

Overview

Unsupervised Domain Adaptation (UDA)

- Train a model on a labeled source sample and an unlabeled target sample.
- Goal: Find a model that performs well on the target domain.

Two Notions of Generalization Errors

- Population-to-population (PP) generalization error: KL based bounds.
- Expected empirical-to-population (EP) generalization error: algorithm-dependent bounds \implies two regularization strategies.

Problem Formulation

Setup

- Source data $Z = (X, Y) \sim \mu$; Target data $Z' = (X', Y') \sim \mu'$; Predictor space $\mathcal{F} = \{f_w : \mathcal{X} \rightarrow \mathcal{Y} | w \in \mathcal{W}\}$
- Source sample: $S = \{Z_i\}_{i=1}^n$; Target sample $S'_{X'} = \{X'_j\}_{j=1}^m$
- Learning algorithm: $\mathcal{A} : \mathcal{Z}^n \times \mathcal{X}^m \rightarrow \mathcal{W}$

Generalization Error

- Population risk of target domain: $R_{\mu'}(w) \triangleq \mathbb{E}_{Z'}[\ell(f_w(X'), Y')]$
- Empirical risk of source domain: $R_S(w) \triangleq \frac{1}{n} \sum_{i=1}^n \ell(f_w(X_i), Y_i)$
- Expected EP error:

$$\text{Err} \triangleq \mathbb{E}_{W, S} [R_{\mu'}(W) - R_S(W)] = \mathbb{E}_{W, S, S'} [R_{\mu'}(W) - R_S(W)]$$

- PP error for w : $\widetilde{\text{Err}}(w) \triangleq R_{\mu'}(w) - R_{\mu}(w)$

Assumptions of the Loss Function

Assumption 1 (Boundedness). $\ell(\cdot, \cdot)$ is bounded in $[0, M]$.

Assumption 2 (Subgaussianity). $\ell(f_w(X), Y)$ is R -subgaussian under μ .

Assumption 3 (Lipschitzness). $\ell(f_w(X), Y)$ is β -Lipschitz continuous i.e., $|\ell(f_w(x_1), y_1) - \ell(f_w(x_2), y_2)| \leq \beta d(z_1, z_2)$ for some metric d on \mathcal{Z} .

Assumption 4 (Triangle and Symmetric). $\ell(\cdot, \cdot)$ satisfies: $\ell(y_1, y_2) = \ell(y_2, y_1)$ and $\ell(y_1, y_2) \leq \ell(y_1, y_3) + \ell(y_3, y_2)$ for any $y_1, y_2, y_3 \in \mathcal{Y}$.

Key Ingredients

Lemma 1 (DV variational formula of KL). $D_{\text{KL}}(Q||P) = \sup_f \mathbb{E}_{\theta \sim Q} [f(\theta)] - \log \mathbb{E}_{\theta \sim P} [\exp f(\theta)]$.

Lemma 2 (KR duality). $\mathbb{W}(P, Q) = \sup_{f \in 1\text{-Lip}(\rho)} \int_{\mathcal{X}} f dP - \int_{\mathcal{X}} f dQ$.

Lemma 3. If $g(\theta)$ is R -subgaussian, then

$$|\mathbb{E}_{\theta \sim Q} [g(\theta')] - \mathbb{E}_{\theta \sim P} [g(\theta)]| \leq \sqrt{2R^2 D_{\text{KL}}(Q||P)}.$$

Bounding PP Error by KL Divergence

Theorem 1. If Assumption 2 holds, then $|\widetilde{\text{Err}}(w)| \leq \sqrt{2R^2 D_{\text{KL}}(\mu' || \mu)}$.

Corollary 1. Let $f_w = g \circ h$ (where $h : \mathcal{X} \rightarrow \mathcal{T}$ and $g : \mathcal{T} \rightarrow \mathcal{Y}$), then

$$R_{\mu}(w) - \sqrt{2R^2 D_{\text{KL}}(\mu' || \mu)} \leq R_{\mu'}(w) \leq R_{\mu}(w) + \sqrt{2R^2 D_{\text{KL}}(\mu' || \mu)}$$

Corollary 2. Assumption 1 $\implies |\widetilde{\text{Err}}(w)| \leq \frac{M}{2} \sqrt{D_{\text{KL}}(\mu || \mu') + D_{\text{KL}}(\mu' || \mu)}$.

Theorem 2. Assumption 4 + $\ell(f_w(X), f_w(X))$ is R -subgaussian $\implies \widetilde{\text{Err}}(w) \leq \sqrt{2R^2 D_{\text{KL}}(P_{X'} || P_X)} + \lambda^*$, where $\lambda^* = \min_{w \in \mathcal{W}} R_{\mu'}(w) + R_{\mu}(w)$.

Bounding PP Error by Wasserstein Distance

Theorem 3. If Assumption 3 holds, then $|\widetilde{\text{Err}}(w)| \leq \beta \mathbb{W}(\mu', \mu)$.

Corollary 3. If Assumption 1 holds and let d be the discrete metric, then

$$|\widetilde{\text{Err}}(w)| \leq M \text{TV}(\mu', \mu) \leq M \sqrt{\min \left\{ \frac{1}{2} D_{\text{KL}}(\mu' || \mu), 1 - e^{-D_{\text{KL}}(\mu' || \mu)} \right\}}$$

Theorem 4. Assumption 4 + $\ell(f_w(X), f_w(X))$ is β -Lipschitz $\implies \widetilde{\text{Err}}(w) \leq \beta \mathbb{W}(P_{X'}, P_X) + \lambda^*$, where $\lambda^* = \min_{w \in \mathcal{W}} R_{\mu'}(w) + R_{\mu}(w)$.

Mutual Information (MI) Bound for EP

Theorem 5. Assume $\ell(f_w(X'), Y')$ is R -subgaussian then

$$|\text{Err}| \leq \underbrace{\frac{1}{nm} \sum_{j=1}^m \sum_{i=1}^n \mathbb{E}_{X'_j} \sqrt{2R^2 I^{X'_j}(W; Z_i)}}_{\text{Generalization error on } \mu} + \underbrace{\sqrt{2R^2 D_{\text{KL}}(\mu' || \mu)}}_{\text{PP error (Theorem 1)}}$$

where $I^{X'_j}(\cdot, \cdot)$ is the disintegrated version of mutual information.

Corollary 4. Let Assumption 1 hold. Then

$$|\text{Err}| \leq \frac{M}{\sqrt{2nm}} \sum_{j=1}^m \sum_{i=1}^n \mathbb{E}_{X'_j} \sqrt{\min \{I^{X'_j}(W; Z_i), L^{X'_j}(W; Z_i)\}} + \frac{M}{\sqrt{2}} \sqrt{\min \{D_{\text{KL}}(\mu || \mu'), D_{\text{KL}}(\mu' || \mu)\}}$$

where $L^{X'_j}(\cdot, \cdot)$ is the disintegrated version of Lautum information.

Stronger Bounds for EP

Theorem 6. Assume ℓ is Lipschitz for both $w \in \mathcal{W}$ and $z \in \mathcal{Z}$, then

$$|\text{Err}| \leq \frac{\beta'}{nm} \sum_{j=1}^m \sum_{i=1}^n \mathbb{E}_{X'_j, Z_i} \mathbb{W}(P_{W|Z_i, X'_j}, P_{W|X'_j}) + \beta \mathbb{W}(\mu, \mu').$$

Further, if Assumption 1 hold. Then

$$\begin{aligned} |\widetilde{\text{Err}}| &\leq \frac{M}{nm} \sum_{j=1}^m \sum_{i=1}^n \mathbb{E}_{X'_j, Z_i} \left[\text{TV}(P_{W|Z_i, X'_j}, P_{W|X'_j}) \right] + M \text{TV}(\mu, \mu') \\ &\leq \frac{1}{nm} \sum_{j=1}^m \sum_{i=1}^n \mathbb{E}_{X'_j, Z_i} \sqrt{\frac{M^2}{2} D_{\text{KL}}(P_{W|Z_i, X'_j} || P_{W|X'_j})} + \sqrt{\frac{M^2}{2} D_{\text{KL}}(\mu || \mu')}. \end{aligned}$$

Applications

Gradient Penalty as an Universal Regularizer

Theorem 7. Consider a “noisy” iterative algorithm for updating W , e.g., SGLD,

$$|\text{Err}| \leq \sqrt{\frac{R^2}{n} \sum_{t=1}^T \frac{\eta_t^2}{\sigma_t^2} \mathbb{E}_{S_{X'}, W_{t-1}, S} \left[\|G_t - \mathbb{E}_{Z_{B_t}} [G_t]\|^2 \right]} + \sqrt{2R^2 D_{\text{KL}}(\mu || \mu')}.$$

Restrict the gradient norm \implies Reduce $|\text{Err}|$!

Controlling Label Information for KL Guided Marginal Alignment

• Nguyen et al. (2022): $D_{\text{KL}}(P_{Y|T} || P_{Y|T}) \leq D_{\text{KL}}(P_{Y|X'} || P_{Y|X})$ if $I(X; Y) = I(T; Y)$.

• $I(X; Y) \neq I(T; Y)$ when ℓ is cross-entropy: $I(X; Y) \geq I(T; Y) = H(Y) - H(Y|T)$.

$$\mathbb{E}_{W, Z_i} [\ell(f_w(T_i), Y_i)] = H(Y_i|T_i) + \mathbb{E}_{T_i, W} [D_{\text{KL}}(P_{Y_i|T_i, W} || Q_{Y_i|T_i, W})] - I(W; Y_i|T_i).$$

Minimizing cross-entropy \Rightarrow Minimizing $H(Y|T)$

• $I^{T_i}(W; Y_i|T_i) \leq \mathcal{O}(\|W - \widetilde{W}\|^2)$: Creating $f_{\widetilde{w}}$ that does not depend on Y .

– Train $f_{\widetilde{w}}$ by pseudo labels of f_w

– Adding $\|W - \widetilde{W}\|^2$ as a regularizer in the training of W .

Experimental Results

Table 1: RotatedMNIST and Digits. Results of baselines are reported from Nguyen et al. (2022).

Method	RotatedMNIST (0° as source domain)					Digits				
	15°	30°	45°	60°	75°	Ave	M \rightarrow U	U \rightarrow M	S \rightarrow M	Ave
ERM	97.5±0.2	84.1±0.8	53.9±0.7	34.2±0.4	22.3±0.5	58.4	73.1±4.2	54.8±6.2	65.9±1.4	64.6
DANN	97.3±0.4	90.6±1.1	68.7±4.2	30.8±0.6	19.0±0.6	61.3	90.7±0.4	91.2±0.8	71.1±0.5	84.3
MMD	97.5±0.1	95.3±0.4	73.6±2.1	44.2±1.8	32.1±2.1	68.6	91.8±0.3	94.4±0.5	82.8±0.3	89.7
CORAL	97.1±0.3	82.3±0.3	56.0±2.4	30.8±0.2	27.1±1.7	58.7	88.0±1.9	83.3±0.1	69.3±0.6	80.2
WD	96.7±0.3	93.1±1.2	64.1±3.3	41.4±7.6	27.6±2.0	64.6	88.2±0.6	60.2±1.8	68.4±2.5	72.3
KL	97.8±0.1	97.1±0.2	93.4±0.8	75.5±2.4	68.1±1.8	86.4	98.2±0.2	97.3±0.5	92.5±0.9	96.0
ERM-GP	97.5±0.1	86.2±0.5	62.0±1.9	34.8±2.1	26.1±1.2	61.2	91.3±1.6	72.7±4.2	68.4±0.2	77.5
KL-GP	98.2±0.2	96.9±0.1	95.0±0.6	88.0±8.1	78.1±2.5	91.2	98.8±0.1	97.8±0.1	93.8±1.1	96.8
KL-CL	98.4±0.2	97.3±0.2	95.6±0.1	83.0±8.2	73.6±4.0	89.6	98.9±0.1	97.7±0.1	93.0±0.3	96.5