ICLR 2024 Spotlight

Improving Domain Generalization with Domain Relations

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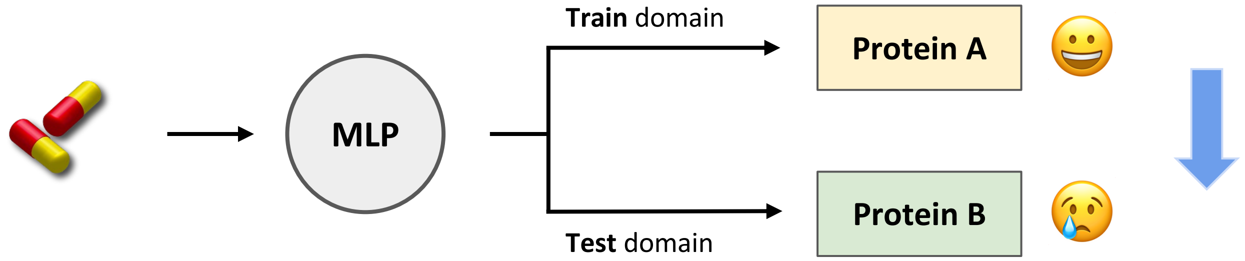
Sangyoon Lee

Motivation

Domain Shift

Applying a trained model to **new domains** (differ from training domains)



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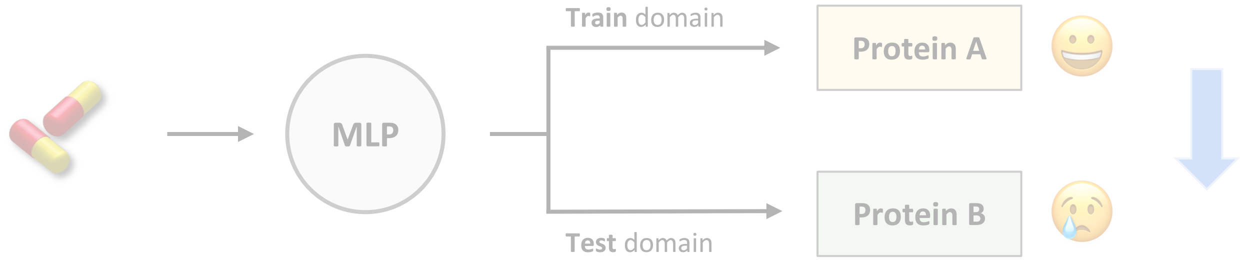


Robust model that can be **generalized** to overall domains.

Motivation

Domain Shift

Prior approach

→ **Single model** that is **domain invariant**

This work ...

Construct a **domain-specific model** for a *new domain* seen at test time.

(1) Model may perform better if they were *specialized to a given domain*.
(2) Different domains can exhibit *strong correlations* with non-general features.

Background

Out-of-Distribution Generalization

Problem: predicting the label $\boldsymbol{y} \in \boldsymbol{\mathcal{Y}}$ based on the input features $\boldsymbol{x} \in \boldsymbol{\mathcal{X}}$

$\boldsymbol{P^{tr}}$: train distribution, $\boldsymbol{P^{ts}}$: test distribution

Traditional Objective = $\arg\min_{\theta \in \Theta} \mathbb{E}_{(x,y)\,\sim \boldsymbol{P^{tr}}}[l(f_\theta(x), y)]$

Distribution shift → $\boldsymbol{P^{tr}} \neq \boldsymbol{P^{ts}}$

This work considers a setting where **overall distribution** is drawn from **a set of domains $\boldsymbol{\mathfrak{D}} = \{\mathbf{1}, \dots, \boldsymbol{D}\}$.**

→ Domain ID of training and test datapoints are available!

Background

Domain Relations and Domain Meta-Data

Key Idea: **Domain Relations** → Domain Shift

Domain meta-data $\mathcal{M} = \{m_i\}_{i=1}^{D}$

: depict the distinctive properties of each domain.

Domain relations (Domain Similarity Matrix $\mathcal{A} = \{a_{ij}\}_{i,j=1}^{D}$**)**

: similarity or relatedness between different domains.

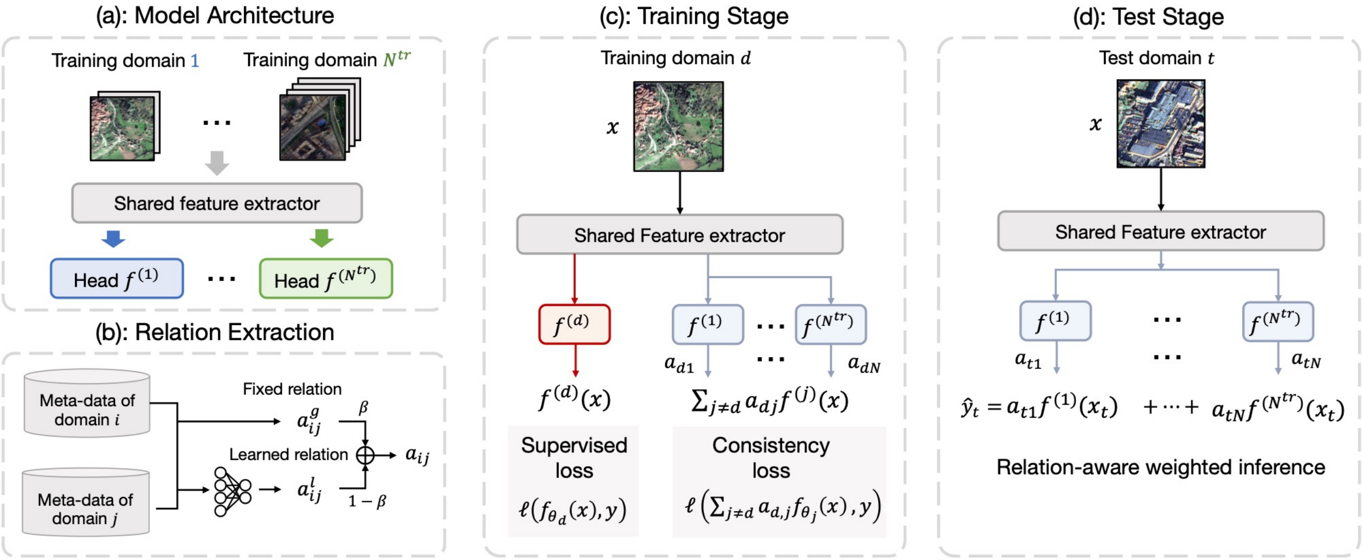
→ strength of the relationship between domains i and j

Method

Leveraging domain distances for out-of-domain generalization

$\boldsymbol{D^3G}$: Leveraging domain distances for out-of-domain generalization

→ improve *out-of-domain generalization* by constructing **domain- specific** models.



Method

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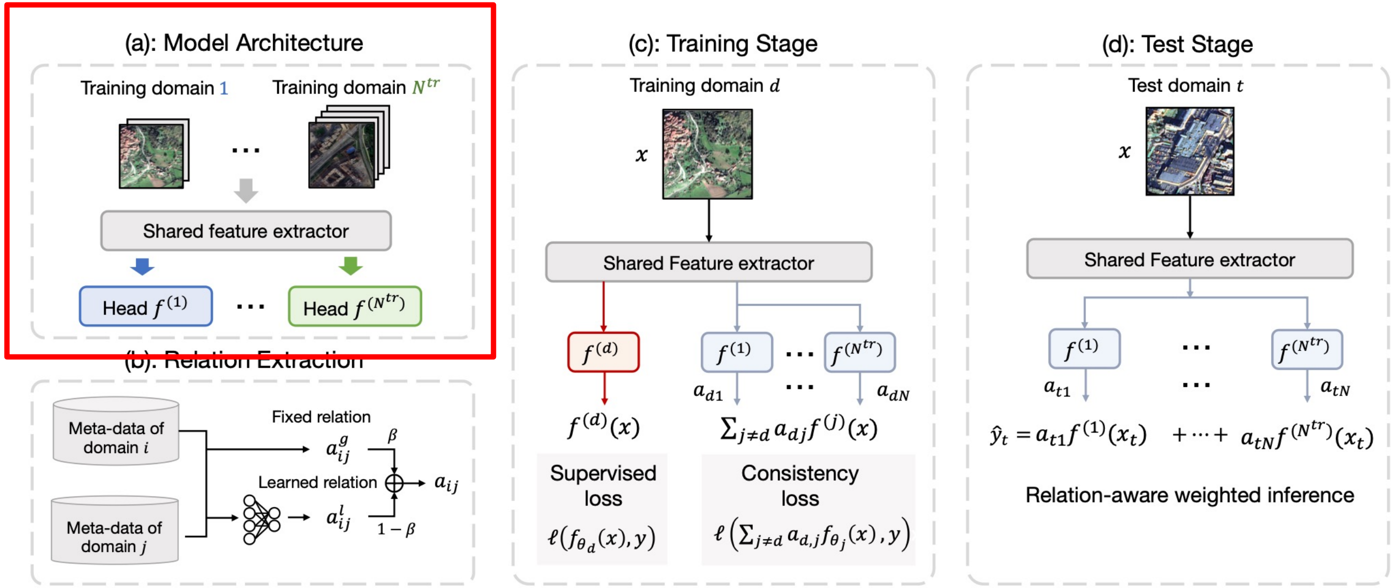

Method

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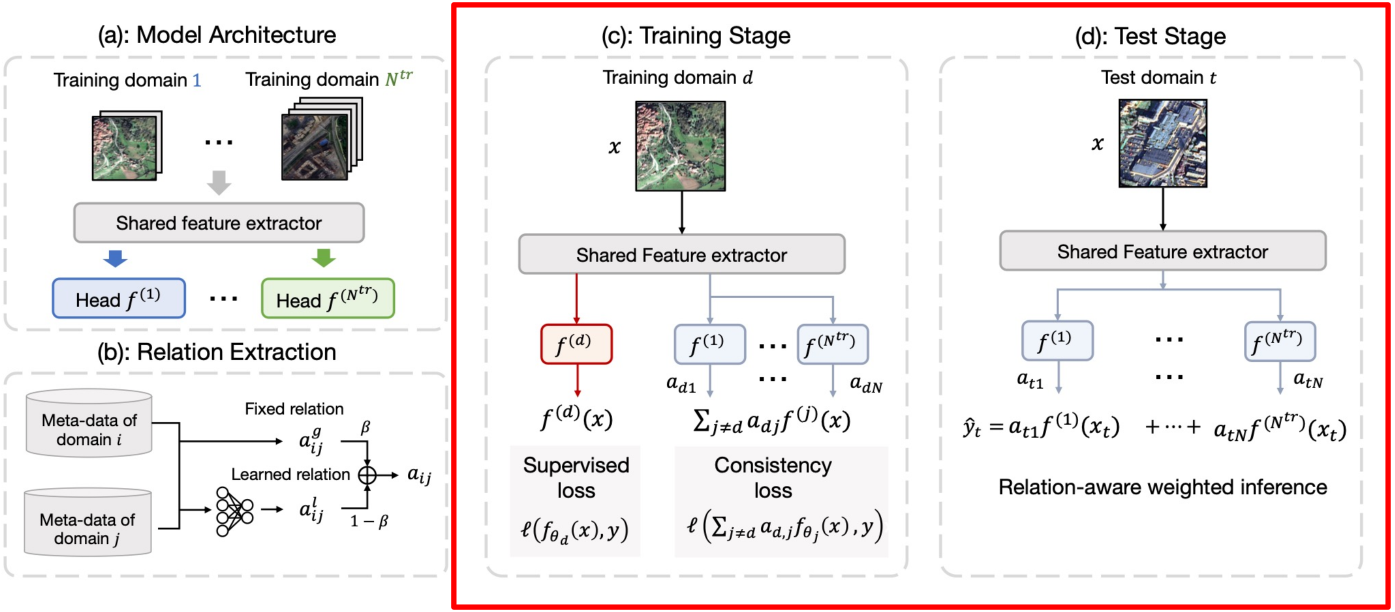

Method

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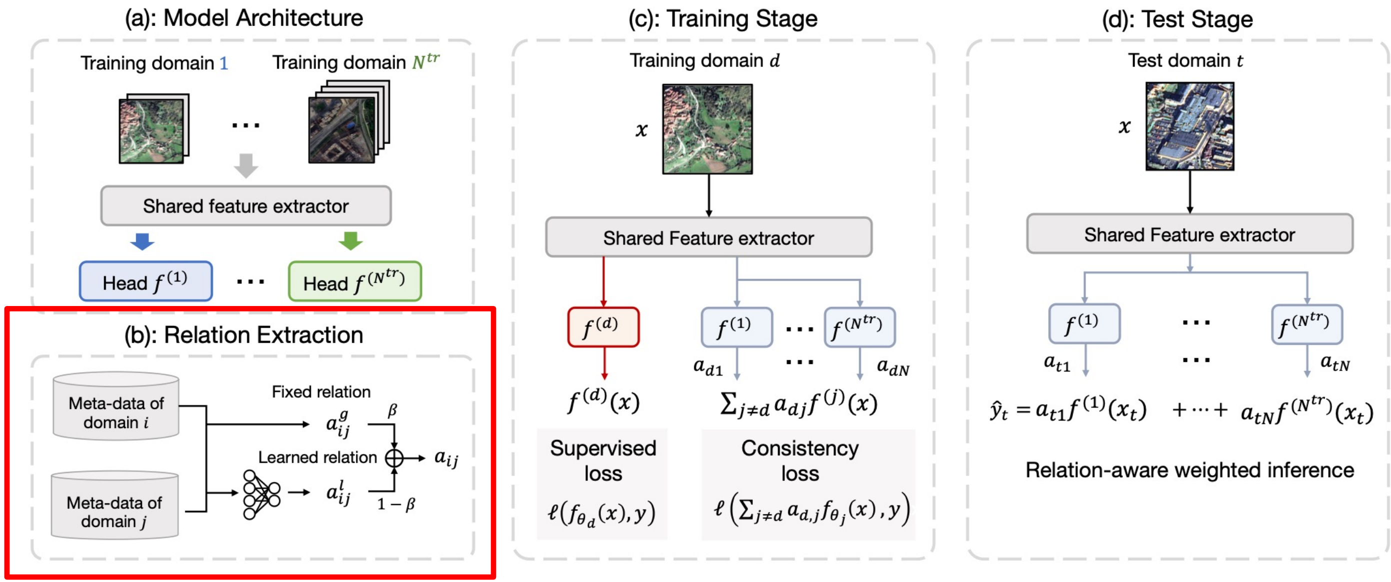


Method

Building Domain-Specific Models

Training Stage.

Multi-headed neural network comprising N^{tr} heads. (N^{tr} : Number of training domains)

Input datapoint (x, y) from domain d → prediction made by d_{th} head : $\boldsymbol{f^{(d)}(x) = h^{(d)}(e(x))}$

Minimizing the **predictivie risk** :

$$\boldsymbol{L_{pred}} = \mathbb{E}_{d\in\mathcal{D}^{tr}}\mathbb{E}_{(x,y)\sim P_d}[l\left(f^{(d)}(x), y\right)].$$

Method

Building Domain-Specific Models

Training Stage. (with limited data)

Difficulties in training *domain-specific predictor*

→ similar domains tend to have similar predictive functions

Relation-aware consistency regularizer

$$\boldsymbol{L_{rel}} = \mathbb{E}_{d \in \mathcal{D}^{tr}} \mathbb{E}_{(x,y) \sim P_d} [l(\frac{\sum_{j=1, j \neq d}^{N^{tr}} a_{dj} f^{(j)}(x)}{\sum_{k=1, k \neq d}^{N^{tr}} a_{dk}}, y)].$$

$$\boldsymbol{L = L_{pred} + \lambda L_{rel}}$$

(1) rely more on predictions made by similar domains

(2) strengthen the relations between predictors and help training predictors for domains with insufficient data

Method

Building Domain-Specific Models

Test Stage.

$\boldsymbol{D^3G}$ constructs test domain-specific models based on the same assumption.

→ similar domains have similar predictive functions.

Prediction $\widehat{\boldsymbol{y}} = \frac{\sum_{d=1}^{N^{tr}} a_{dt} f^{(d)}(x)}{\sum_{k=1}^{N^{tr}} a_{kt}}$

Method

Extracting and Refining Domain Relations

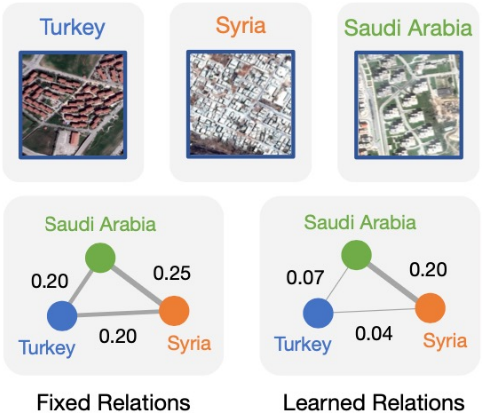
Domain Relations : $\mathcal{A} = \{a_{ij}\}_{i,j=1}^{D}$

→ Derived from **domain meta-data**

How to define?

Domain Relations = **Fixed Relations** + **Learned Relations**

$$a_{ij} = \beta a_{ij}^{g} + (1-\beta) a_{ij}^{l}$$



Method

Extracting and Refining Domain Relations

Fixed relations (directly collecting from domain-meta data)

(1) a relation graph in domain meta-data

(2) pairwise similarity calculated from each domain's meta-data

$\Rightarrow$ a_{ij}^{g}

Learned relations

fixed relations may not fully reflect accurate application-specific domain relation

$$\boldsymbol{a_{ij}^{l}} = \frac{\boldsymbol{1}}{\boldsymbol{R}}\sum_{\boldsymbol{r=1}}^{\boldsymbol{R}} \mathbf{cos}(\boldsymbol{w_r} \odot \boldsymbol{g}(\boldsymbol{m_i}), \boldsymbol{w_r} \odot \boldsymbol{g}(\boldsymbol{m_j}))$$

Algorithm

Training and Test Procedure of D^3G

Algorithm 1 Training and Test Procedure of D^{3}G

Require: Training and test data, relation combining coefficient β, loss balanced coefficient λ, meta-data $\{m_d\}_{d=1}^{D}$ of all domains, learning rate γ

/* *Training stage* */
Initialize all learnable parameters
Extract fixed relations $\{a_{ij}^{g}\}_{i,j=1}^{N^{tr}}$.
while not converge **do**
  Compute learned relations $\{a_{ij}^{l}\}_{i,j=1}^{N^{tr}}$ and obtain the final domain relations by equation 6.
  for each example (x, y, d) **do**
    Calculated supervised loss $\mathcal{L}_{pred}$ by equation 2.
    Computed consistency loss $\mathcal{L}_{rel}$ by equation 3 using domain relations.
  Update learnable parameters with learning rate γ.
/* *Test stage* */
for each test domain t **do**
  Obtain the relations between the test domain and training domains $\{a_{dt}\}_{d=1}^{N^{tr}}$
  for each example (x, y, t) **do**
    Computed the prediction $\hat{y}$ by equation 4.

Algorithm

Training and Test Procedure of D^3G

Algorithm 1 Training and Test Procedure of $\mathrm{D}^3\mathrm{G}$

Require: Training and test data, relation combining coefficient β, loss balanced coefficient λ, meta-data $\{m_d\}_{d=1}^{D}$ of all domains, learning rate γ

```
/* Training stage                                                                   */
Initialize all learnable parameters
Extract fixed relations {a^g_ij}_{i,j=1}^{N^tr}.
while not converge do
    Compute learned relations {a^l_ij}_{i,j=1}^{N^tr} and obtain the final domain relations by equation 6.
    for each example (x, y, d) do
        Calculated supervised loss L_pred by equation 2.
        Computed consistency loss L_rel by equation 3 using domain relations.
    Update learnable parameters with learning rate γ.
/* Test stage                                                                       */
for each test domain t do
    Obtain the relations between the test domain and training domains {a_dt}_{d=1}^{N^tr}
    for each example (x, y, t) do
        Computed the prediction ŷ by equation 4.
```

$$\boldsymbol{a_{ij}^l = \frac{1}{R}\sum_{r=1}^{R} \cos(w_r \odot g(m_i), w_r \odot g(m_j))}$$

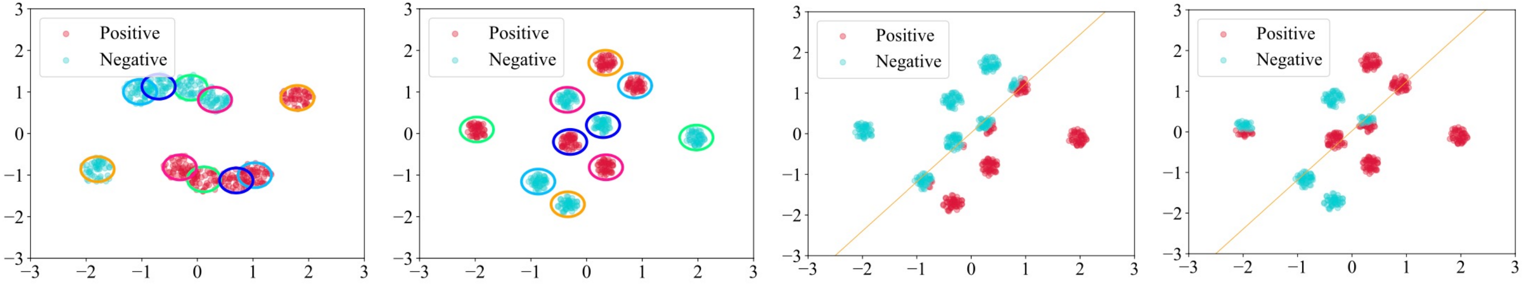
$$\boldsymbol{a_{ij} = \beta a_{ij}^g + (1-\beta) a_{ij}^l}$$

$$\boldsymbol{L = L_{pred} + \lambda L_{rel}}$$

$$\hat{\boldsymbol{y}} = \frac{\sum_{d=1}^{N^{tr}} a_{dt} f^{(d)}(x)}{\sum_{k=1}^{N^{tr}} a_{kt}}$$

Experiments

Illustrative Toy Task



(a) Training Distribution (b) Test Distribution (c) GroupDRO (d) D^{3}G

Model	ERM	GroupDRO	IRM	IB-IRM	IB-ERM	V-REx	DANN	CORAL
Accuracy	44.0%	47.7%	43.9%	45.4%	43.1%	44.0%	43.1%	43.5%
Model	MMD	RSC	CAD	SelfReg	Mixup	LISA	MAT	RaMoE
Accuracy	41.3%	58.2%	43.3%	40.7%	41.3%	47.4%	39.6%	53.7%
Model	mDSDI	AFFAR	GRDA	DRM	LLE	DDN	TRO	**D^{3}G (ours)**
Accuracy	45.2%	58.2%	59.5%	61.4%	58.8%	<u>66.2%</u>	56.3%	**77.5%**

Experiments

Performance between D^3G and other baselines

	TPT-48 (MSE ↓)		FMoW (Worst Acc. ↑)		ChEMBL-STRING (ROC-AUC ↑)	
	N (24) → S (24)	E (24) → W (24)	FMoW-Asia	FMoW-WILDS	$\text{PPI}_{>50}$	$\text{PPI}_{>100}$
	Region Shift	Region Shift	Region Shift	Region-Time Shift	Protein Shift	Protein Shift
ERM	0.445 ± 0.029	0.328 ± 0.033	26.05 ± 3.84%	34.87 ± 0.41%	74.11 ± 0.35%	71.91 ± 0.24%
GroupDRO	0.413 ± 0.045	0.434 ± 0.082	26.24 ± 1.85%	31.16 ± 2.12%	73.98 ± 0.25%	71.55 ± 0.59%
IRM	0.429 ± 0.043	0.262 ± 0.034	25.02 ± 2.38%	32.54 ± 1.92%	52.71 ± 0.50%	51.73 ± 1.54%
IB-IRM	0.416 ± 0.009	0.272 ± 0.026	26.30 ± 1.51%	34.94 ± 1.38%	52.12 ± 0.91%	52.33 ± 1.06%
IB-ERM	0.458 ± 0.032	0.273 ± 0.030	26.78 ± 1.34%	35.52 ± 0.79%	74.69 ± 0.14%	73.32 ± 0.21%
V-REx	0.412 ± 0.042	0.343 ± 0.021	26.63 ± 0.93%	37.64 ± 0.92%	71.46 ± 1.47%	69.37 ± 0.85%
DANN	0.394 ± 0.019	0.515 ± 0.156	25.62 ± 1.59%	33.78 ± 1.55%	73.49 ± 0.45%	72.22 ± 0.10%
CORAL	0.401 ± 0.022	0.283 ± 0.048	25.87 ± 1.97%	36.53 ± 0.15%	75.42 ± 0.15%	73.10 ± 0.14%
MMD	0.409 ± 0.067	0.279 ± 0.026	25.06 ± 2.19%	35.48 ± 1.81%	75.11 ± 0.27%	73.30 ± 0.50%
RSC	0.421 ± 0.040	0.330 ± 0.068	25.73 ± 0.70%	34.59 ± 0.42%	74.83 ± 0.68%	72.47 ± 0.38%
CAD	n/a	n/a	26.13 ± 1.82%	35.17 ± 1.73%	75.17 ± 0.64%	72.92 ± 0.39%
SelfReg	n/a	n/a	24.81 ± 1.77%	37.33 ± 0.87%	75.42 ± 0.42%	72.63 ± 0.71%
Mixup	0.574 ± 0.030	0.357 ± 0.011	26.99 ± 1.27%	35.67 ± 0.53%	74.40 ± 0.54%	71.31 ± 1.06%
LISA	0.467 ± 0.032	0.345 ± 0.014	26.05 ± 2.09%	34.59 ± 1.28%	74.30 ± 0.59%	71.45 ± 0.44%
MAT	0.423 ± 0.027	0.291 ± 0.024	25.92 ± 2.83%	35.07 ± 0.84%	74.73 ± 0.30%	72.07 ± 0.81%
AdaGraph	n/a	n/a	25.91 ± 0.59%	35.42 ± 0.55%	74.02 ± 0.42%	72.10 ± 0.06%
RaMoE	0.372 ± 0.035	0.311 ± 0.060	26.65 ± 0.46%	36.51 ± 0.71%	74.99 ± 0.22%	71.48 ± 0.49%
mDSDI	0.445 ± 0.027	0.315 ± 0.089	25.54 ± 0.46%	36.35 ± 0.45%	75.09 ± 0.47%	71.23 ± 0.69%
ADDAR	0.403 ± 0.061	0.287 ± 0.040	25.87 ± 1.01%	35.77 ± 0.70%	74.55 ± 0.54%	71.93 ± 0.33%
GRDA	0.373 ± 0.040	0.355 ± 0.068	26.57 ± 0.70%	34.41 ± 0.42%	75.01 ± 0.68%	73.57 ± 0.38%
DRM	0.571 ± 0.038	0.557 ± 0.027	25.22 ± 2.33%	36.39 ± 0.76%	74.34 ± 0.48%	72.41 ± 0.76%
LLE	0.603 ± 0.041	0.467 ± 0.047	26.37 ± 1.19%	35.83 ± 1.00%	74.01 ± 0.63%	71.68 ± 0.61%
DDN	0.537 ± 0.024	0.601 ± 0.038	26.77 ± 1.72%	35.13 ± 0.62%	75.17 ± 0.61%	72.71 ± 0.59%
TRO	0.371 ± 0.054	0.281 ± 0.066	26.87 ± 1.26%	37.48 ± 0.55%	74.85 ± 0.27%	72.49 ± 0.36%
D^3G (ours)	**0.342 ± 0.019**	**0.236 ± 0.063**	**28.12 ± 0.28%**	**39.47 ± 0.57%**	**78.67 ± 0.16%**	**77.24 ± 0.30%**

Domain-invariant learning approaches

Domain-specific learning approaches

Conclusion

Contributions

1) Novel method called $\boldsymbol{D^3G}$

2) Leverages the connections between different domains & employs **a domain-relationship aware weighting** system

(With **domain meta-data**)

3) Evaluate the **effectiveness** of $\boldsymbol{D^3G}$

Q&A

Out-of-distribution Generalization

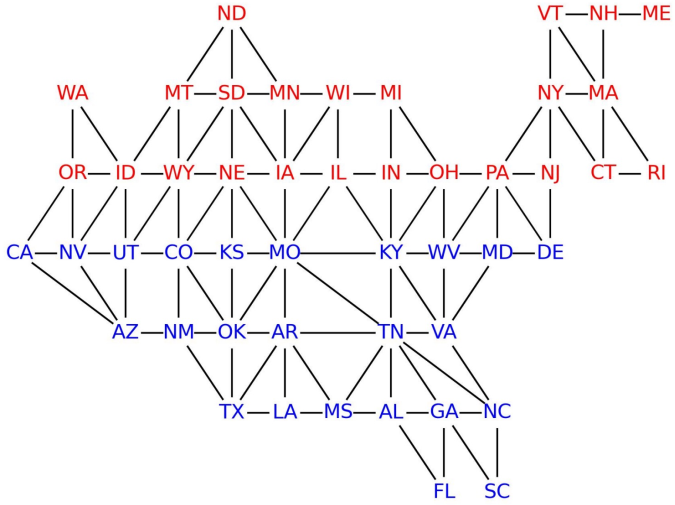
Previous works

(1) minimizing the divergence of feature distributions

(2) generating more domains and enhancing the consistency among representations

(3) find a predictor that is invariant across domains by imposing an explicit regularizer

Appendix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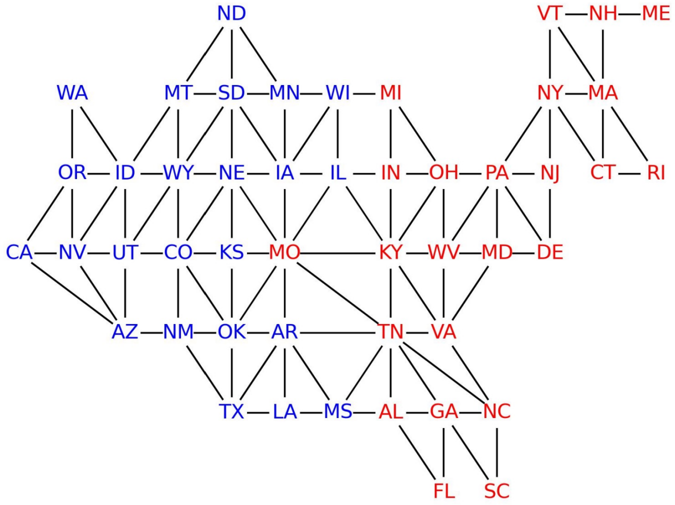
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Appendix

Table 10: Comparison of using different relations. The results on FMoW and ChEMBL-STRING are reported. In this case, when no relations are used, we take the average of predictions across all domains.

Fixed relations	Learned relations	FMoW (Worst Acc. ↑) FMoW-Asia	FMoW-WILDS	ChEMBL-STRING (ROC-AUC ↑) $\text{PPI}_{>50}$	$\text{PPI}_{>100}$
		$26.93 \pm 0.47\%$	$35.32 \pm 0.66\%$	$76.17 \pm 0.21\%$	$73.38 \pm 0.13\%$
✓		$27.43 \pm 0.41\%$	$39.37 \pm 0.34\%$	$77.66 \pm 0.32\%$	$76.59 \pm 0.40\%$
	✓	$21.18 \pm 2.30\%$	$36.41 \pm 1.09\%$	$77.09 \pm 0.94\%$	$75.57 \pm 1.20\%$
✓	✓	$\mathbf{28.12 \pm 0.28\%}$	$\mathbf{39.47 \pm 0.57\%}$	$\mathbf{78.67 \pm 0.16\%}$	$\mathbf{77.24 \pm 0.30\%}$

Table 11: Full results of comparison between D^3G with domain-specific fine-tuning.

Model	FMoW (Worst Acc. ↑) FMoW-Asia	FMoW-WILDS	ChEMBL (ROC-AUC ↑) $\text{PPI}_{>50}$	$\text{PPI}_{>100}$
ERM	$26.05 \pm 3.84\%$	$34.87 \pm 0.41\%$	$74.11 \pm 0.35\%$	$71.91 \pm 0.24\%$
CORAL	$25.87 \pm 1.97\%$	$36.53 \pm 0.15\%$	$75.42 \pm 0.15\%$	$73.10 \pm 0.14\%$
RW-FT	$27.03 \pm 1.03\%$	$36.39 \pm 1.28\%$	$76.31 \pm 0.35\%$	$74.30 \pm 0.40\%$
D^3G	$\mathbf{28.12 \pm 0.28\%}$	$\mathbf{39.47 \pm 0.57\%}$	$\mathbf{78.67 \pm 0.16\%}$	$\mathbf{77.24 \pm 0.30\%}$