Invariant Learning via the Probability of Sufficient and Necessary Causes

(NeurIPS 2023 Spotlight!)

Mengyue Yang

University College London

Email: mengyue.yang.20@ucl.ac.uk

Website: https://ymy4323460.github.io/

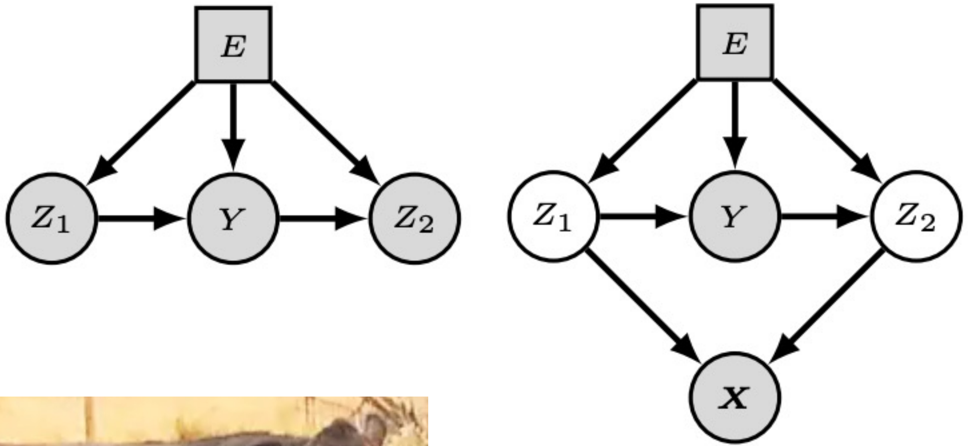
Paper link: https://arxiv.org/pdf/2309.12559.pdf

Invariant Learning

- The OOD generalization task

Train

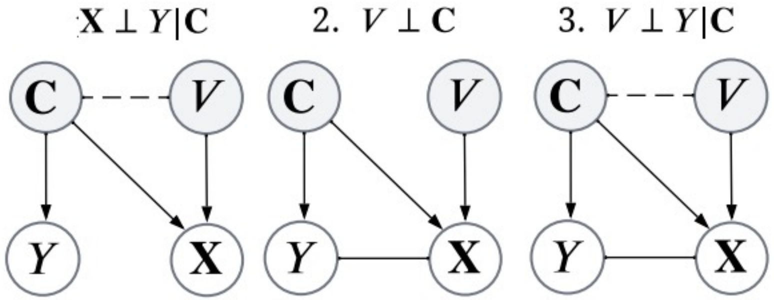
Test



Invariant Learning

- Invariant causal assumption across source and test distribution
  - $P_s(Y|C = c) = P_t(Y|C = c)$
- Extract causal feature for OOD generalization.
  - Infer causal feature from observation data
  - Predict label y from causal feature

$$y = \text{sign}[\mathbb{E}_{\mathbf{c} \sim P_t(\mathbf{C}|\mathbf{X}=\mathbf{x})} \mathbf{w}^\top \mathbf{c}].$$



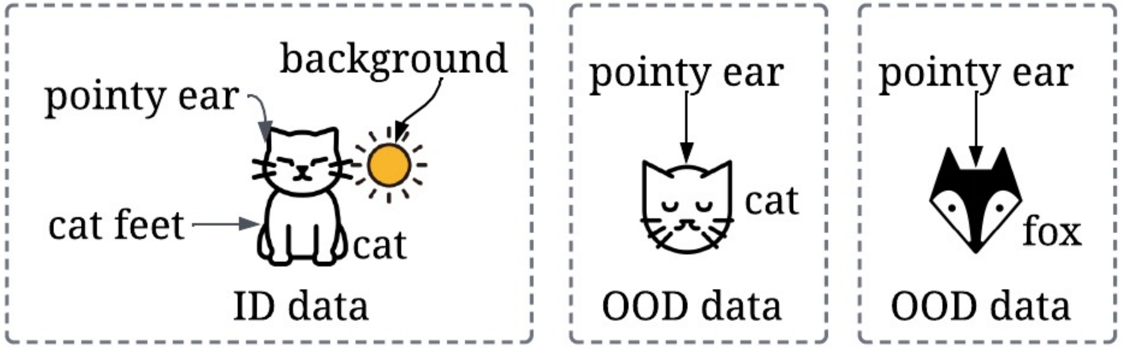
(b) Causal graph

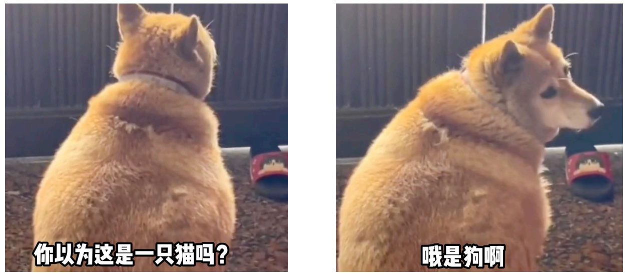
Causal representation

- Is causal representation enough in invariant learning?
- What kind of causal information is essential?

-- The sufficient and necessary causes!

'pointy ear' is necessary cause, 'cat feet' is sufficient cause
'background' is supurious correlation





Is that a cat? No!

Causal representation

- **A** is a Sufficient cause of **B** means when we know event **A**, the result **B** will happen.
- **A** is a Necessary cause of **B** means when the result **B** comes out, the event **A** must happened.

Pointy ear is necessary but insufficient

Cat feet is sufficient but unnecessary

Short label is sufficient and necessary

	ID train	OOD test	OOD test
pointy ear	True	True	True
cat feet	True	False	False
short mouth	True	False	True
label	Cat	Fox	Cat

Causal representation

- Defining the sufficient and necessary causes.
  - Chapter 9 in book: Causality
  - Considering the counterfactual probability on binary variables X and Y

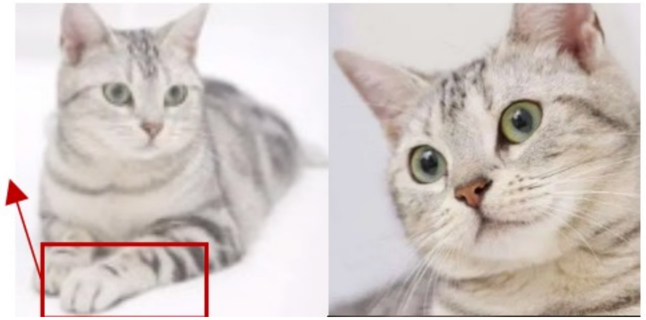
Definition 2.1 (Probability of Necessary and Sufficient (PNS) (Pearl, 2009)). Let the specific implementations of causal variable $\mathbf{C}$ as $\mathbf{c}$ and $\bar{\mathbf{c}}$, where $\bar{\mathbf{c}} \neq \mathbf{c}$. The probability that $\mathbf{C}$ is the necessary and sufficiency cause of Y on test domain $\mathcal{T}$ is

$$\begin{aligned} \mathrm{PNS}(\mathbf{c}, \bar{\mathbf{c}}) := & \underbrace{P_t(Y_{do(\mathbf{C}=\mathbf{c})} = y \mid \mathbf{C} = \bar{\mathbf{c}}, Y \neq y)}_{\text{sufficiency}} P_t(\mathbf{C} = \bar{\mathbf{c}}, Y \neq y) \\ & + \underbrace{P_t(Y_{do(\mathbf{C}=\bar{\mathbf{c}})} \neq y \mid \mathbf{C} = \mathbf{c}, Y = y)}_{\text{necessity}} P_t(\mathbf{C} = \mathbf{c}, Y = y). \end{aligned} \tag{2}$$

Causal representation

- Understanding PNS

The 'cat feet' patch is sufficient but unnecessary



We assume $P(Y_{do(C=1)} = 1) = 1$ and $P(Y_{do(C=0)} = 0) = 0.5$, $P(Y = 1) = 0.75$, $P(C = 1, Y = 1) = 0.5$, $P(C = 0, Y = 0) = 0.25$, $P(C = 0, Y = 1) = 0.25$.

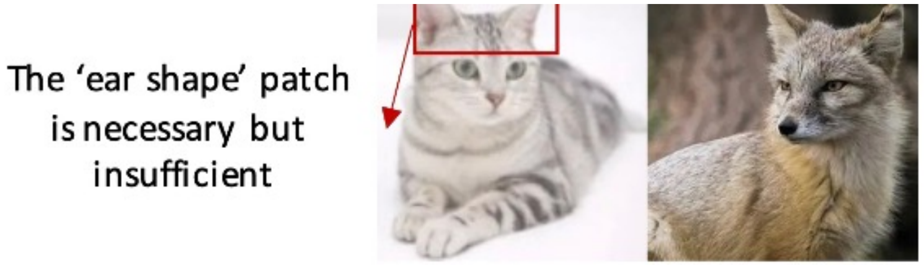
Now, applying the concept of the probability of sufficiency and necessity, we obtain:

Probability of necessity: $P(Y_{do(C=0)} = 0|Y = 1, C = 1) = \frac{P(Y=1)-P(Y_{do(C=0)}=1)}{P(Y=1,C=1)} = \frac{0.5-0.5}{P(Y=1,C=1)} = 0$

Probability of sufficiency: $P(Y_{do(\mathbf{C}=1)} = 1|Y = 0, C = 0) = \frac{P(Y_{do(C=1)}=1)-P(Y=1)}{P(Y=0,C=0)} = \frac{1-0.75}{P(Y=1,C=1)} = 1$

Causal representation

- Understanding PNS



we assume $P(Y_{do(C=1)} = 1) = 0.5$ and $P(Y_{do(C=0)} = 0) = 1$.

Now, applying the concept of the probability of sufficiency and necessity, we obtain:

Probability of necessity: $P(Y_{do(C=0)} = 0 | Y = 1, X = 1) = 1$

Probability of sufficiency: $P(Y_{do(C=1)} = 1 | Y = 0, X = 0) = 0.5$

In this example, we can state that variable C has a probability of being a necessary cause.

Causal representation

- How to identify PNS from observational data
  - Exogeneity : X is the cause of Y
  - Monotonicity : Changes on X lead to monotonic changes on Y

Definition 9.2.9 (Exogeneity)
A variable X is said to be exogenous *relative to Y in model M if and only if*

$$\{Y_x, Y_{x'}\} \perp\!\!\!\perp X.$$

Definition 9.2.13 (Monotonicity)
A variable Y is said to be monotonic *relative to variable X in a causal model M if and only if the function $Y_x(u)$ is monotonic in x for all u. Equivalently, Y is monotonic relative to X if and only if*

$$y'_x \wedge y_{x'} = false. \tag{9.20}$$

Causal representation

- How to identify PNS from observational data
  - Exogeneity : X is the cause of Y
  - Monotonicity : Changes on X lead to monotonically changes on Y

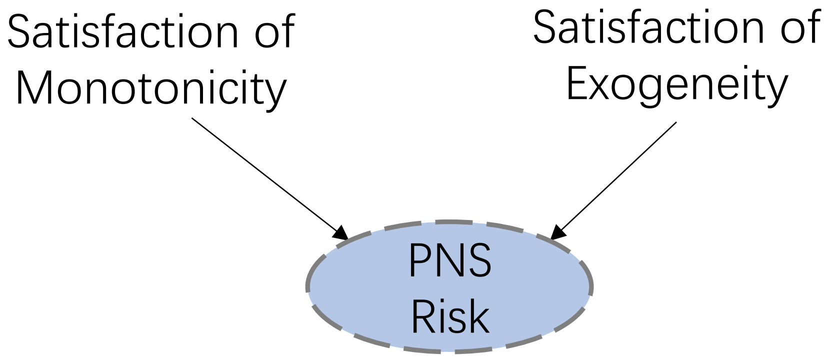
Lemma 2.4 (Pearl (2009)). *If* $\mathbf{C}$ *is exogenous relative to* Y*, and* Y *is monotonic relative to* $\mathbf{C}$*, then*

$$PNS(\mathbf{c}, \bar{\mathbf{c}}) = \underbrace{P_t(Y = y|\mathbf{C} = \mathbf{c})}_{\textit{sufficiency}} - \underbrace{P_t(Y = y|\mathbf{C} = \bar{\mathbf{c}})}_{\textit{necessity}} . \tag{3}$$

The PNS risk modeling

- Defining the PNS risk on test domain

$$R_t(\mathbf{w},\phi,\xi) := \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{T}}\big[\mathbb{E}_{\mathbf{c}\sim P_t(\mathbf{C}|\mathbf{X}=\mathbf{x})}\mathrm{I}[\mathrm{sign}(\mathbf{w}^\top\mathbf{c})\neq y] + \mathbb{E}_{\bar{\mathbf{c}}\sim P_t(\bar{\mathbf{C}}|\mathbf{X}=\mathbf{x})}\mathrm{I}[\mathrm{sign}(\mathbf{w}^\top\bar{\mathbf{c}})=y]\big].$$



- Defining Monotonicity measurement.

$$M_t^{\mathbf{w}}(\phi,\xi) := \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{T}}\mathbb{E}_{\mathbf{c}\sim P_t^{\phi}(\mathbf{C}|\mathbf{X}=\mathbf{x})}\mathbb{E}_{\bar{\mathbf{c}}\sim P_t^{\xi}(\bar{\mathbf{C}}|\mathbf{X}=\mathbf{x})}\mathrm{I}[\mathrm{sign}(\mathbf{w}^\top\mathbf{c})=\mathrm{sign}(\mathbf{w}^\top\bar{\mathbf{c}})],$$

then we have

$$R_t(\mathbf{w},\phi,\xi) = M_t^{\mathbf{w}}(\phi,\xi) + 2SF_t(\mathbf{w},\phi)NC_t(\mathbf{w},\xi) \leq M_t^{\mathbf{w}}(\phi,\xi) + 2SF_t(\mathbf{w},\phi).$$

Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Satisfaction of Monotonicity

- Connecting the Monotonicity measurement with PNS risk

$$M_t^{\mathbf{w}}(\phi,\xi) = SF_t(\mathbf{w},\phi)(1-NC_t(\mathbf{w},\xi)) + (1-SF_t(\mathbf{w},\phi))NC_t(\mathbf{w},\xi). \tag{14}$$

The following equation understands the above decomposition.

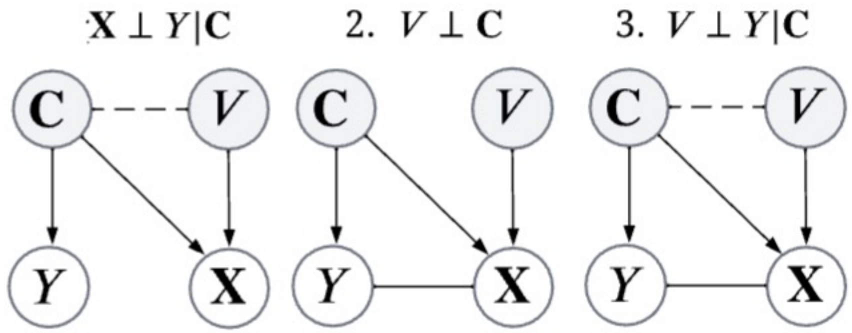
$$\begin{aligned} &P(\text{sign}(\mathbf{w}^\top \mathbf{c}) = \text{sign}(\mathbf{w}^\top \bar{\mathbf{c}})) \\ =&P(\text{sign}(\mathbf{w}^\top \mathbf{c}) = y)P(\text{sign}(\mathbf{w}^\top \bar{\mathbf{c}}) = y) + P(\text{sign}(\mathbf{w}^\top \mathbf{c}) \neq y)P(\text{sign}(\mathbf{w}^\top \bar{\mathbf{c}}) \neq y). \end{aligned} \tag{15}$$

We can further derive Eq.14 as follows.

$$\begin{aligned} M_t^{\mathbf{w}}(\phi,\xi) =& SF_t(\mathbf{w},\phi)(1-NC_t(\mathbf{w},\xi)) + (1-SF_t(\mathbf{w},\phi))NC_t(\mathbf{w},\xi) \\ =& \underbrace{SF_t(\mathbf{w},\phi) + NC_t(\mathbf{w},\xi)}_{R_t(\mathbf{w},\phi,T)} - 2SF_t(\mathbf{w},\phi)NC_t(\mathbf{w},\xi) \\ =& R_t(\mathbf{w},\phi,\xi) - 2SF_t(\mathbf{w},\phi)NC_t(\mathbf{w},\xi). \end{aligned} \tag{16}$$

Satisfaction of Exogeneity

- Exogeneity under different causal assumption
  - 1. C contain all information of Y in X
  - 2. There are no spurious correlation between causal information and domain knowledge
  - 3. C contain not all information of Y in X



Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Satisfaction of Exogeneity

- Exogeneity under different causal assumption
  - 1. PNS Risk can directly satisfies exogeneity
  - 2. Additional constraint of independency between V and C like MMD
  - 3. Additional constraint of conditional independence is required like IRM constraint.

Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Generalization analysis

- PNS risk defined on unknown test domain

$$R_t(\mathbf{w}, \phi, \xi) := \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{T}}\big[\mathbb{E}_{\mathbf{c}\sim P_t(\mathbf{C}|\mathbf{X}=\mathbf{x})}\mathrm{I}[\mathrm{sign}(\mathbf{w}^\top\mathbf{c}) \neq y] \\ +\mathbb{E}_{\bar{\mathbf{c}}\sim P_t(\bar{\mathbf{C}}|\mathbf{X}=\mathbf{x})}\mathrm{I}[\mathrm{sign}(\mathbf{w}^\top\bar{\mathbf{c}}) = y]\big].$$

- Connecting source domain and test domain

Theorem 3.2. *The risk on the test domain is bounded by the risk on the source domain, i.e.,*

$$R_t(\mathbf{w}, \phi, \xi) \leq \lim_{k\to+\infty} \beta_k(\mathcal{T}\|\mathcal{S})([M_s^{\mathbf{w}}(\phi, \xi)]^{1-\frac{1}{k}} + 2[SF_s(\mathbf{w}, \phi)]^{1-\frac{1}{k}}) + \eta_{t\backslash s}(\mathbf{X}, Y),$$

where

$$\eta_{t\backslash s}(\mathbf{X}, Y) := P_t(\mathbf{X}\times Y \notin \mathrm{supp}(\mathcal{S})) \cdot \sup R_{t\backslash s}(\mathbf{w}, \phi, \xi).$$

Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Generalization analysis

- Using dataset from source domain to evaluate the risk

(1) $|SF_s(\mathbf{w},\phi) - \widehat{SF}_s(\mathbf{w},\phi)|$ *is upper bounded by*

$$\mathbb{E}_{\mathcal{S}^n}\mathrm{KL}(\hat{P}_s^{\phi}(\mathbf{C}|\mathbf{X}=\mathbf{x})\|\pi_{\mathbf{C}}) + \frac{\ln(n/\epsilon)}{2(n-1)} + C.$$

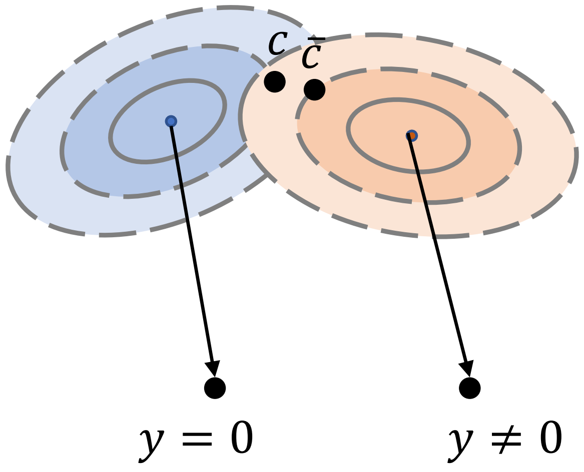
(2) $|M_s^{\mathbf{w}}(\phi,\xi) - \widehat{M}_s^{\mathbf{w}}(\phi,\xi)|$ *is upper bounded by*

$$\mathbb{E}_{\mathcal{S}^n}\mathrm{KL}(\hat{P}_s^{\phi}(\mathbf{C}|\mathbf{X}=\mathbf{x})\|\pi_{\mathbf{C}}) + \mathbb{E}_{\mathcal{S}^n}\mathrm{KL}(\hat{P}_s^{\xi}(\bar{\mathbf{C}}|\mathbf{X}=\mathbf{x})\|\pi_{\bar{\mathbf{C}}}) + \frac{\ln(n/\epsilon)}{2(n-1)} + 2C.$$

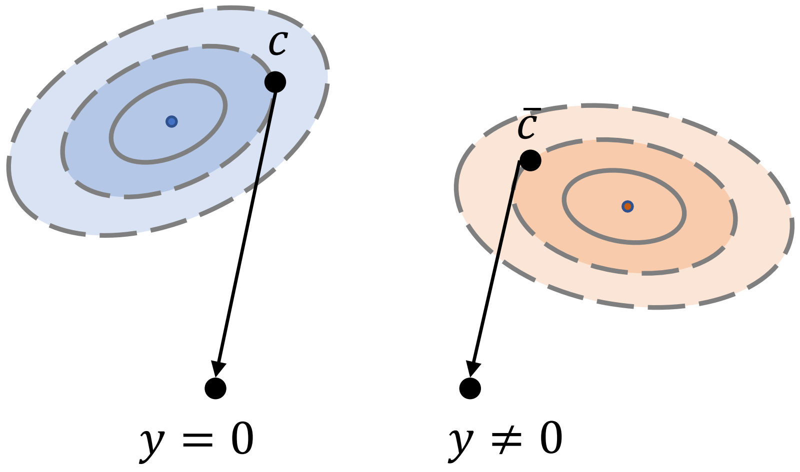
Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Optimization process

- Consider the failure case of learned PNS
  - The small perturbation induce changes on prediction



Failure case



Sematic separatable case

Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Optimization process

- Consider the failure case of learned PNS
  - Under the case of Sematic separatable, It is worth to evaluate PNS risk

Assumption 4.1 (δ-Semantic Separability). For any domain index $d \in \{s, t\}$, the variable $\mathbf{C}$ is δ-semantic separable, if for any $\mathbf{c} \sim P_d(\mathbf{C}|Y = y)$ and $\bar{\mathbf{c}} \sim P_d(\mathbf{C}|Y \neq y)$, the following inequality holds almost surely: $\|\bar{\mathbf{c}} - \mathbf{c}\|_2 > \delta$.

  - When Sematic separatable satisfies in data, then we should add additional constraint on representation avoid to learn trivial PNS.

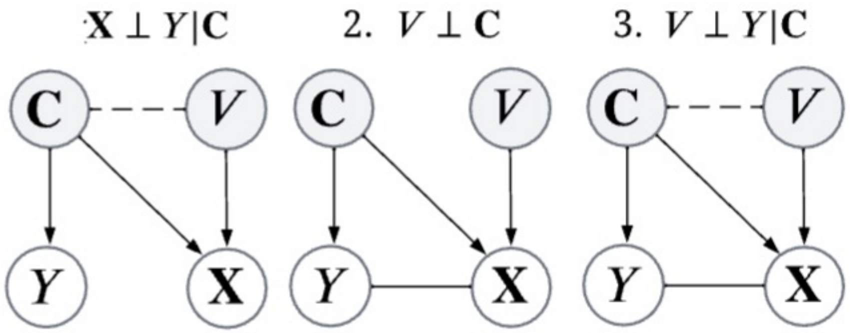
Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Optimization process

- Final objective

$$\min_{\phi,\mathbf{w}} \max_{\xi} \quad \widehat{M}_s^{\mathbf{w}}(\phi,\xi) + \widehat{SF}_s(\mathbf{w},\phi) + \lambda L_{\mathrm{KL}}, \quad \text{subject to} \quad \|\mathbf{c} - \bar{\mathbf{c}}\|_2 > \delta,$$

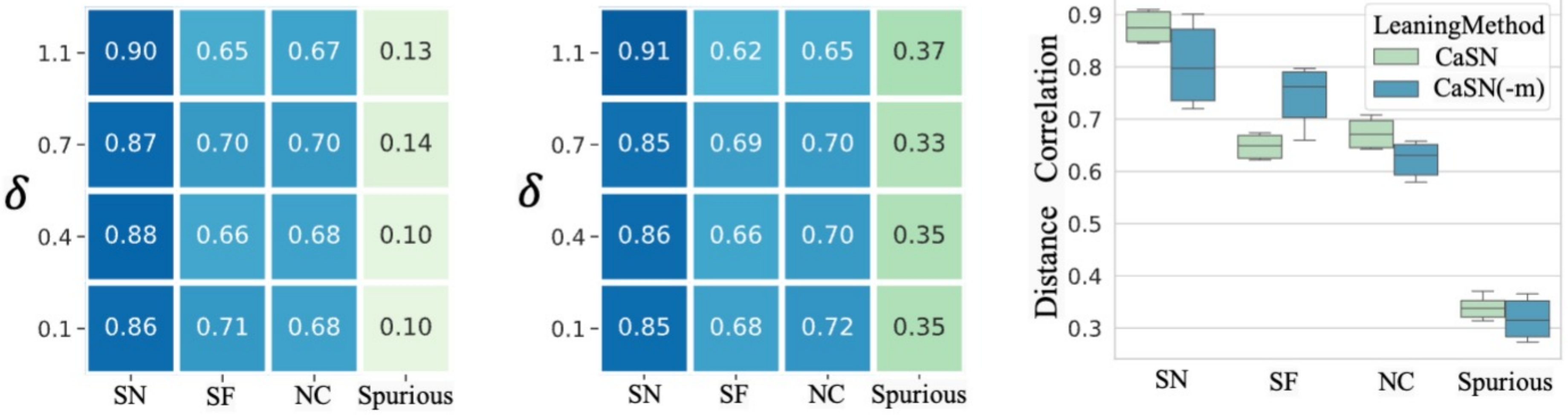
- For different causal assumption we need to add additional constraint



Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Experiment

- Can we learn the sufficient and necessary causes?



(a) Spurious degree $s = 0.1$ (b) Spurious degree $s = 0.7$ (c) Results of CaSN and the CaSN(-m)

Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Experiment

- The OOD generalization ability

Table 1: Results on PACS and VLCS dataset

Dataset			**PACS**						**VLCS**			
Algorithm	**A**	**C**	**P**	**S**	**Avg**	**Min**	**C**	**L**	**S**	**V**	**Avg**	**Min**
ERM	84.7 $\pm$ 0.4	80.8 $\pm$ 0.6	97.2 $\pm$ 0.3	79.3 $\pm$ 1.0	85.5	79.3	97.7 $\pm$ 0.4	64.3 $\pm$ 0.9	73.4 $\pm$ 0.5	74.6 $\pm$ 1.3	77.5	64.3
IRM	84.8 $\pm$ 1.3	76.4 $\pm$ 1.1	96.7 $\pm$ 0.6	76.1 $\pm$ 1.0	83.5	76.4	98.6 $\pm$ 0.1	64.9 $\pm$ 0.9	**73.4** $\pm$ **0.6**	**77.3** $\pm$ **0.9**	78.5	64.9
GroupDRO	83.5 $\pm$ 0.9	79.1 $\pm$ 0.6	96.7 $\pm$ 0.3	78.3 $\pm$ 2.0	84.4	79.1	97.3 $\pm$ 0.3	63.4 $\pm$ 0.9	69.5 $\pm$ 0.8	76.7 $\pm$ 0.7	76.7	63.4
Mixup	86.1 $\pm$ 0.5	78.9 $\pm$ 0.8	**97.6** $\pm$ **0.1**	75.8 $\pm$ 1.8	84.6	78.9	98.3 $\pm$ 0.6	64.8 $\pm$ 1.0	72.1 $\pm$ 0.5	74.3 $\pm$ 0.8	77.4	64.8
MLDG	86.4 $\pm$ 0.8	77.4 $\pm$ 0.8	97.3 $\pm$ 0.4	73.5 $\pm$ 2.3	83.6	77.4	97.4 $\pm$ 0.2	65.2 $\pm$ 0.7	71.0 $\pm$ 1.4	75.3 $\pm$ 1.0	77.2	65.2
MMD	86.1 $\pm$ 1.4	79.4 $\pm$ 0.9	96.6 $\pm$ 0.2	76.5 $\pm$ 0.5	84.6	79.4	97.7 $\pm$ 0.1	64.0 $\pm$ 1.1	72.8 $\pm$ 0.2	75.3 $\pm$ 3.3	77.5	64.0
DANN	86.4 $\pm$ 0.8	77.4 $\pm$ 0.8	97.3 $\pm$ 0.4	73.5 $\pm$ 2.3	83.6	77.4	**99.0** $\pm$ 0.3	65.1 $\pm$ 1.4	73.1 $\pm$ 0.3	77.2 $\pm$ 0.6	**78.6**	65.1
CDANN	84.6 $\pm$ 1.8	75.5 $\pm$ 0.9	96.8 $\pm$ 0.3	73.5 $\pm$ 0.6	82.6	75.5	97.1 $\pm$ 0.3	65.1 $\pm$ 1.2	70.7 $\pm$ 0.8	77.1 $\pm$ 1.5	77.5	65.1
CaSN (base)	**87.1** $\pm$ **0.6**	80.2 $\pm$ 0.6	96.2 $\pm$ 0.8	80.4 $\pm$ 0.2	**86.0**	80.2	97.5 $\pm$ 0.6	64.8 $\pm$ 1.9	70.2 $\pm$ 0.5	76.4 $\pm$ 1.7	77.2	64.8
CaSN (irm)	82.1 $\pm$ 0.3	77.9 $\pm$ 1.8	93.3 $\pm$ 0.8	**80.6** $\pm$ **1.0**	83.5	77.9	97.8 $\pm$ 0.3	65.7 $\pm$ 0.8	72.3 $\pm$ 0.4	77.0 $\pm$ 1.4	78.2	65.7
CaSN (mmd)	84.7 $\pm$ 0.1	**81.4** $\pm$ **1.2**	95.7 $\pm$ 0.2	80.2 $\pm$ 0.6	85.5	**81.4**	98.2 $\pm$ 0.7	**65.9** $\pm$ **0.6**	71.2 $\pm$ 0.3	76.9 $\pm$ 0.7	78.1	**65.9**

Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).

Probable application/Future work

- The scenario which need more stable than accuracy
  - Auto drive
  - OOD generalization
  - Domain adaptation
  - Dynamic system
- Future work
  - More causal assumption
  - More general case

Yang, Mengyue, et al. "Invariant Learning via Probability of Sufficient and Necessary Causes." *arXiv preprint* (NeurIPS2023 Spotlight).