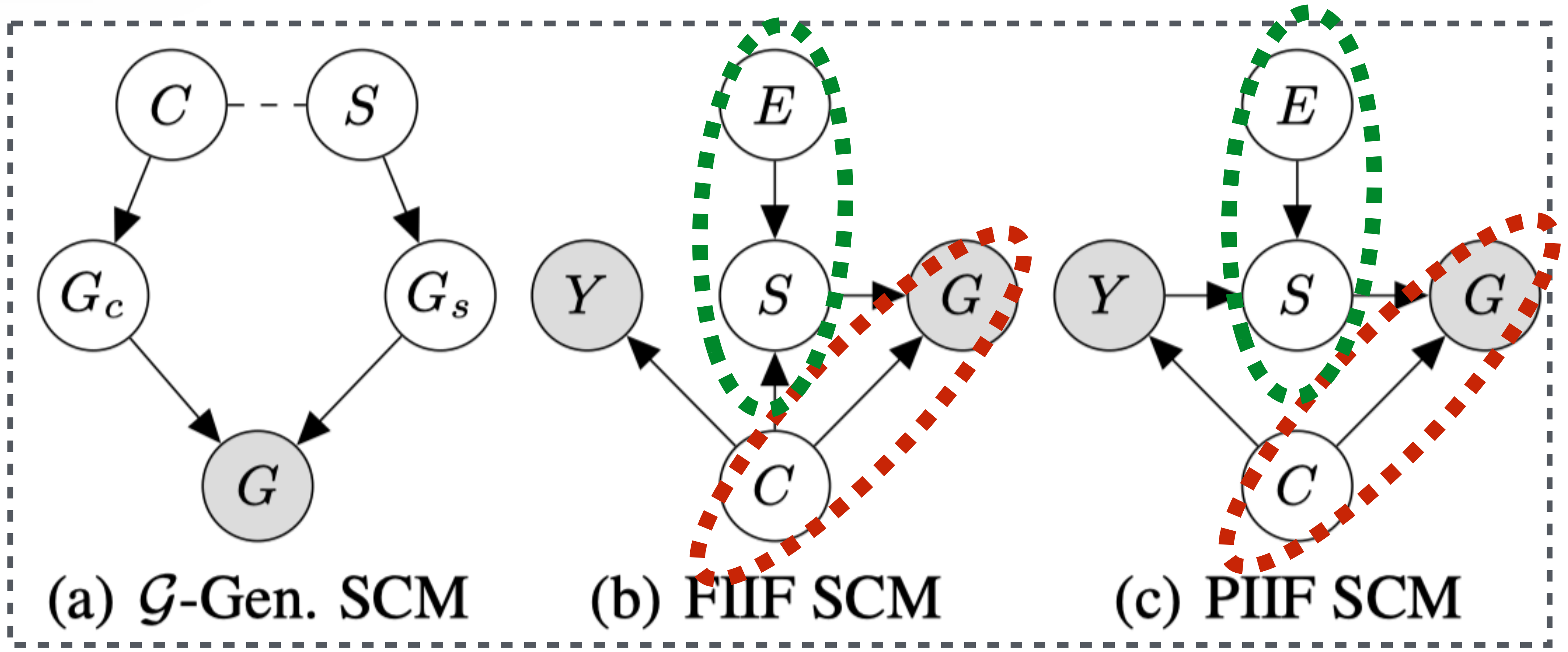
CIGA: Causality Inspired Invariant Graph LeArning

Graph Generation Process:

$$f_{\text{gen}} : \mathcal{Z} \rightarrow \mathcal{G}$$

Invariant features C

S Spurious features



Structural Causal Models

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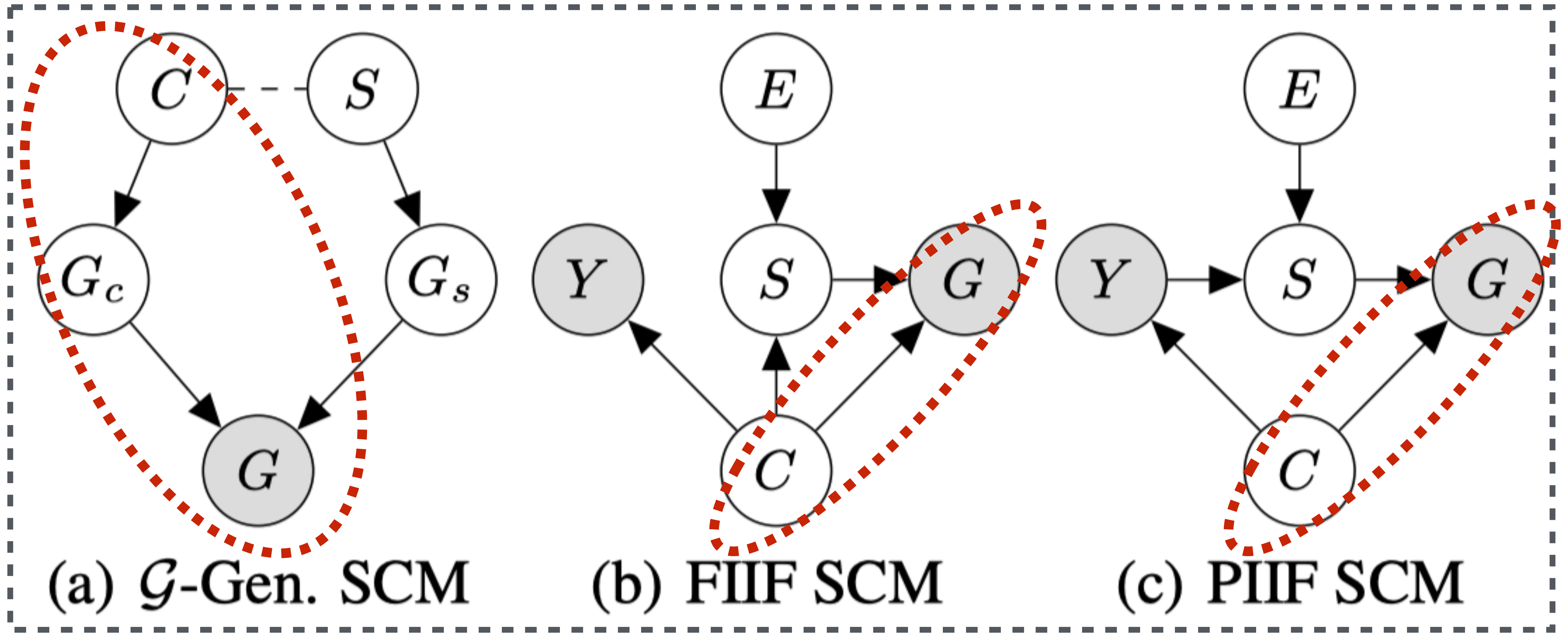
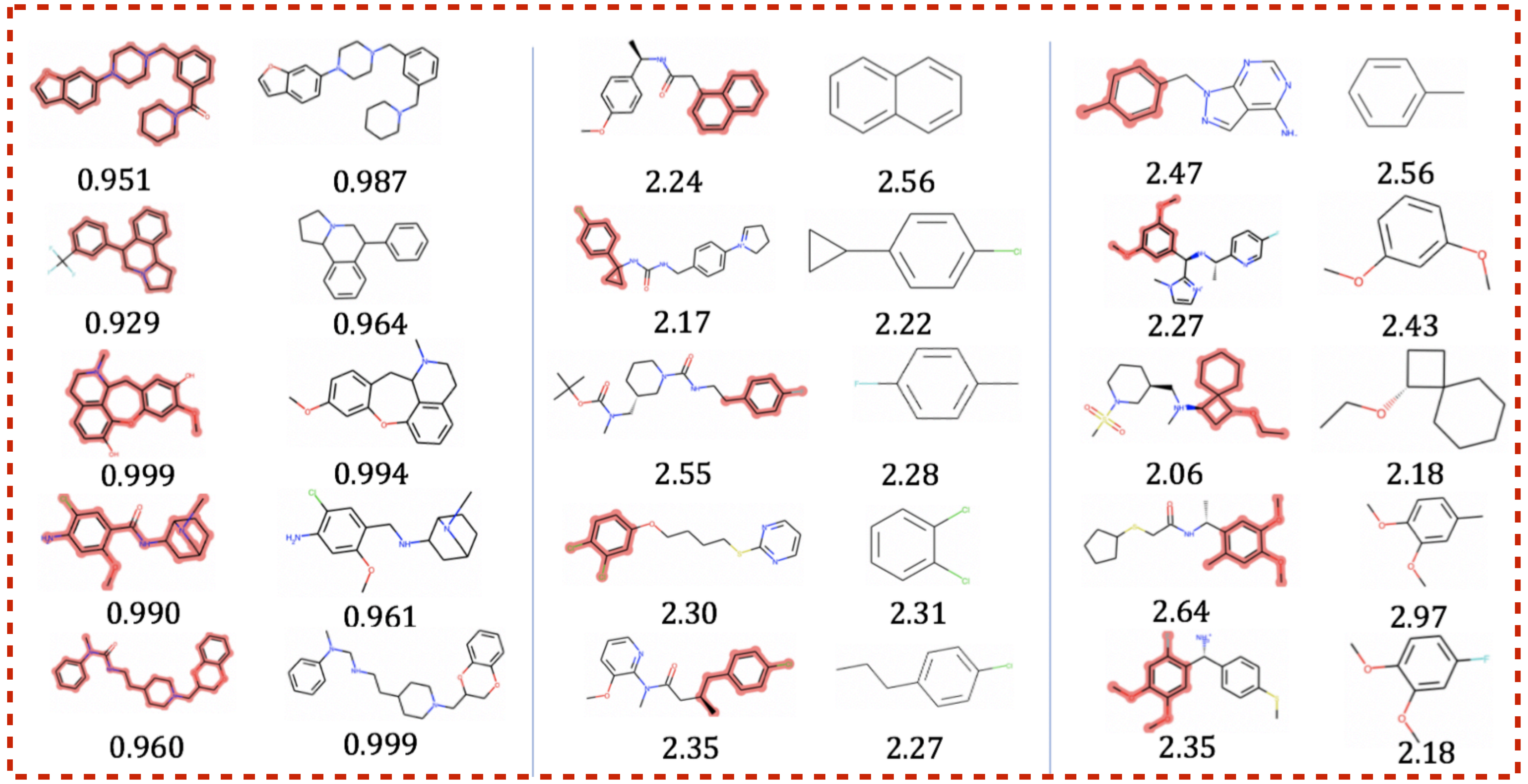


Structural Causal Models

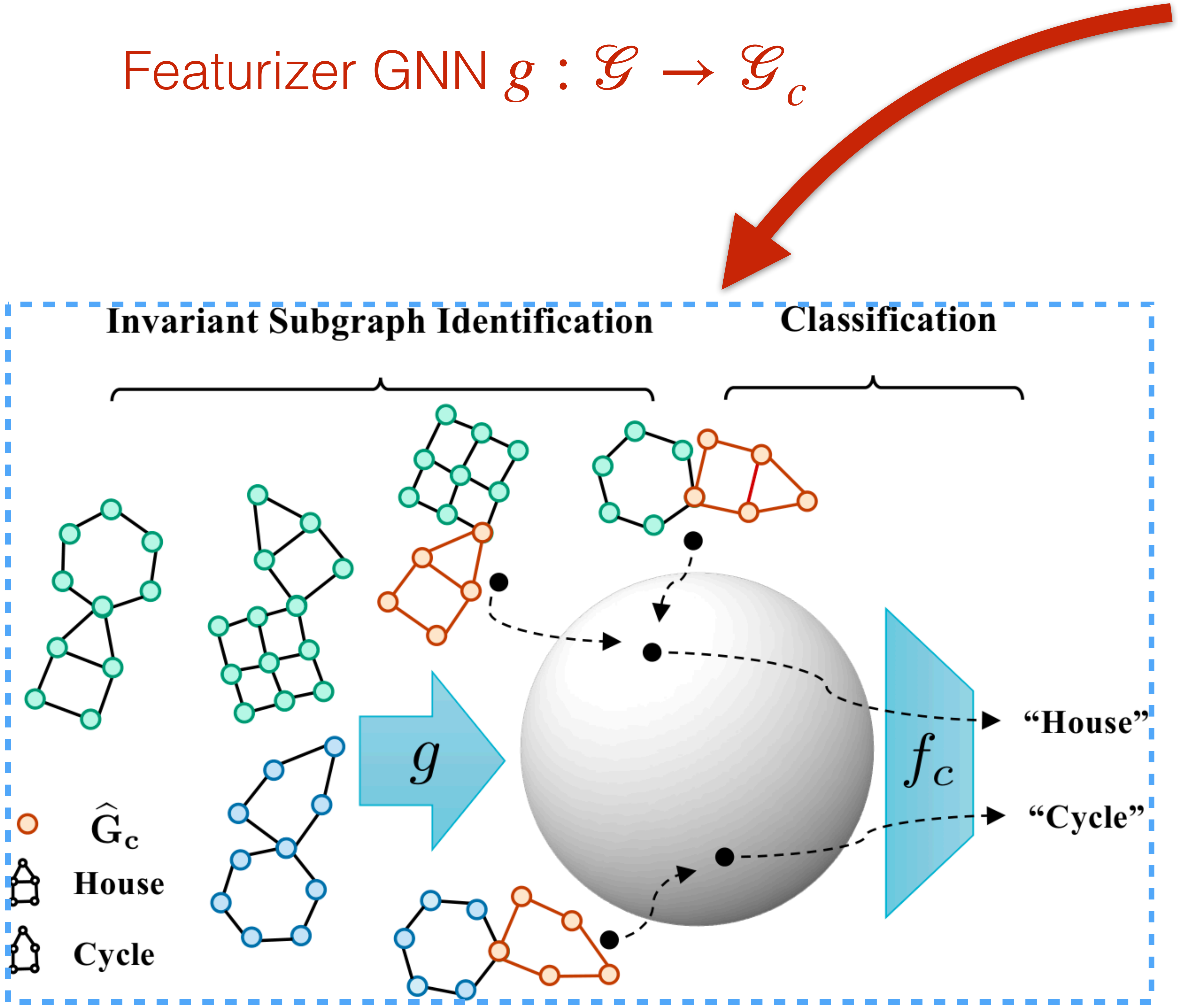
Realistic examples

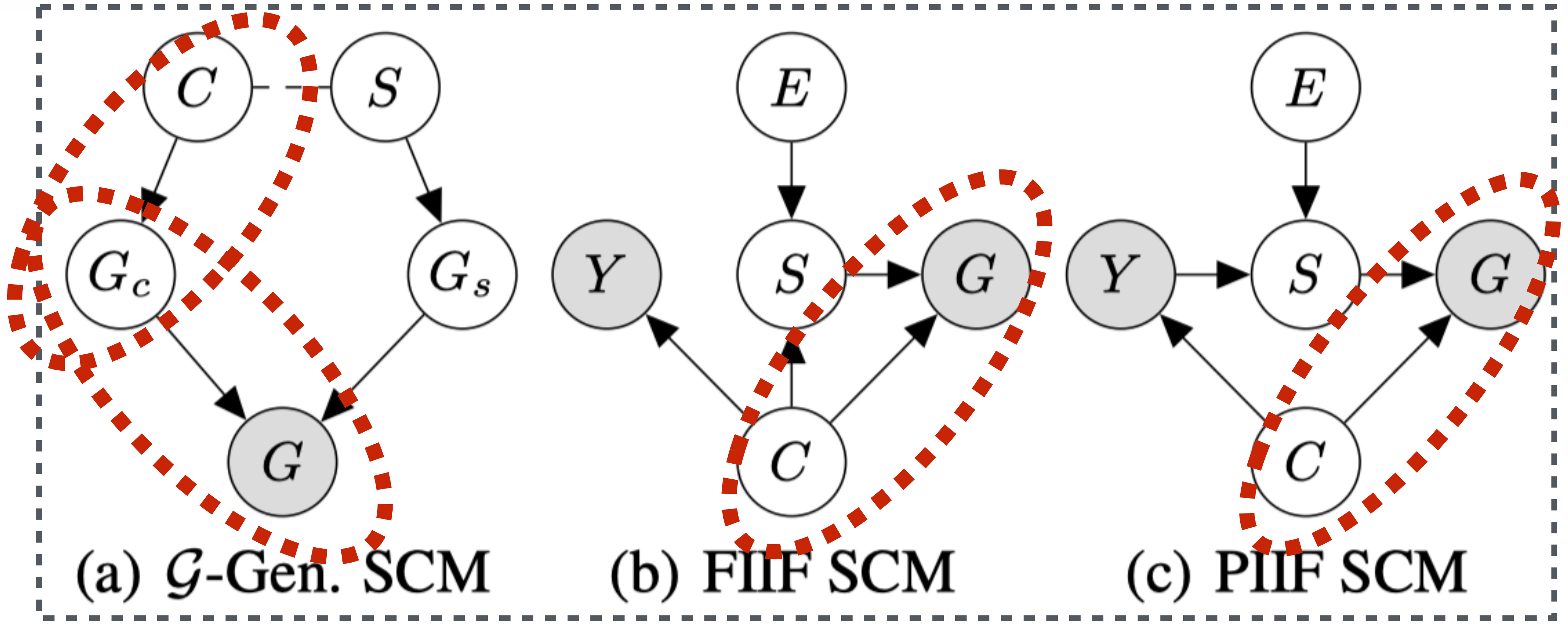


CIGA: Causality Inspired Invariant Graph LeArning

Step 1: Invariant subgraph identification

Featurizer GNN $g : \mathcal{G} \rightarrow \mathcal{G}_c$





Structural Causal Models

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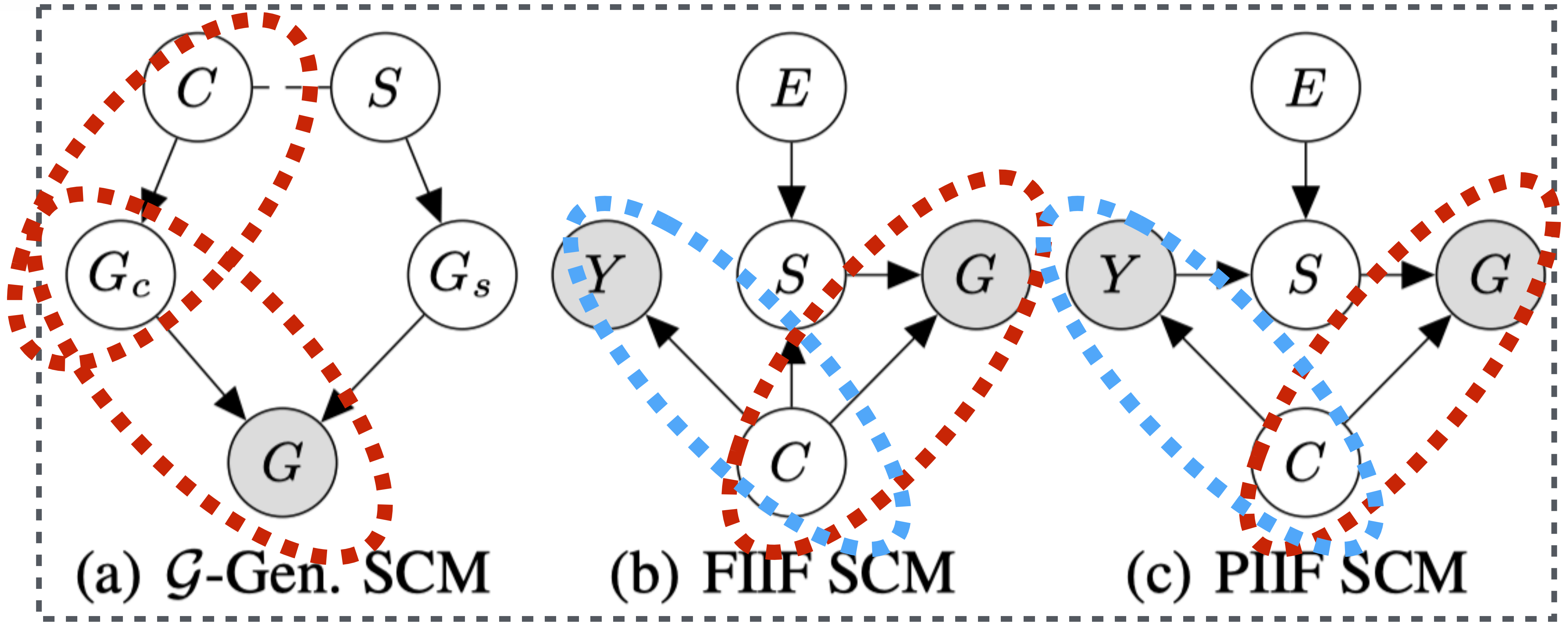
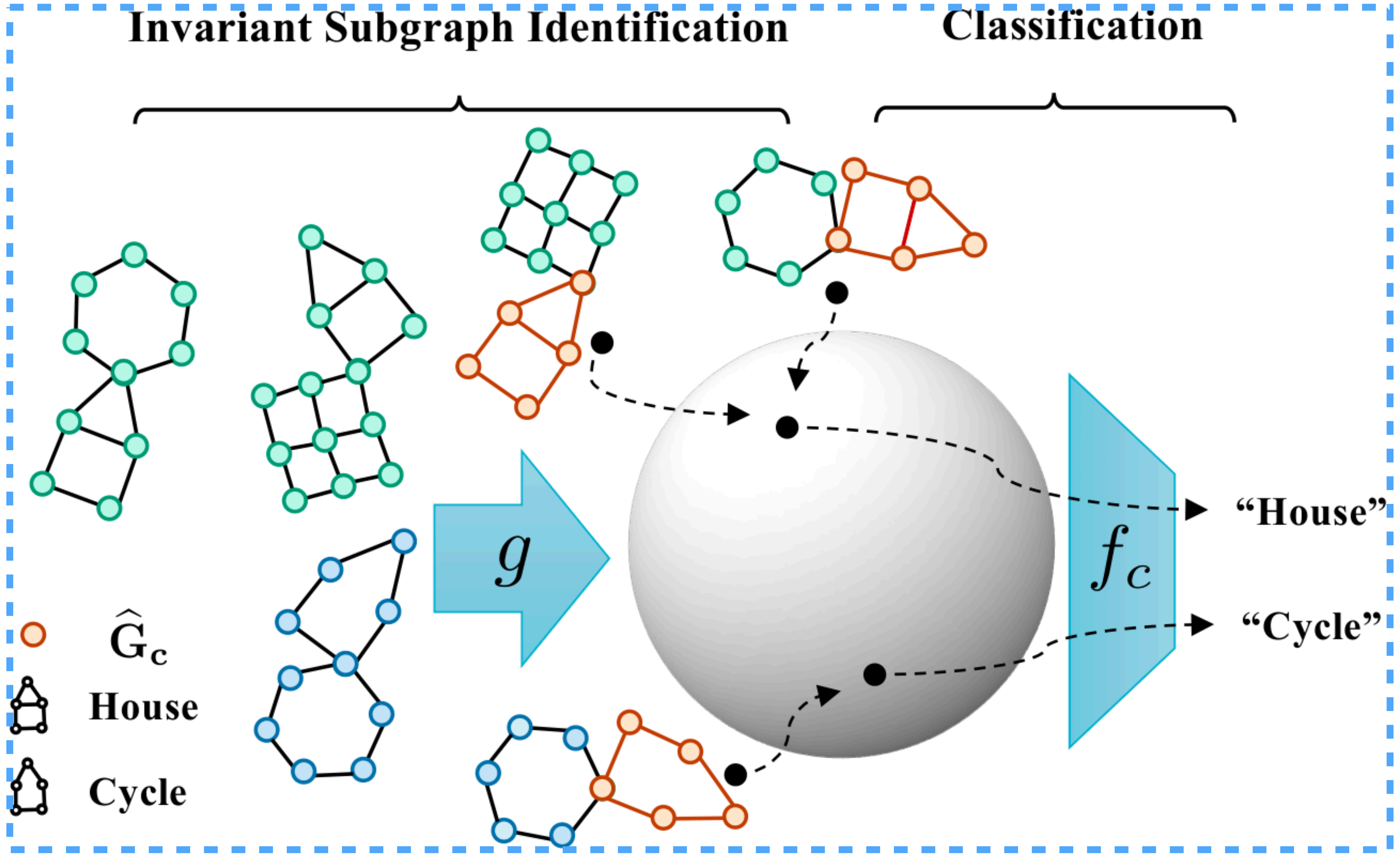


Structural Causal Models

Step 2: Label prediction

Classifier GNN $f_c : \mathcal{G}_c \to \mathcal{Y}$



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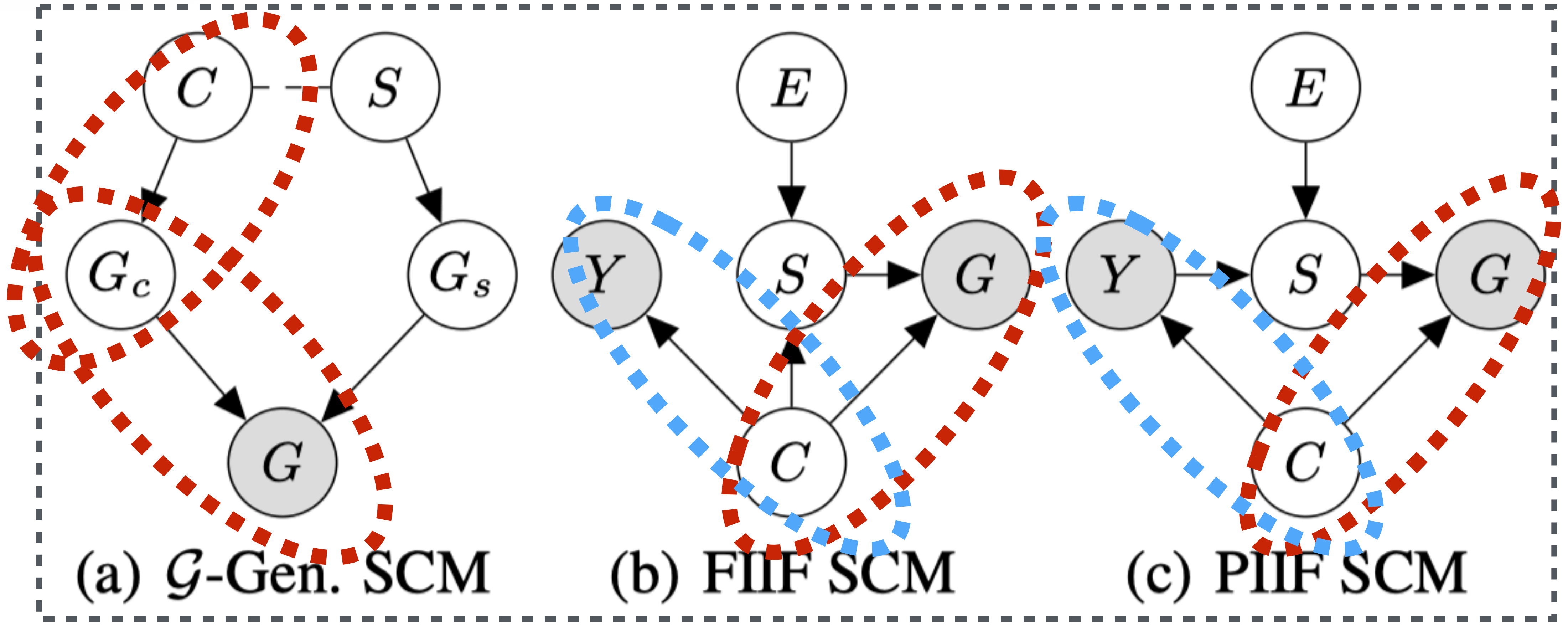
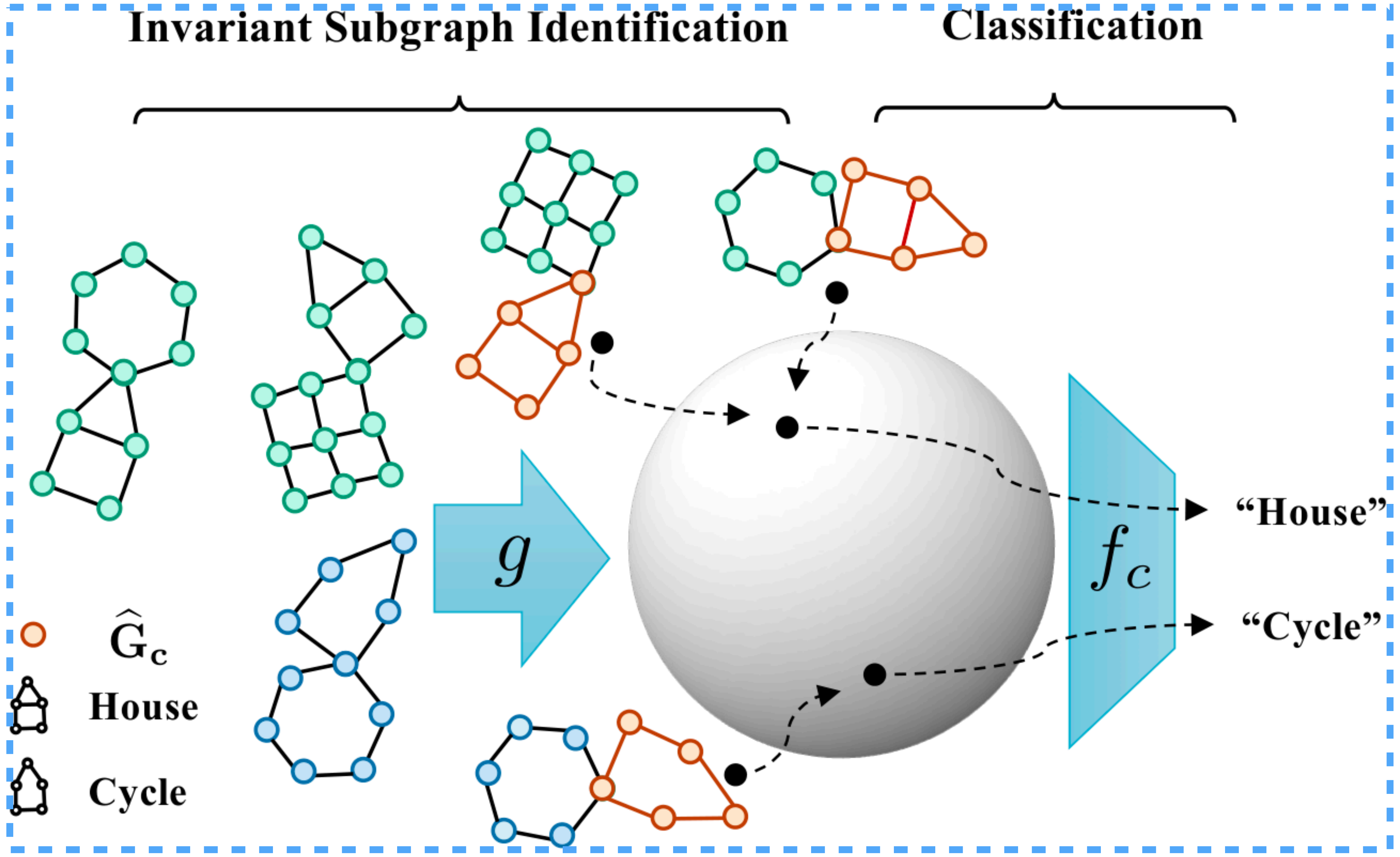


Structural Causal Models



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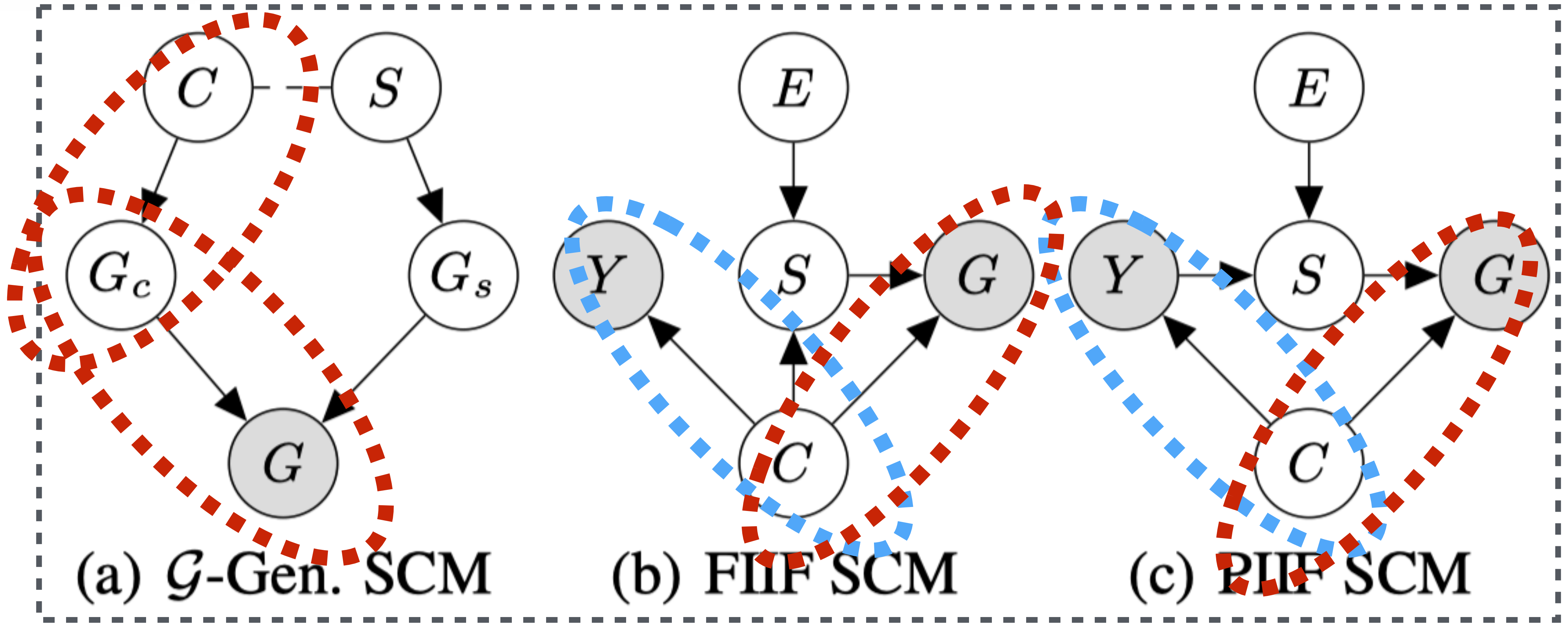
Overall objective

$$\max_{f_c,\, g} I(\widehat{G}_c; Y),\ \text{s.t. } \widehat{G}_c \perp E,\ \widehat{G}_c = g(G),$$

Informative

Invariant

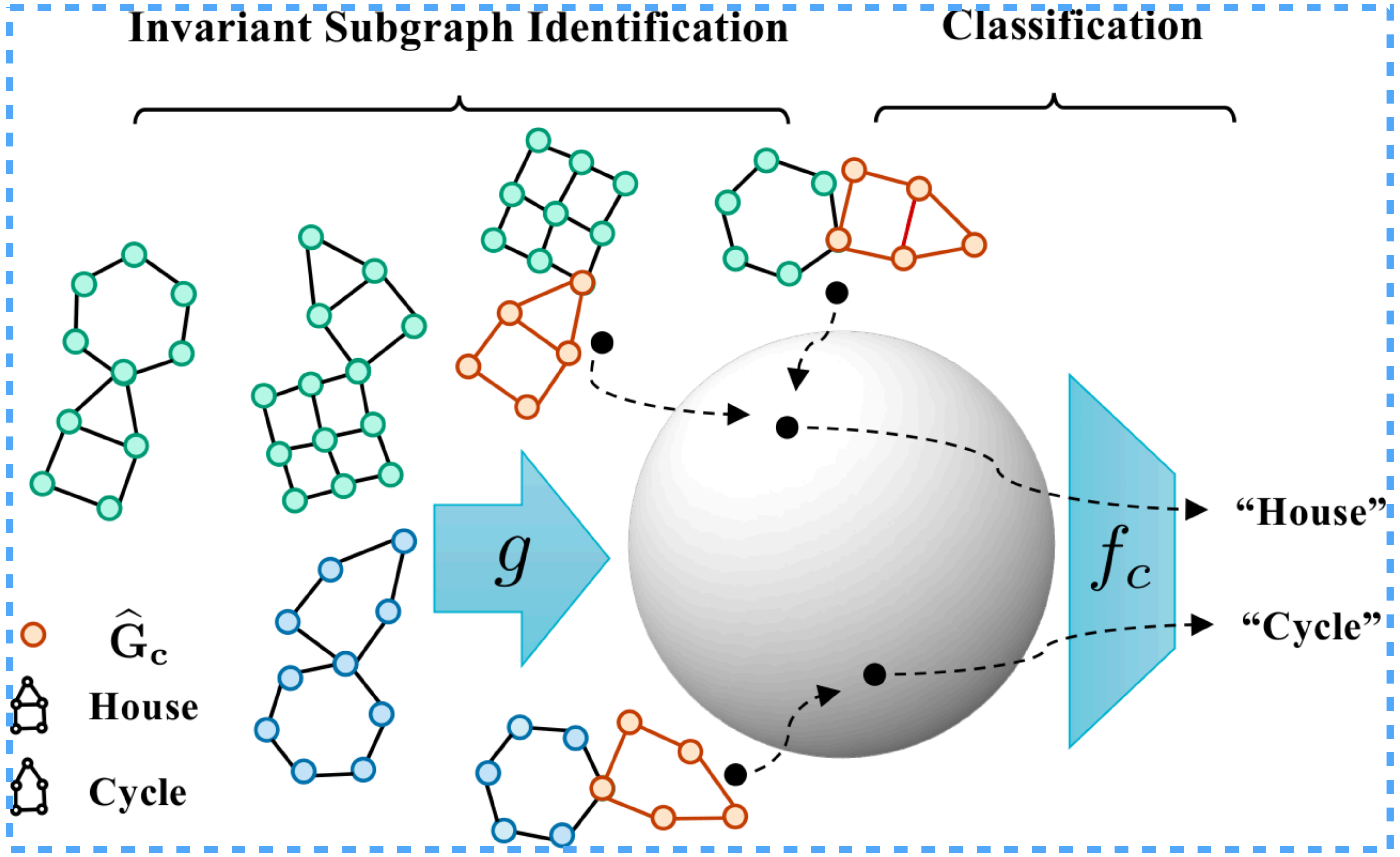
CIGA: Causality Inspired Invariant Graph LeArning



Structural Causal Models

CIGAv1: when $|G_c| = s_c$ is known and fixed

$$\max_{f_c, g} I(\widehat{G}_c; Y), \text{ s.t. } \widehat{G}_c \in \underset{\widehat{G}_c = g(G), |\widehat{G}_c| \le s_c}{\arg\max} I(\widehat{G}_c; \widetilde{G}_c | Y),$$



CIGAv2: eliminate the size constraint

$$\max_{f_c, g} I(\widehat{G}_c; Y) + I(\widehat{G}_s; Y), \text{ s.t. } \widehat{G}_c \in \arg\max_{\widehat{G}_c = g(G)} I(\widehat{G}_c; \widetilde{G}_c | Y),$$
$$I(\widehat{G}_s; Y) \le I(\widehat{G}_c; Y),\ \widehat{G}_s = G - g(G),$$

CIGA: Causality Inspired Invariant Graph LeArning

Theoretical results (Informal):
Given the previous SCMs, each solution to CIGAv1 or CIGAv2 elicits a GNN that is generalizable against various distribution shifts, with some mild assumptions on training environments, and the expressivity of GNNs encoders.

Table 1: OOD generalization performance on structure and mixed shifts for synthetic graphs.

	SPMotif-Struc†			SPMotif-Mixed†			
	bias=0.33	bias=0.60	bias=0.90	bias=0.33	bias=0.60	bias=0.90	Avg
ERM	59.49 (3.50)	55.48 (4.84)	49.64 (4.63)	58.18 (4.30)	49.29 (8.17)	41.36 (3.29)	52.24
ASAP	64.87 (13.8)	64.85 (10.6)	**57.29 (14.5)**	66.88 (15.0)	59.78 (6.78)	**50.45 (4.90)**	60.69
DIR	58.73 (11.9)	48.72 (14.8)	41.90 (9.39)	67.28 (4.06)	51.66 (14.1)	38.58 (5.88)	51.14
IRM	57.15 (3.98)	61.74 (1.32)	45.68 (4.88)	58.20 (1.97)	49.29 (3.67)	40.73 (1.93)	52.13
V-Rex	54.64 (3.05)	53.60 (3.74)	48.86 (9.69)	57.82 (5.93)	48.25 (2.79)	43.27 (1.32)	51.07
EIIL	56.48 (2.56)	60.07 (4.47)	55.79 (6.54)	53.91 (3.15)	48.41 (5.53)	41.75 (4.97)	52.73
IB-IRM	58.30 (6.37)	54.37 (7.35)	45.14 (4.07)	57.70 (2.11)	50.83 (1.51)	40.27 (3.68)	51.10
CNC	70.44 (2.55)	**66.79 (9.42)**	50.25 (10.7)	65.75 (4.35)	59.27 (5.29)	41.58 (1.90)	59.01
CIGAv1	**71.07 (3.60)**	63.23 (9.61)	51.78 (7.29)	**74.35 (1.85)**	**64.54 (8.19)**	49.01 (9.92)	**62.33**
CIGAv2	**77.33 (9.13)**	**69.29 (3.06)**	**63.41 (7.38)**	**72.42 (4.80)**	**70.83 (7.54)**	**54.25 (5.38)**	**67.92**
Oracle (IID)		88.70 (0.17)			88.73 (0.25)		

†Higher accuracy and lower variance indicate better OOD generalization ability.

CIGA outperforms previous methods under ***structure and mixed shifts*** by a significant margin up to ***10%***.

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Theoretical results (Informal):
Given the previous SCMs, each solution to CIGAv1 or CIGAv2 elicits a GNN that is generalizable against various distribution shifts, with some mild assumptions on training environments, and the expressivity of GNNs encoders.

Table 2: OOD generalization performance on complex distribution shifts for real-world graphs.

Datasets	Drug-Assay	Drug-Sca	Drug-Size	CMNIST-sp	Graph-SST5	Twitter	Avg (Rank)†
ERM	71.79 (0.27)	68.85 (0.62)	66.70 (1.08)	13.96 (5.48)	43.89 (1.73)	60.81 (2.05)	54.33 (6.00)
ASAP	70.51 (1.93)	66.19 (0.94)	64.12 (0.67)	10.23 (0.51)	44.16 (1.36)	60.68 (2.10)	52.65 (8.33)
GIB	63.01 (1.16)	62.01 (1.41)	55.50 (1.42)	15.40 (3.91)	38.64 (4.52)	48.08 (2.27)	47.11 (10.0)
DIR	68.25 (1.40)	63.91 (1.36)	60.40 (1.42)	15.50 (8.65)	41.12 (1.96)	59.85 (2.98)	51.51 (9.33)
IRM	72.12 (0.49)	68.69 (0.65)	66.54 (0.42)	31.58 (9.52)	43.69 (1.26)	63.50 (1.23)	57.69 (4.50)
V-Rex	72.05 (1.25)	68.92 (0.98)	66.33 (0.74)	10.29 (0.46)	43.28 (0.52)	63.21 (1.57)	54.01 (6.17)
EIIL	72.60 (0.47)	68.45 (0.53)	66.38 (0.66)	30.04 (10.9)	42.98 (1.03)	62.76 (1.72)	57.20 (5.33)
IB-IRM	72.50 (0.49)	68.50 (0.40)	66.64 (0.28)	**39.86 (10.5)**	40.85 (2.08)	61.26 (1.20)	58.27 (5.33)
CNC	72.40 (0.46)	67.24 (0.90)	65.79 (0.80)	12.21 (3.85)	42.78 (1.53)	61.03 (2.49)	53.56 (7.50)
CIGAv1	**72.71 (0.52)**	**69.04 (0.86)**	**67.24 (0.88)**	19.77 (17.1)	**44.71 (1.14)**	**63.66 (0.84)**	**56.19 (2.50)**
CIGAv2	**73.17 (0.39)**	**69.70 (0.27)**	**67.78 (0.76)**	**44.91 (4.31)**	**45.25 (1.27)**	**64.45 (1.99)**	**60.88 (1.00)**
Oracle (IID)	85.56 (1.44)	84.71 (1.60)	85.83 (1.31)	62.13 (0.43)	48.18 (1.00)	64.21 (1.77)	

†Averaged rank is also reported in the blankets because of dataset heterogeneity. Lower rank is better.

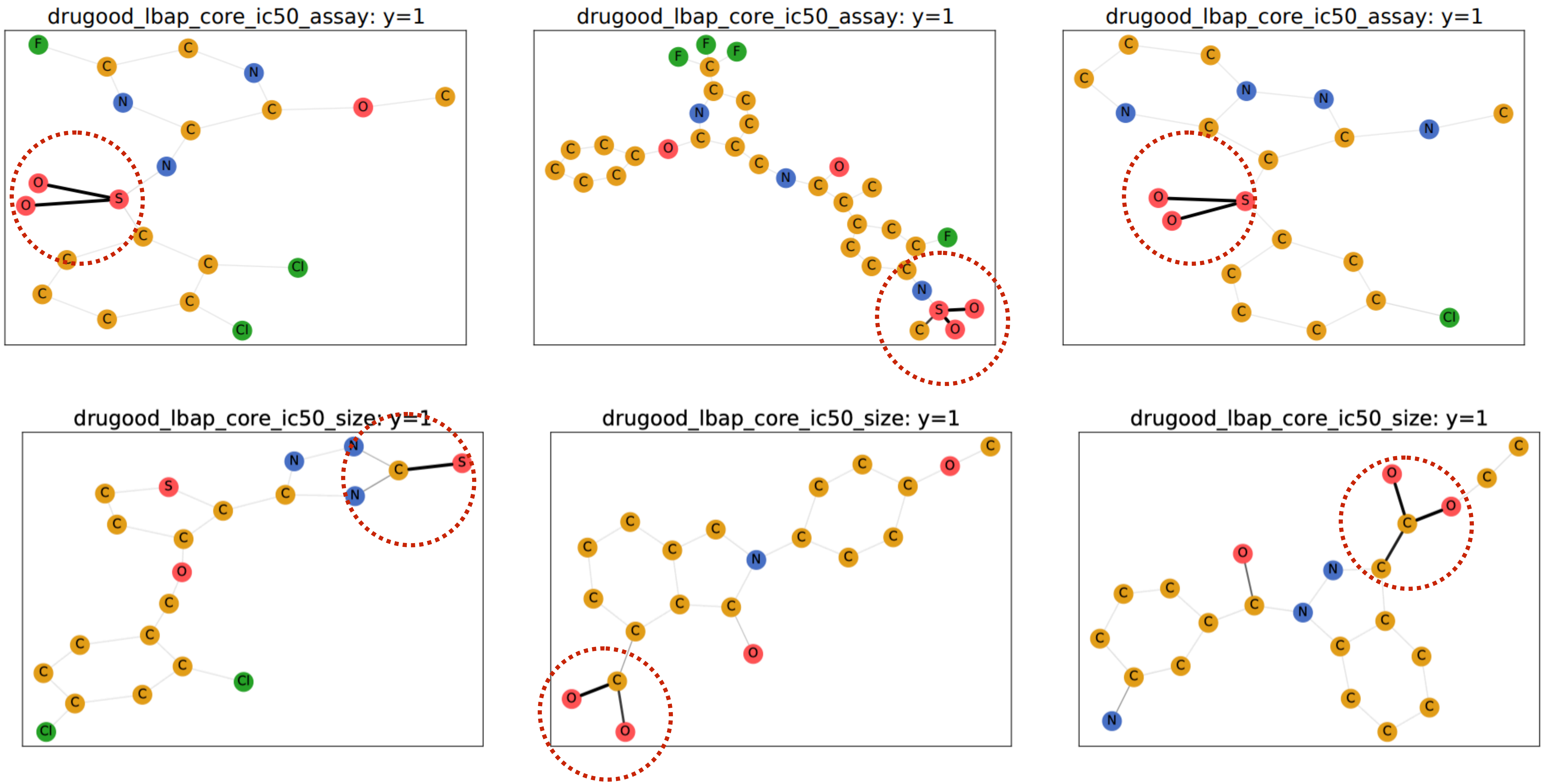
Table 3: OOD generalization performance on graph size shifts for real-world graphs in terms of Matthews correlation coefficient.

Datasets	NCI1	NCI109	PROTEINS	DD	Avg
ERM	0.15 (0.05)	0.16 (0.02)	0.22 (0.09)	0.27 (0.09)	0.20
ASAP	0.16 (0.10)	0.15 (0.07)	0.22 (0.16)	0.21 (0.08)	0.19
GIB	0.13 (0.10)	0.16 (0.02)	0.19 (0.08)	0.01 (0.18)	0.12
DIR	0.21 (0.06)	0.13 (0.05)	0.25 (0.14)	0.20 (0.10)	0.20
IRM	0.17 (0.02)	0.14 (0.01)	0.21 (0.09)	0.22 (0.08)	0.19
V-Rex	0.15 (0.04)	0.15 (0.04)	0.22 (0.06)	0.21 (0.07)	0.18
EIIL	0.14 (0.03)	0.16 (0.02)	0.20 (0.05)	0.23 (0.10)	0.19
IB-IRM	0.12 (0.04)	0.15 (0.06)	0.21 (0.06)	0.15 (0.13)	0.16
CNC	0.16 (0.04)	0.16 (0.04)	0.19 (0.08)	0.27 (0.13)	0.20
WL kernel	**0.39 (0.00)**	0.21 (0.00)	0.00 (0.00)	0.00 (0.00)	0.15
GC kernel	0.02 (0.00)	0.00 (0.00)	0.29 (0.00)	0.00 (0.00)	0.08
$\Gamma_{\text{1-hot}}$	0.17 (0.08)	**0.25 (0.06)**	0.12 (0.09)	0.23 (0.08)	0.19
Γ_{GIN}	0.24 (0.04)	0.18 (0.04)	0.29 (0.11)	**0.28 (0.06)**	0.25
Γ_{RPGIN}	0.26 (0.05)	0.20 (0.04)	0.25 (0.12)	0.20 (0.05)	0.23
CIGAv1	0.22 (0.07)	**0.23 (0.09)**	**0.40 (0.06)**	**0.29 (0.08)**	**0.29**
CIGAv2	**0.27 (0.07)**	0.22 (0.05)	**0.31 (0.12)**	0.26 (0.08)	**0.27**
Oracle (IID)	0.32 (0.05)	0.37 (0.06)	0.39 (0.09)	0.33 (0.05)	

CIGA outperforms previous methods under other ***realistic shifts*** by a significant margin up to ***10%***.

Interpretable Studies of CIGA

CIGA finds interesting critical functional groups/sub-molecules in OOD molecular affinity prediction.



(Ji et al., 2022;)

Summary

Through the lens of causality, we establish general SCMs to characterize the distribution shifts on graphs, and generalize the invariance principle to graphs.

We instantiate the invariance principle through a novel framework CIGA, where the prediction is decomposed into the subgraph identification and classification.

We show that the provable identification of the underlying invariant subgraph can be achieved using a contrastive strategy both theoretically and empirically.

Paper Code

Thank you!

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