Learning Causal Semantic Representation for out-of-Distribution Prediction

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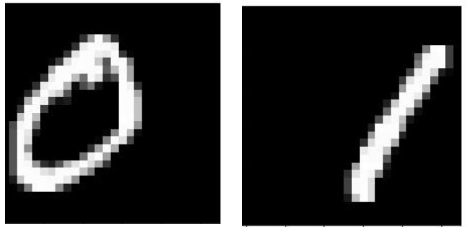
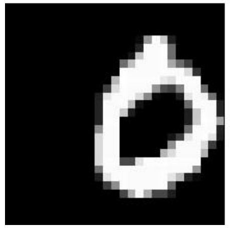
Introduction

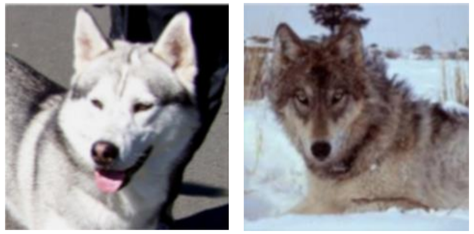
Train:



Test:



Train:



Test:

The problem:

- Deep supervised learning lacks robustness to out-of-distribution (OOD) samples.

Reason behind:

- The learned representation mixes both *semantic factor* s (e.g., shape) and *variation factor* v (e.g., position, background), since both are **correlated** to y.
- But only s **causes** y: intervening v does not change y.

Goal:

- Learning the **causal** representation for OOD prediction.

(a) Husky classified as wolf (b) Explanation

[Ribeiro'16]

Introduction

In this work,

- Causal Semantic Generative model (CSG): describes latent causal structure.
- Methods for OOD prediction (OOD generalization and domain adaptation).
- Theory for identifying the semantic factor and the subsequent benefits for OOD prediction.

Related Work

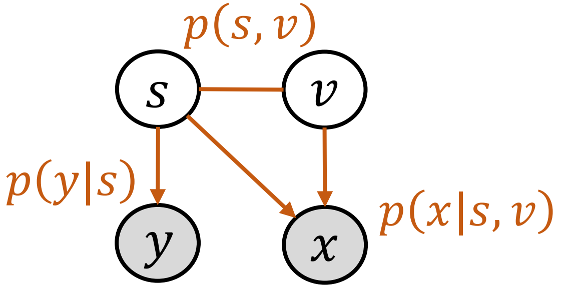
- Domain adaptation/generalization.
  - Based on observation-level causality: not suitable for general data like images.
  - Based on domain-invariant representation: inference invariance; insufficient to identify latent factors.
  - Based on latent generative models: inference invariance; semantic-variation independence; lack of identifiability guarantee.
- Learning disentangled representation.
  - Impossible in unsupervised learning, despite some empirical success.
  - With an auxiliary variable [Khemakhem'20a,b]: require sufficiently many different values of the variable (thus unsuitable for y); no description for domain change.

Related Work

- Generative supervised learning.
  - Few utilized the causal implications of the model.
  - Some aim at estimating causal/treatment effect: not suitable for OOD prediction.
- Causality with latent variables.
  - Most works still focus on the consequence on observation-level causality.
  - Works that identify latent variables do not have semantic-variation split.
- Causal discriminative learning.
  - Lack of identifiability guarantee and structure to capture causal relations.

The Model

- Formal definition of causality:
  "two variables have a causal relation*, if externally intervening the cause (by changing variables out of the considered system) may change the effect, but not* vice versa" [Pearl'09; Peters'17].

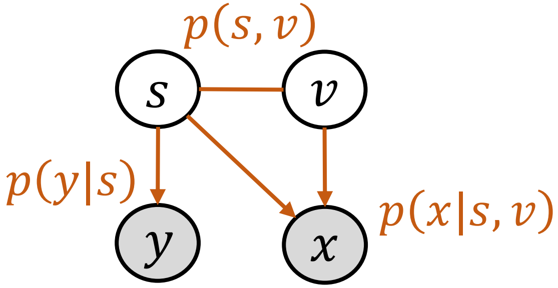


- Causal Semantic Generative (CSG) Model
  - The need of latent variable z: neither $x \to y$ (breaking a camera sensor unit $x \nrightarrow$ label y) nor $y \to x$ (labeling noise $y \nrightarrow$ image x).
    (For labeling process from image x: labelers are doing inference; preference may change from person to person.)
  - $z \to (x, y)$: changing object shape or background z in the scene $\to$ image x, label y; breaking sensor x or labeling noise $y \nrightarrow$ object shape z in the scene.
    (Particularly, different from works with $y \to s$: our y may be a noisy observation.)
  - No x-y edge: attribute all x-y relations to latent factors ("purely common cause", promotes identification) (breaking sensor x / labeling noise y while fixing all factors $z \nrightarrow$ label y / image x).
  - $z = (s, v)$: not all factors *cause* y (changing background $v \nrightarrow$ label y).
  - s-v has a relation, which is often spurious (a desk shape s tends to appear with a workspace background v; a desk shape s can also appear in bedrooms v).
  - Denoted as $p := \langle p_{s,v}, p_{x|s,v}, p_{y|s} \rangle$.

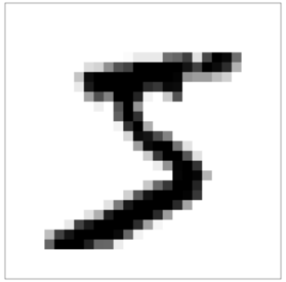
The Model

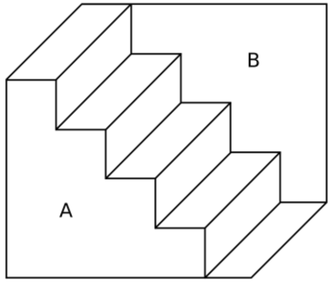
- **Causal invariance** principle:

  Causal mechanisms $p(x|s,v)$ *and* $p(y|s)$ *are domain-invariant, while the prior* $p(s,v)$ *is the handle of intervention for domain shift.*

  - Stems from the *Independent Causal Mechanisms* principle: intervention on $p(s,v)$ does not affect $p(x|s,v)$ and $p(y|s)$.
  - Seemingly variant mechanisms can be explained by including more latent factors.
  - Comparison to **inference invariance**:
    - Domain adapt./gen., invariant risk min.: use a *shared* encoder across domains.
    - In its supportive examples (inferring object position from image, extracting F0 from audio), generative mechanisms are almost deterministic and invertible.
    - When they are not, inference is ambiguous and rely on domain-specific prior.



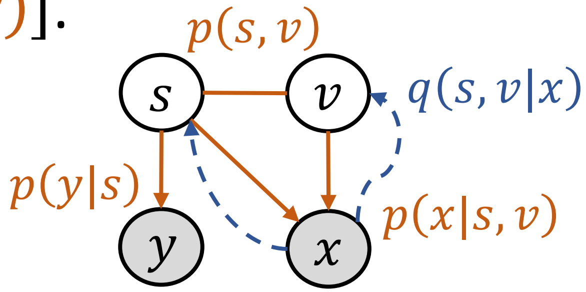


Inference ambiguity in Noisy (“5” or “3”?) and Degenerate (A or B nearer?) generative mechanisms.

Method

$= \int p(s, v) p(x|s, v) p(y|s) \, \mathrm{d}s \mathrm{d}v$ is hard to evaluate.

Fitting training data distribution $p^*(x, y)$ by $\max_p \mathbb{E}_{p^*(x,y)}[\log p(x, y)]$.



- Standard ELBO: using a tractable *inference model* $q(s, v|x, y)$,

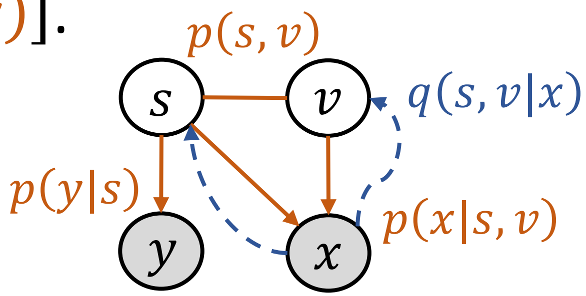
  $$\log p(x, y) \geq \mathcal{L}_{p,q}(x, y) := \mathbb{E}_{q(s,v|x,y)}\left[\log \frac{p(s,v,x,y)}{q(s,v|x,y)}\right].$$

  - $\max_q \mathcal{L}_{p,q}(x, y)$ makes $q(s, v|x, y) \to p(s, v|x, y)$, $\mathcal{L}_{p,q}(x, y) \to \log p(x, y)$.
  - Prediction is still hard: hard to leverage $q(s, v|x, y)$.

Method

$= \int p(s,v)p(x|s,v)p(y|s) \,\mathrm{d}s\mathrm{d}v$ is hard to evaluate.

Fitting training data distribution $p^*(x,y)$ by $\max_p \mathbb{E}_{p^*(x,y)}[\log p(x,y)]$.



- Using a $q(s,v,y|x)$ model:
  - For prediction: ancestral sampling.
  - For learning: $\mathbb{E}_{p^*(x,y)}\left[\mathcal{L}_{p,\, q(s,v|x,y) = q(s,v,y|x) / \int q(s,v,y|x) \,\mathrm{d}s\mathrm{d}v}(x,y)\right]$

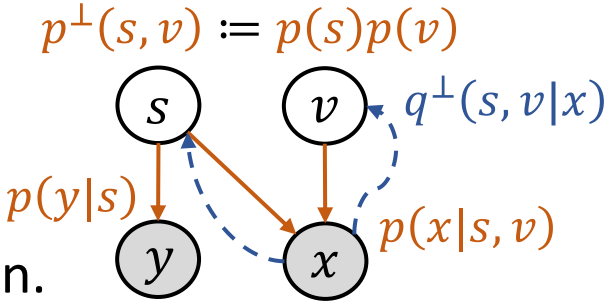
$$= \mathbb{E}_{p^*(x)}\left[\mathbb{E}_{p^*(y|x)}[\log q(y|x)] + \mathbb{E}_{q(s,v,y|x)}\left[\frac{p^*(y|x)}{q(y|x)} \log \frac{p(s,v,x,y)}{q(s,v,y|x)}\right]\right].$$

  - First term = (negative) cross-entropy: makes $q(y|x) \to p^*(y|x)$.
  - Second term $= \mathcal{L}_{p,\, q(s,v,y|x)}(x)$ when $q(y|x) = p^*(y|x)$: makes $q(s,v,y|x) \to p(s,v,y|x)$, $\mathcal{L}_{p,\, q(s,v,y|x)}(x) \to p(x)$.
  - Since $p(s,v,y|x) = p(s,v|x)p(y|s)$, let $q(s,v,y|x) = q(s,v|x)p(y|s)$:

$$\mathcal{L}_{p,\, q(s,v|x,y) = [q(s,v|x),p]}(x,y) = \log q(y|x) + \frac{1}{q(y|x)} \mathbb{E}_{q(s,v|x)}\left[p(y|s) \log \frac{p(s,v)p(x|s,v)}{q(s,v|x)}\right].$$

Method

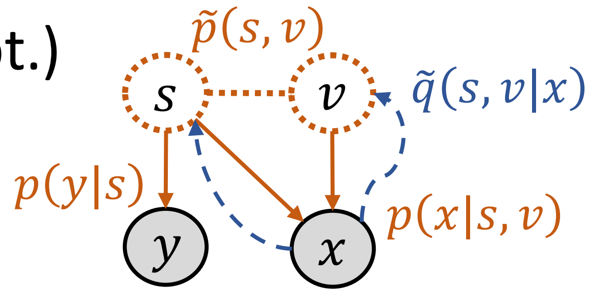
CSG-ind: for prediction in the *unknown* test domain (OOD gen.)



- Use an independent prior $p^\perp(s,v) \coloneqq p(s)p(v)$:
  - Discard the spurious s-v correlation; *defensive* choice.
  - Larger entropy than $p(s,v)$: reduce training-domain-specific information.
  - Randomized experiment by independently soft-intervening s or v.
- Method: avoid two inference models.
  - $q(s,v|x)$ is required for training, and $q^\perp(s,v|x)$ is required for prediction.
  - Avoid $q(s,v|x)$ model: let $q(s,v|x) = \frac{p(s,v)}{p^\perp(s,v)} \frac{p^\perp(x)}{p(x)} q^\perp(s,v|x)$.
  - Following the relation b/w their targets, s.t. $q(s,v|x)$ achieves its target once $q^\perp(s,v|x)$ does.

    $$\mathcal{L}_{p,\,q(s,v|x,y)=[q^\perp(s,v|x),p]}(x,y)$$
    $$= \log \pi(y|x) + \frac{1}{\pi(y|x)} \mathbb{E}_{q^\perp(s,v|x)}\left[\frac{p(s,v)}{p^\perp(s,v)} p(y|s) \log \frac{p^\perp(s,v)p(x|s,v)}{q^\perp(s,v|x)}\right],$$
    where $\pi(y|x) \coloneqq \mathbb{E}_{q^\perp(s,v|x)}\left[\frac{p(s,v)}{p^\perp(s,v)} p(y|s)\right]$.
  - Prediction: $p^\perp(y|x) \approx \mathbb{E}_{q^\perp(s,v|x)}[p(y|s)]$.

Method



CSG-DA: for prediction in test domain with unsupv. data (dom. adapt.)

- Learn the test-domain prior $\tilde{p}(s, v)$ by fitting $\tilde{p}^*(x)$:

  $$\log \tilde{p}(x) \geq \mathcal{L}_{\tilde{p}, \tilde{q}}(x) := \mathbb{E}_{\tilde{q}(s, v|x)}\left[\log \frac{\tilde{p}(s,v)p(x|s, v)}{\tilde{q}(s, v|x)}\right].$$

- Prediction: $\tilde{p}(y|x) \approx \mathbb{E}_{\tilde{q}(s,v|x)}[p(y|s)]$.
- On the training domain: avoid two inference models.
  - Let $q(s, v|x) = \frac{\tilde{p}(x)}{p(x)} \frac{p(s,v)}{\tilde{p}(s,v)} \tilde{q}(s, v|x)$:

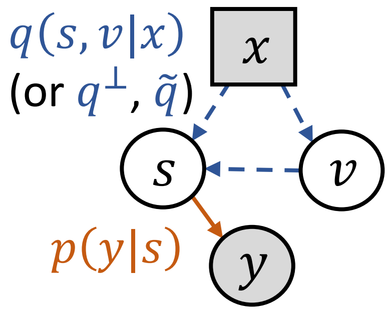
    $$\mathcal{L}_{p,\, q(s, v|x, y) = [\tilde{q}(s, v|x), p]}(x, y)$$
    $$= \log \pi(y|x) + \frac{1}{\pi(y|x)} \mathbb{E}_{\tilde{q}(s, v|x)}\left[\frac{p(s,v)}{\tilde{p}(s,v)} p(y|s) \log \frac{\tilde{p}(s,v)p(x|s, v)}{\tilde{q}(s, v|x)}\right],$$

    where $\pi(y|x) = \mathbb{E}_{\tilde{q}(s, v|x)}\left[\frac{p(s,v)}{\tilde{p}(s,v)} p(y|s)\right]$.

Method

Implementation details.

- Instantiating the model by parsing a general discriminative model:
  - In CSG, $y \perp (x, v) | s$, so no $v \to y$. We then have $p(y|s)$.
  - In CSG, $s \not\perp v \mid x$, so let $v \to s$. We then have $q(s, v|x)$.
  - Use an additional model for $p(x|s, v)$.



(computation direction)

- Implementing the prior.
  - Multivariate Gaussian: $p(s, v) = \mathcal{N}\left(\begin{pmatrix} s \\ v \end{pmatrix} \middle| \begin{pmatrix} \mu_s \\ \mu_v \end{pmatrix}, \Sigma = \begin{pmatrix} \Sigma_{ss} & \Sigma_{sv} \\ \Sigma_{vs} & \Sigma_{vv} \end{pmatrix}\right)$ (no causal direction).
  - Parameterize $\Sigma = LL^\top, L = \begin{pmatrix} L_{ss} & 0 \\ M_{vs} & L_{vv} \end{pmatrix}$ (L_{ss}, L_{vv} are lower-triangular with positive diagonals).
  - $p(v|s) = \mathcal{N}(v | \mu_{v|s}, \Sigma_{v|s})$, where $\mu_{v|s} = \mu_v + M_{vs} L_{ss}^{-1}(s - \mu_s)$, $\Sigma_{v|s} = L_{vv} L_{vv}^\top$.
- Model selection.
  - Use a validation set from the training domain.
  - For CSG-ind/DA, use $p(y|x) \propto \pi(y|x)$ for evaluating validation accuracy.

Theory

Identifiability on the training domain.

- **Definition** (semantic-identification). A learned CSG p is said to be *semantic-identified*, if there exists a homeomorphism Φ on $\mathcal{S} \times \mathcal{V}$, s.t.: (i) $\Phi^{\mathcal{S}}(s, v)$ is constant of v, and (ii) Φ is a *reparameterization* for the ground-truth CSG p^*:
$\Phi_\#\left[p^*_{s,v}\right] = p_{s,v}, p^*(x|s, v) = p(x|\Phi(s, v)), p^*(y|s) = p\left(y\middle|\Phi^{\mathcal{S}}(s)\right).$
  - Reparameterization: describes the degree of freedom given $p(x, y) = p^*(x, y)$.
  - v-constancy: Φ is *semantic-preserving* (the learned s holds equivalent info. to ground-truth).
  - **Proposition**: equivalent relation if $\mathcal{V}$ is connected and is either open or closed in $\mathbb{R}^{d_\mathcal{V}}$.

- Related concepts:
  - Neither sufficient nor necessary to **statistical independence**.
  - Weaker than **disentanglement**: the learned v can be entangled with ground-truth s.

Theory

Identifiability on the training domain.

Assumptions.

- (**A1**)[*additive noise*] There exist functions f and g with bounded derivatives up to 3rd-order, and indep. r.v.s μ and ν, s.t.:
  $p(x|s,v) = p_\mu\big(x - f(s,v)\big)$, and
  $p(y|s) = p_\nu\big(y - g(s)\big)$ for continuous y or $\mathrm{Cat}\big(y|g(s)\big)$ for categorical y.
  - Required to disable the anti-causal direction.
  - Excludes GAN, flow-based models.
- (**A2**)[*bijectivity*] f is bijective and g is injective.
  - A common sufficient condition for the fundamental requirement of causal minimality. (Otherwise, s and v are allowed to have dummy dimensions.)
  - The manifold hypothesis relaxes f to be injective, and allows $d_\mathcal{S} + d_\mathcal{V} < d_\mathcal{X}$.

Theory

Identifiability on the training domain.

- **Theorem** (semantic-identifiability). With A1 and A2, a CSG p is *semantic-identified*, if it is well-learned s.t. $p(x, y) = p^*(x, y)$, under the conditions that $\log p(s, v)$ and $\log p^*(s, v)$ are bounded up to the 2nd-order, and that:
  (i) $\frac{1}{\sigma_\mu^2} \to \infty$, where $\sigma_\mu^2 \coloneqq \mathbb{E}[\mu^\top \mu]$, **or**
  (ii) p_μ has an a.e. non-zero characteristic function (e.g., a Gaussian distribution).
  - (**Appropriate condition**) One cannot identify s in *extreme cases* (all “0”’s are on the left and all “1”’s are on the right): excluded by the condition on $\log p^*(s, v)$.
  - (**Intuition**) In other cases, v for each s is diverse, so mixing s with v worsens training accuracy.
  - Condition (i) requires a *strong* causal mechanism: nearly deterministic and invertible. Condition (ii) covers more than inference invariance.
  - Does not contradict the impossibility result of disentanglement [Locatello’19]: only identify s as a whole; asymmetry from missing $v \to y$.

Theory

Benefit for OOD generalization.

- The test-domain ground-truth CSG $\tilde{p}^* = \langle \tilde{p}^*_{s,v}, p^*_{x|s,v}, p^*_{y|s} \rangle$ (from causal invariance).
- **Theorem** (OOD generalization error) With A1 and A2, for a *semantic-identified* CSG p from the training domain, we have up to $O(\sigma_\mu^4)$,
  $\mathbb{E}_{\tilde{p}^*(x)} \left\| \mathbb{E}[y|x] - \widetilde{\mathbb{E}}^*[y|x] \right\|_2^2 \leq \sigma_\mu^4 B'^4_{f^{-1}} B'^2_g \mathbb{E}_{\tilde{p}_{s,v}} \left\| \nabla \log(\tilde{p}_{s,v} / p_{s,v}) \right\|_2^2$,
  where $B'_{f^{-1}}$, B'_g bounds the Jacobian 2-norms of f^{-1}, g, and $\tilde{p}_{s,v} \coloneqq \Phi_\# [\tilde{p}^*_{s,v}]$.
  - When the causal mechanism $p(x|s,v)$ is strong, the bound is small.
  - $\mathbb{E}_{\tilde{p}_{s,v}} \left\| \nabla \log(\tilde{p}_{s,v} / p_{s,v}) \right\|_2^2$: Fisher-Divergence$(\tilde{p}_{s,v} \| p_{s,v})$, "OODness" for prediction.
  - $\mathbb{E}_{\tilde{p}_{s,v}} \left\| \nabla \log(\tilde{p}_{s,v} / p_{s,v}) \right\|_2^2$: similar to forward KL$(\tilde{p}_{s,v} \| p_{s,v})$, prefers $p_{s,v}$ to have a large support. $p^\perp_{s,v}$ has a larger support than $p_{s,v}$: CSG-ind tends to have a smaller error bound!

Theory

Benefit for domain adaptation.

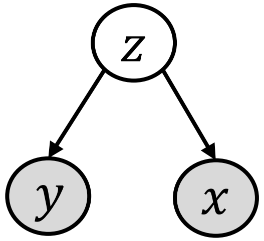
- **Theorem** (domain adaptation error) Under the conditions for identifiability, for a *semantic-identified* CSG p from the training domain, if the test-domain prior $\tilde{p}_{s,v}$ is well-learned s.t. $\tilde{p}_x = \tilde{p}_x^*$, then $\tilde{p}_{s,v} = \Phi_\#\left[\tilde{p}_{s,v}^*\right]$, and $\widetilde{\mathbb{E}}[y|x] = \widetilde{\mathbb{E}}^*[y|x]$, $\forall x \in \mathrm{supp}(\tilde{p}_x^*)$.

Experiments

Baselines:

- For OOD generalization,
  - CE (cross entropy): standard supervised learning.
  - CNBB (ConvNet with Batch Balancing): a causal discriminative method.
- For domain adaptation,
  - DANN, DAN, CDAN, MDD, BNM: classical domain adaptation methods.
- For an ablation study,
  - CSGz (and CSGz-DA): a generative method without separating z as s and v.

CSGz / CSGz-DA



Datasets:

- Shifted MNIST.
  - Training dataset: “0”s are horiz. shifted by $\delta_0 \sim \mathcal{N}(-5,1^2)$ px, “1”s by $\delta_1 \sim \mathcal{N}(5,1^2)$ px.
  - Test datasets: (1) $\delta_0 = \delta_1 = 0$; (2) $\delta_0, \delta_1 \sim \mathcal{N}(0,2^2)$.
- ImageCLEF-DA.
- PACS.

Experiments

OOD generalization

task		CE	CNBB	CSGz	CSG	CSG-ind
Shifted-MNIST	$\delta_0 = \delta_1 = 0$	42.9±3.1	54.7±3.3	53.0±6.7	81.4±7.4	**82.6±4.0**
	$\delta_0, \delta_1 \sim \mathcal{N}(0, 2^2)$	47.8±1.5	59.2±2.4	54.8±5.6	61.7±3.6	**62.3±2.2**
ImageCLEF-DA	**C→P**	65.5±0.3	72.7±1.1	73.3±1.0	73.6±0.6	**74.0±1.3**
	P→C	91.2±0.3	91.7±0.2	91.6±0.9	92.3±0.4	**92.7±0.2**
	I→P	74.8±0.3	75.4±0.6	77.0±0.2	76.9±0.3	**77.2±0.2**
	P→I	83.9±0.1	88.7±0.5	90.4±0.3	90.4±0.3	**90.9±0.2**
PACS	others→**P**	**97.8±0.0**	96.9±0.2	97.7±0.3	97.7±0.2	**97.8±0.2**
	others→**A**	88.1±0.1	73.1±0.3	87.3±0.8	**88.5±0.6**	**88.6±0.6**
	others→**C**	77.9±1.3	50.2±1.2	84.3±0.9	84.4±0.9	**84.6±0.8**
	others→**S**	79.1±0.9	43.3±1.2	80.6±1.4	80.7±1.0	**81.1±1.2**

Domain adaptation

task		DANN	DAN	CDAN	MDD	BNM	CSGz-DA	CSG-DA
Shifted-MNIST	$\delta_0 = \delta_1 = 0$	40.9±3.0	40.4±2.0	41.0±0.5	41.9±0.8	40.8±1.0	78.0±27.2	**97.6±4.0**
	$\delta_0, \delta_1 \sim \mathcal{N}(0, 2^2)$	46.2±0.7	45.6±0.7	46.3±0.6	45.8±0.3	45.7±1.0	68.1±17.4	**72.0±9.2**
ImageCLEF-DA	**C→P**	74.3±0.5	69.2±0.4	74.5±0.3	74.1±0.7	**75.2±1.4**	74.3±0.3	**75.1±0.5**
	P→C	91.5±0.6	89.8±0.4	**93.5±0.4**	92.1±0.6	**93.5±2.8**	92.7±0.4	**93.4±0.3**
	I→P	75.0±0.6	74.5±0.4	76.7±0.3	76.8±0.4	76.7±1.4	77.0±0.3	**77.4±0.3**
	P→I	86.0±0.3	82.2±0.2	90.6±0.3	90.2±1.1	**91.0±0.8**	90.6±0.4	**91.1±0.5**
PACS	others→**P**	97.6±0.2	97.6±0.4	97.0±0.4	97.6±0.3	87.6±4.2	97.6±0.4	**97.9±0.2**
	others→**A**	85.9±0.5	84.5±1.2	84.0±0.9	88.1±0.8	86.4±0.4	88.0±0.8	**88.8±0.7**
	others→**C**	79.9±1.4	81.9±1.9	78.5±1.5	83.2±1.1	83.6±1.7	**84.6±0.9**	**84.7±0.8**
	others→**S**	75.2±2.8	77.4±3.1	71.8±3.9	80.2±2.2	59.1±1.5	80.9±1.2	**81.4±0.8**

More suitable scenarios: diverse v for each s (easier identification) for solving spurious correlation problem.

Thanks!

References

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