
Quantifying and Improving Transferability in Domain Generalization

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Abstract

Out-of-distribution generalization is one of the key challenges when transferring a model from the lab to the real world. Existing efforts mostly focus on building invariant features among source and target domains. Based on invariant features, a high-performing classifier on source domains could hopefully behave equally well on a target domain. In other words, we hope the invariant features to be *transferable*. However, in practice, there are no perfectly transferable features, and some algorithms seem to learn “more transferable” features than others. How can we understand and quantify such *transferability*? In this paper, we formally define transferability that one can quantify and compute in domain generalization. We point out the difference and connection with common discrepancy measures between domains, such as total variation and Wasserstein distance. We then prove that our transferability can be estimated with enough samples and give a new upper bound for the target error based on our transferability. Empirically, we evaluate the transferability of the feature embeddings learned by existing algorithms for domain generalization. Surprisingly, we find that many algorithms are not quite learning transferable features, although few could still survive. In light of this, we propose a new algorithm for learning transferable features and test it over various benchmark datasets, including RotatedMNIST, PACS, Office-Home and WILDS-FMoW. Experimental results show that the proposed algorithm achieves consistent improvement over many state-of-the-art algorithms, corroborating our theoretical findings.¹

1 Introduction

One of the cornerstone assumptions underlying the recent success of deep learning models is that the test data should share the same distribution as the training data. However, faced with ubiquitous distribution shifts in various real-world applications, such assumption hardly holds in practice. For example, a self-driving recognition system trained using data collected in the daytime may continually degrade its performance during nightfall. The system may also encounter weather or traffic conditions in a new city that never appear in the training set. In light of these potentially unseen scenarios, it is

¹Code available at <https://github.com/Gordon-Guojun-Zhang/Transferability-NeurIPS2021>.

of paramount importance that the trained model can generalize *Out-Of-Distribution* (OOD): even if the target domain is not exactly the same as the source domain(s), the learned model should hopefully behave robustly under slight distribution shift.

To this end, one line of works focuses on learning the so-called *invariant representations* [2, 16, 57, 58]. At a colloquial level, the goal here is to learn feature embeddings that lead to indistinguishable feature distributions from different domains. In practice, both the feature embeddings and the domain discriminators are often parametrized by neural networks, leading to an adversarial game between these two. Furthermore, in order to avoid degenerate solutions, the learned features are required to be informative about the output variable as well. This is enforced by placing a predictor over the features and minimize the corresponding supervised loss simultaneously [17, 32, 48, 49].

Another line of recent works aims to learn features that can induce *invariant predictors*, first termed as the invariant risk minimization (IRM) [3, 39] paradigm. Roughly speaking, the goal of IRM is to discover a feature embedding, upon which the optimal predictors, i.e., the Bayes predictor, are invariant across the training domains. Again, at the same time, the features should be informative about the output variable as well. However, the optimization problem of IRM is rather difficult, and several follow-up works have proposed different relaxations to the original formulation [1, 26].

Despite being extensively studied, both theoretical [41, 59] and empirical [20, 23] works have shown the insufficiency of existing algorithms for domain generalization (DG). Methods based on invariant features ignore the potential shift in the marginal label distributions across domains [59] and the methods based on invariant predictors are not robust to covariate shift [26]. Perhaps surprisingly, empirical works have shown that with proper data augmentation and careful model tuning, the very basic algorithm of empirical risk minimization (ERM) demonstrates superior performance on domain generalization over existing methods on benchmark image datasets [20, 23]. This sharp gap between theory and practice calls for a fundamental understanding of the following question:

What kind of invariance should we look for, in order to ensure that a good model on source domains also achieves decent accuracy on a related target domain?

In this work we attempt to answer the above question by proposing a criterion for models to look at, dubbed as *transferability*, which asks for an invariance of the *excess risks* of a predictor across domains. Different from existing proposals of invariant features and invariant predictors, which seek to find feature embeddings that respectively induce invariant marginal and conditional distributions, our notion of transferability depends on the excess risk, hence it directly takes into account the joint distribution over both the features and the labels. We show how it can be used to naturally derive a new upper bound for the target error, and then we discuss how to estimate the transferability empirically with enough samples. Our definition also inspires a method that aims to find more transferable features via representation learning using adversarial training.

Empirically, we perform experiments to measure the transferability of several existing algorithms, on both small and large scale datasets. We show that many algorithms, including ERM, are not quite transferable under the definition (Fig. 1, see more details in §5): when we go away from the optimal classifier (with distance δ in the parameter space), it could happen that the source accuracy remains high but the target accuracy drops significantly. This implies that during the training process, an existing algorithm may find a good source classifier with low target accuracy, hence violating the requirement for invariance of excess risks. In contrast, our algorithm is more transferable, and achieves consistent improvement over existing state-of-the-art algorithms, corroborating our findings.

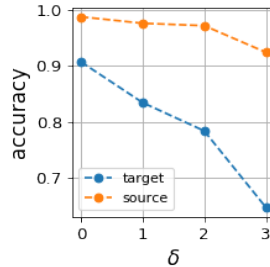


Figure 1: The target and source (test) accuracies of ERM on MNIST.

2 What is Transferability?

In this section we present our definition of transferability in the classification setting. The setup of domain generalization is the following:

Settings and Notation Given n labeled source domains $\mathcal{S}_1, \dots, \mathcal{S}_n$, the problem of domain generalization is to learn a model from these source domains, in the hope that it performs well on an

unseen target domain \mathcal{T} that is “similar” to the source domains. Throughout the paper, we assume that both the source domains and the unseen target domain share the same input and output spaces, denoted as \mathcal{X} and \mathcal{Y} , respectively. For multi-class classification, the output space $\mathcal{Y} = [K]$ is a set of labels for multi-class classification. For binary classification, we consider $\mathcal{Y} = \{-1, +1\}$. Denote \mathcal{H} as the hypothesis class. We define the classification error of a classifier $h \in \mathcal{H}$ on a domain \mathcal{D} (or \mathcal{S} for source domains, or \mathcal{T} for target domains) as:²

$$\epsilon_{\mathcal{D}}(h) = \mathbb{E}_{(x,y) \sim \mathcal{D}}[\ell(h(x), y)]. \quad (1)$$

For $\ell(h(x), y) = \mathbb{1}(h(x) \neq y)$, where $\mathbb{1}(\cdot)$ is the usual indicator function, we use $\epsilon_{\mathcal{D}}^{0-1}(h)$ to denote it is the 0-1 loss.

In domain generalization, we often have several source domains. For the ease of presentation, we only consider a single source domain in this section, and later extend to the general case in Section 5. Given two domains, the source domain \mathcal{S} and the target domain \mathcal{T} , the task of domain generalization is to transfer a classifier h that performs well on \mathcal{S} to \mathcal{T} . We ask: how much of the success of h on \mathcal{S} can be transferred to \mathcal{T} ?

Note that in order to evaluate the transferability from \mathcal{S} to \mathcal{T} , we need information from the target domain, similar to the test phase in traditional supervised learning. We believe a good criterion of transferability should satisfy the following properties:

1. *Quantifiable*: the notion should be quantifiable and can be computed in practice;
2. Any near-optimal source classifier should be near-optimal on the target domain.
3. If the two domains are similar, as measured by e.g., total variation, then they are transferable to each other, but the converse may not be true.

At first glance the second criterion above might seem too strong and restrictive. However, we argue that in the task of domain generalization, we only have labeled source data and there is no clue to distinguish a classifier from another if both of them perform equally well on the source domain. Based on the second property, we first propose the following definition of transferability:

Definition 1 (transferability). \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{T}})_{\mathcal{H}}$ -transferable to \mathcal{T} if for $\delta_{\mathcal{S}} > 0$, there exists $\delta_{\mathcal{T}} > 0$ such that $\operatorname{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})_{\mathcal{H}} \subseteq \operatorname{argmin}(\epsilon_{\mathcal{T}}, \delta_{\mathcal{T}})_{\mathcal{H}}$, where:

$$\operatorname{argmin}(\epsilon_{\mathcal{D}}, \delta_{\mathcal{D}})_{\mathcal{H}} := \{h \in \mathcal{H} : \epsilon_{\mathcal{D}}(h) \leq \inf_{h \in \mathcal{H}} \epsilon_{\mathcal{D}}(h) + \delta_{\mathcal{D}}\}.$$

In the literature the set $\operatorname{argmin}(\epsilon_{\mathcal{D}}, \delta_{\mathcal{D}})_{\mathcal{H}}$ is also known as a $\delta_{\mathcal{D}}$ -minimal set [24] of $\epsilon_{\mathcal{D}}$, which represents the near-optimal set of classifiers. Note that the δ -minimal set depends on the hypothesis class \mathcal{H} . Throughout the paper, we omit the subscript \mathcal{H} in the definition when there is no confusion. Def. 1 says that near-optimal source classifiers are also near-optimal target classifiers. Furthermore, it is easy to verify that our transferability is transitive: if \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{P}})$ -transferable to \mathcal{P} , and \mathcal{P} is $(\delta_{\mathcal{P}}, \delta_{\mathcal{T}})$ -transferable to \mathcal{T} , then \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{T}})$ -transferable to \mathcal{T} .

Next we define transfer measures, which we will show to be equivalent with Def. 1 in Prop. 5.

Definition 2 (quantifiable transfer measures). Given some $\Gamma \subseteq \mathcal{H}$, $\epsilon_{\mathcal{S}}^* := \inf_{h \in \Gamma} \epsilon_{\mathcal{S}}(h)$ and $\epsilon_{\mathcal{T}}^* := \inf_{h \in \Gamma} \epsilon_{\mathcal{T}}(h)$ we define the one-sided transfer measure, symmetric transfer measure and the realizable transfer measure respectively as:

$$T_{\Gamma}(\mathcal{S} \parallel \mathcal{T}) := \sup_{h \in \Gamma} \epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* - (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*), \quad (2)$$

$$T_{\Gamma}(\mathcal{S}, \mathcal{T}) := \max\{T_{\Gamma}(\mathcal{S} \parallel \mathcal{T}), T_{\Gamma}(\mathcal{T} \parallel \mathcal{S})\} = \sup_{h \in \Gamma} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^* - (\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^*)|, \quad (3)$$

$$T_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) := \sup_{h \in \Gamma} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h)|. \quad (4)$$

The distinction between Γ and \mathcal{H} will become apparent in Prop. 5. Note that the one-sided transfer measure is not symmetric. If we want the two domains \mathcal{S} and \mathcal{T} to be mutually transferable to each other, we can use the symmetric transfer measure. We call both quantities as *transfer measures*. Furthermore, the symmetric transfer measure reduces to (4) in the realizable case when $\epsilon_{\mathcal{S}}^* = \epsilon_{\mathcal{T}}^* = 0$. In statistical learning theory, $\epsilon_{\mathcal{D}}(h) - \epsilon_{\mathcal{D}}^*$ is often known as an *excess risk* [24], which is the relative error compared to the optimal classifier. The transfer measures can thus be represented with the difference of excess risks. With Def. 2, we can immediately obtain the following result that upper bounds the target error:

²Throughout the paper, we will use the terms domain and distribution interchangeably.

Proposition 3 (target error bound). *Given $\Gamma \subseteq \mathcal{H}$, for any $h \in \Gamma$, the target error is bounded by:*

$$\epsilon_{\mathcal{T}}(h) \leq \epsilon_{\mathcal{S}}(h) + \epsilon_{\mathcal{T}}^* - \epsilon_{\mathcal{S}}^* + \mathsf{T}_{\Gamma}(\mathcal{S}||\mathcal{T}) \leq \epsilon_{\mathcal{S}}(h) + \epsilon_{\mathcal{T}}^* - \epsilon_{\mathcal{S}}^* + \mathsf{T}_{\Gamma}(\mathcal{S}, \mathcal{T}). \quad (5)$$

The first error bound of such type for a target domain uses \mathcal{H} -divergence [8, 9, 12] for binary classification (or more rigorously, the $\mathcal{H}\Delta\mathcal{H}$ -divergence). The main difference between ours and \mathcal{H} -divergence is that \mathcal{H} -divergence only concerns about the marginal input distributions, whereas the transfer measures depend on the joint distributions over both the inputs and the labels. We note that Proposition 3 is general and works in the multi-class case as well. Moreover, even in the binary classification case we can prove that our Proposition 3 is tighter than \mathcal{H} -divergence (see Proposition 27 in the appendix).

In practice we may not know the optimal errors. In this case, we can use the realizable transfer measure to upper bound the symmetric transfer measure (note that $\epsilon_{\mathcal{S}}^*$ or $\epsilon_{\mathcal{T}}^*$ may not be zero):

Proposition 4. *For $\Gamma \subseteq \mathcal{H}$ and domains \mathcal{S}, \mathcal{T} we have: $\mathsf{T}_{\Gamma}(\mathcal{S}, \mathcal{T}) \leq 2\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T})$.*

Since Def. 1 essentially asks that the excess risks of approximately optimal classifiers on the source domain are comparable between the source and target domains, we can show that Def. 1 and Def. 2 are equivalent if Γ is a δ -minimal set:

Proposition 5 (equivalence between transferability and transfer measures). *Let $\delta_{\mathcal{S}} > 0$ and $\Gamma = \operatorname{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})$ and suppose $\inf_{h \in \Gamma} \epsilon_{\mathcal{T}}(h) = \inf_{h \in \mathcal{H}} \epsilon_{\mathcal{T}}(h)$. If $\mathsf{T}_{\Gamma}(\mathcal{S}||\mathcal{T}) \leq \delta$ or $\mathsf{T}_{\Gamma}(\mathcal{S}, \mathcal{T}) \leq \delta$, then \mathcal{S} is $(\delta_{\mathcal{S}}, \delta + \delta_{\mathcal{S}})$ -transferable to \mathcal{T} . Furthermore, if \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{T}})$ -transferable to \mathcal{T} , then $\mathsf{T}_{\Gamma}(\mathcal{S}||\mathcal{T}) \leq \delta_{\mathcal{T}}$ and $\mathsf{T}_{\Gamma}(\mathcal{S}, \mathcal{T}) \leq \max\{\delta_{\mathcal{S}}, \delta_{\mathcal{T}}\}$.*

In Prop. 5, we do not require $\Gamma = \mathcal{H}$ since it is unnecessary to impose that all classifiers in \mathcal{H} have similar excess risks on source and target domains. Instead, we only constrain Γ to be a δ -minimal set, i.e., Γ includes approximately optimal classifiers of \mathcal{S} . See also Example 8. An additional assumption is that Γ also includes the optimal classifier of \mathcal{T} which can be ensured by controlling $\delta_{\mathcal{S}}$.

2.1 Comparison with other discrepancy measures between domains

In this subsection, we compare the realizable transfer measure (4) with other discrepancy measures between domains and focus on the 0-1 loss $\epsilon_{\mathcal{D}}^{0-1}$. We first note that $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T})$ can be written as an integral probability metric (IPM) [36, 46]. The l.h.s. of (4) can be written as:

$$\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) := d_{\mathcal{F}_{\Gamma}}(\mathcal{S}, \mathcal{T}), \text{ where } d_{\mathcal{F}}(\mathcal{S}, \mathcal{T}) = \sup_{f \in \mathcal{F}} \left| \sum_y \int f(x, y)(p_{\mathcal{S}}(x, y) - p_{\mathcal{T}}(x, y))dx \right|, \quad (6)$$

and $\mathcal{F}_{\Gamma} := \{(x, y) \mapsto \mathbb{1}(h(x) \neq y), h \in \Gamma\}$. Typical IPMs [46] include MMD, Wasserstein distance, Dudley metric and the Kolmogorov–Smirnov distance (see Appendix B.2 for more details). However, \mathcal{F}_{Γ} is fundamentally different from these IPMs since it relies on an underlying function class Γ . Our realizable transfer measure shares some similarity with Arora et al. [4], where a changeable function class is used, but the exact choices of the function class are different.

Even though the transferability can be written in terms of IPM, it is in fact a pseudo-metric:

Proposition 6 (pseudo-metric). *For a general loss $\epsilon_{\mathcal{D}}$ as in (1), $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T})$ is a pseudo-metric, i.e., for any distributions $\mathcal{S}, \mathcal{T}, \mathcal{P}$ on the same underlying space, we have $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{S}) = 0$, $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) = \mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{T}, \mathcal{S})$ (symmetry), and $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) \leq \mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{P}) + \mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{P}, \mathcal{T})$ (triangle inequality).*

However in general $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T})$ is not a metric since $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) = 0$ even if $\mathcal{S} \neq \mathcal{T}$. For instance, taking $\Gamma = \{h^*\}$ to be the optimal classifier on both \mathcal{S} and \mathcal{T} . we have $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) = 0$, but \mathcal{S} and \mathcal{T} could differ a lot (see Figure 2). In the next result we discuss the connection between realizable transfer measures and total variation (c.f. Appendix B.2).

Proposition 7 (equivalence with total variation). *For binary classification with labels $\{-1, 1\}$, given the 0-1 loss $\epsilon_{\mathcal{D}} = \epsilon_{\mathcal{D}}^{0-1}$, we have $\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) \leq d_{\text{TV}}(\mathcal{S}, \mathcal{T})$ for domains \mathcal{S}, \mathcal{T} and any $\Gamma \subseteq \mathcal{H}$. Denote \mathcal{H}_t to be the set of all binary classifiers. Then we have $d_{\text{TV}}(\mathcal{S}, \mathcal{T}) \leq 4\mathsf{T}_{\mathcal{H}_t}^{\mathbb{F}}(\mathcal{S}, \mathcal{T})$.*

Prop. 7 tells us that transfer measures (see also Prop. 4) are no stronger than total variation, and in the realizable case, (3) is equivalent to the similarity of domains (as measured by total variation) if Γ is unconstrained. We can moreover show that transfer measures are strictly weaker, if we choose Γ to be some δ -minimal set:

Example 8 (very dissimilar joint distributions but transferable). We study the distributions described in Figure 2. The joint distributions are very dissimilar, i.e., for any X, Y in the domain, $|p_S(X, Y) - p_T(X, Y)| = 0.8$. Define

$$h_\rho(X) = \begin{cases} 1 & \text{if } -1 \leq X < \rho \\ -1 & \text{if } \rho \leq X < 1 \end{cases}. \quad (7)$$

We choose the hypothesis class $\mathcal{H} = \{h_\rho, \rho \in [-1, 1]\}$ and $\Gamma = \{h_\rho, |\rho| \leq \delta/0.8\}$ (for small δ , say $\delta < 0.01$) to be some neighborhood of the optimal source classifier $h^* = h_0$. Then $T_\Gamma(\mathcal{S}, \mathcal{T}) = \sup_{h \in \Gamma} |\epsilon_S(h) - \epsilon_T(h)| = \delta$, and \mathcal{S} is $(\delta_S, \delta + \delta_S)$ -transferable to \mathcal{T} on Γ for any $\delta_S > 0$ according to Prop. 5. Note that $\epsilon_S^* = \epsilon_T^* = 0$.

3 Computing Transferability

In the last section we proposed a new concept called transferability. However, although Def. 1 provides a theoretically sound result for transferability, it is hard to verify it in practice, since we cannot exhaust all approximately good classifiers, especially for rich models such as deep neural networks. Nevertheless, Prop. 3 and Prop. 5 provide a framework to compute transferability through transfer measures, despite their simplicity. In this section we discuss how to compute these quantities by making necessary approximations based on transfer measures. There are two difficulties we need to overcome: (1) In practice we only have finite samples drawn from true distributions; (2) We need a surrogate loss such as cross entropy for training and the 0-1 loss for evaluation. In §3.1 we show that our transfer measures can be estimated with enough samples, and in §3.2 we discuss transferability with a surrogate loss. These results will be used in our algorithms in the next section.

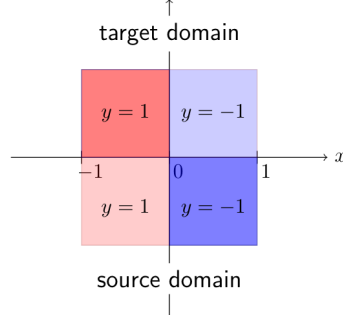


Figure 2: Visualization of Example 8. **Source domain:** $P_S(Y = 1, -1 \leq X < 0) = 0.1$, $P_S(Y = -1, 0 \leq X < 1) = 0.9$. **Target domain:** $P_T(Y = 1, -1 \leq X < 0) = 0.9$, $P_T(Y = -1, 0 \leq X < 1) = 0.1$. The dark and light colors show the intensity of the probability mass. The vertical axis denotes whether it is the target or source domain (above or below x -axis).

3.1 Estimation of transferability

We show how to estimate the transfer measure $T_\Gamma(\mathcal{S}||\mathcal{T})$ from finite samples. Other versions of transfer measures in Def. 1 follow analogously (see Appendix A for more details).

Lemma 9 (reduction of estimation error). Given general loss ϵ_D as in (1), suppose $\hat{\mathcal{S}}$ and $\hat{\mathcal{T}}$ are i.i.d. sample distributions drawn from distributions of \mathcal{S} and \mathcal{T} , then for any $\Gamma \subseteq \mathcal{H}$ we have:

$$T_\Gamma(\mathcal{S}||\mathcal{T}) \leq T_\Gamma(\hat{\mathcal{S}}||\hat{\mathcal{T}}) + 2\text{est}_\Gamma(\mathcal{S}) + 2\text{est}_\Gamma(\mathcal{T}),$$

with the estimation errors $\text{est}_\Gamma(\mathcal{S}) = \sup_{h \in \Gamma} |\epsilon_S(h) - \epsilon_{\hat{\mathcal{S}}}(h)|$, $\text{est}_\Gamma(\mathcal{T}) = \sup_{h \in \Gamma} |\epsilon_T(h) - \epsilon_{\hat{\mathcal{T}}}(h)|$.

This lemma tells us that estimating transferability is no harder than computing the estimation errors of both domains. If the function class Γ has uniform convergence property [44], then we can guarantee efficient estimation of transferability. We first bound the sample complexity through Rademacher complexity, which is a standard tool in bounding estimation errors [5]:

Theorem 10 (estimation error with Rademacher complexity). Given the 0-1 loss $\epsilon_D = \epsilon_D^{0-1}$, suppose $\hat{\mathcal{S}}$ and $\hat{\mathcal{T}}$ are sample sets with m and k samples drawn i.i.d. from distributions \mathcal{S} and \mathcal{T} , respectively. For any $\Gamma \subseteq \mathcal{H}$ the following holds with probability $1 - \delta$:

$$T_\Gamma(\mathcal{S}||\mathcal{T}) \leq T_\Gamma(\hat{\mathcal{S}}||\hat{\mathcal{T}}) + 4\mathfrak{R}_m(\mathcal{F}_\Gamma) + 4\mathfrak{R}_k(\mathcal{F}_\Gamma) + 2\sqrt{\frac{\log(4/\delta)}{2m}} + 2\sqrt{\frac{\log(4/\delta)}{2k}},$$

where $\mathcal{F}_\Gamma := \{(x, y) \mapsto \mathbb{1}(h(x) \neq y), h \in \Gamma\}$. If furthermore, Γ is a set of binary classifiers with labels $\{-1, 1\}$, then $2\mathfrak{R}_m(\mathcal{F}_\Gamma) = \mathfrak{R}_m(\Gamma)$, $2\mathfrak{R}_k(\mathcal{F}_\Gamma) = \mathfrak{R}_k(\Gamma)$.

We also provide estimation error results using Vapnik–Chervonenkis (VC) dimension and Natarajan dimension in Appendix B.3. It is worth mentioning that the VC dimension of piecewise-polynomial neural networks has been upper bounded in Bartlett et al. [7]. Since transfer measures can be estimated, in later sections we do not distinguish the sample sets $\hat{\mathcal{S}}, \hat{\mathcal{T}}$ and the underlying distributions \mathcal{S}, \mathcal{T} .

3.2 Transferability with a surrogate loss

Due to the intractability of minimizing the 0-1 loss, we need to use a surrogate loss [6] for training in practice. In this section, we discuss this nuance w.r.t. transferability. We will focus on the most commonly used surrogate loss, cross entropy (CE), although some of the results can be easily adapted to other loss functions. To distinguish a surrogate loss from the 0-1 loss, we use $\epsilon_{\mathcal{D}}$ from now on for a surrogate loss and $\epsilon_{\mathcal{D}}^{0-1}$ for the 0-1 loss. One of the difficulties is the non-equivalence between δ -minimal sets w.r.t. the 0-1 loss and a surrogate loss, i.e. $\operatorname{argmin}(\epsilon_{\mathcal{D}}, \delta_{\mathcal{D}})$ might be quite different from $\operatorname{argmin}(\epsilon_{\mathcal{D}}^{0-1}, \delta_{\mathcal{D}})$. Moreover, it is not practical to find all elements in $\operatorname{argmin}(\epsilon_{\mathcal{D}}^{0-1}, \delta_{\mathcal{D}})$ since the loss is nonconvex and nonsmooth. In light of these difficulties, we propose a more practical notion of transferability based on surrogate loss $\epsilon_{\mathcal{D}}$:

Proposition 11 (transfer measure with a surrogate loss). *Given surrogate loss $\epsilon_{\mathcal{D}} \geq \epsilon_{\mathcal{D}}^{0-1}$ on a general domain \mathcal{D} . Suppose $\Gamma = \operatorname{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})$ and denote $\epsilon_{\mathcal{T}}^* = \inf_{h \in \Gamma} \epsilon_{\mathcal{T}}(h)$, $\epsilon_{\mathcal{S}}^* = \inf_{h \in \Gamma} \epsilon_{\mathcal{S}}(h)$, $(\epsilon_{\mathcal{T}}^{0-1})^* = \inf_{h \in \mathcal{H}} \epsilon_{\mathcal{T}}^{0-1}(h)$. If the following holds:*

$$\mathsf{T}_{\Gamma}(\mathcal{S} \parallel \mathcal{T}) = \sup_{h \in \Gamma} \epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* - (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*) \leq \delta, \quad (8)$$

then we have $\operatorname{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}}) \subseteq \operatorname{argmin}(\epsilon_{\mathcal{T}}^{0-1}, \delta + \delta_{\mathcal{S}} + \epsilon_{\mathcal{T}}^* - (\epsilon_{\mathcal{T}}^{0-1})^*)$.

This proposition implies that if the transfer measure is small, then a near-optimal classifier of the surrogate loss in the source domain would be near-optimal in the target domain for the 0-1 loss. It also gives us a practical framework to guarantee transferability, which we will discuss in more depth in Section 4. Assume $\epsilon_{\mathcal{D}} : \mathcal{H} \rightarrow \mathbb{R}$ to be Lipschitz continuous and strongly convex, which is satisfied for the cross entropy loss (see Appendix B.4). We are able to translate the δ -minimal set to L_p balls in the function space:

$$C_1 \|h - h^*\|_{2, \mathcal{D}} \leq \epsilon_{\mathcal{D}}(h) - \epsilon_{\mathcal{D}}(h^*) \leq C_2 \|h - h^*\|_{1, \mathcal{D}}, \quad (9)$$

where C_1 and C_2 are absolute constants and h^* is an optimal classifier. The function norms $\|\cdot\|_{1, \mathcal{D}}$ and $\|\cdot\|_{2, \mathcal{D}}$ are the usual L_p norms over distribution \mathcal{D} . Since the classifier $h = q(\theta, \cdot)$ is usually parameterized with, say a neural network, we further upper bound the function norms by the distance of parameters, that is, for $1 \leq p < \infty$, $h = q(\theta, \cdot)$ and $h' = q(\theta', \cdot)$, we have $\|h - h'\|_{p, \mathcal{D}} \leq L \|\theta - \theta'\|_2$, with L some Lipschitz constant of q (Appendix B.4). Combined with (9), we obtain:

$$\epsilon_{\mathcal{D}}(h) - \epsilon_{\mathcal{D}}(h') \leq LC_2 \|\theta - \theta'\|_2. \quad (10)$$

In other words, if the parameters are close enough, then the losses should not differ too much. We denote $\|\cdot\|_2$ as the Euclidean norm, and for later convenience we will omit the subscript in $\|\cdot\|_2$.

4 Algorithms for Evaluating and Improving Transferability

The notion of transferability is defined w.r.t. domains, hence by learning feature embeddings that induce certain feature distributions, one can aim to improve transferability of two given domains. In this section we design algorithms to evaluate and improve transferability by learning such transformations. To start with, let $g : \mathcal{X} \rightarrow \mathcal{Z}$ be a feature embedding (a.k.a. featurizer), where \mathcal{Z} is understood to be a feature space. By a joint distribution \mathcal{D}^g (or $\mathcal{S}^g, \mathcal{T}^g$) we mean a distribution on $g(\mathcal{X}) \times \mathcal{Y}$. Formally, we are dealing with push-forwards of distributions:

$$\mathcal{S}^g := (g, \operatorname{id})\#\mathcal{S}, \quad \mathcal{T}^g := (g, \operatorname{id})\#\mathcal{T}, \quad (11)$$

where $(g, \operatorname{id}) : (x, y) \mapsto (g(x), y)$ is a function on $\mathcal{X} \times \mathcal{Y}$. \mathcal{S} and \mathcal{T} here are joint distributions on $\mathcal{X} \times \mathcal{Y}$, and here we specify \mathcal{X} to be the space of the original signal such as an image. Since \mathcal{S} and \mathcal{T} cannot be changed, what we are evaluating here is the feature embedding g . The key quantity is transfer measures as in (8):

$$\mathsf{T}_{\Gamma}(\mathcal{S}^g \parallel \mathcal{T}^g) = \sup_{h \in \Gamma} \epsilon_{\mathcal{T}^g}(h) - \epsilon_{\mathcal{T}^g}^* - (\epsilon_{\mathcal{S}^g}(h) - \epsilon_{\mathcal{S}^g}^*), \quad \Gamma = \operatorname{argmin}(\epsilon_{\mathcal{S}^g}, \delta_{\mathcal{S}^g}). \quad (12)$$

Although Γ is hard to compute, we can use (10) to obtain a lower bound of (12). That is, given a parametrization of the classifier $h = q(\theta, \cdot)$ and the optimal classifier $h^* = q(\theta^*, \cdot)$, we have:

$$\begin{aligned} \mathsf{T}_\Gamma(\mathcal{S}^g \parallel \mathcal{T}^g) &\geq \sup_{\|\theta - \theta^*\| \leq \delta} \epsilon_{\mathcal{T}^g}(h) - \epsilon_{\mathcal{S}^g}(h) - \epsilon_{\mathcal{T}^g}^* + \epsilon_{\mathcal{S}^g}^* \\ &\geq \sup_{\|\theta - \theta^*\| \leq \delta} \epsilon_{\mathcal{T}^g}(h) - \epsilon_{\mathcal{S}^g}(h) - \epsilon_{\mathcal{T}^g}(\widehat{h}^*) \\ &\approx \sup_{\|\theta - \theta^*\| \leq \delta} \epsilon_{\mathcal{T}^g}(h) - \epsilon_{\mathcal{S}^g}(h) - \epsilon_{\mathcal{T}^g}(\widehat{h}^*) \end{aligned} \quad (13)$$

where $\delta > 0$ depends on Γ and the constant in (10). In the second and the third lines, we approximated the optimal errors $\epsilon_{\mathcal{T}^g}^*$ and $\epsilon_{\mathcal{S}^g}^*$ with $0 \leq \epsilon_{\mathcal{S}^g}^* \leq \epsilon_{\mathcal{S}^g}(\widehat{h}^*)$, $0 \leq \epsilon_{\mathcal{T}^g}^* \leq \epsilon_{\mathcal{T}^g}(\widehat{h}^*)$, and we use the learned classifier $\widehat{h}^* = q(\widehat{\theta}^*, \cdot)$ as a surrogate for the optimal classifier. As a result, if the r.h.s. of (13) is large, then \mathcal{S}^g is not quite transferable to \mathcal{T}^g .

Algorithm 1: Algorithm for evaluating transferability among multiple domains

Input: learned feature embedding g , learned classifier $\widehat{h}^* = q(\widehat{\theta}^*, \cdot)$, target sample training set $\mathcal{T} = \mathcal{S}_0$, sample training sets $\mathcal{S}_1, \dots, \mathcal{S}_n$, ascent optimizer, minimal errors $\epsilon_{\mathcal{S}_i}^* \approx \epsilon_{\mathcal{S}_i}(\widehat{h}^*)$, adversarial radius δ

Initialize: a classifier $h = q(\theta, \cdot)$ and $\theta = \widehat{\theta}^*$, $\text{gap} = -\infty$

for t in $1 \dots T$ **do**

Find $\max_i \epsilon_{\mathcal{S}_i}(h \circ g)$ and $\min_i \epsilon_{\mathcal{S}_i}(h \circ g)$ and corresponding indices j and k

Run an ascent optimizer on h to maximize $\text{gap}_0 = \epsilon_{\mathcal{S}_j}(h \circ g) - \epsilon_{\mathcal{S}_k}(h \circ g)$

Project θ onto the Euclidean ball $\|\theta - \widehat{\theta}^*\| \leq \delta$

if $\text{gap}_0 > \text{gap}$ **then**

$\text{gap} = \text{gap}_0$, save accuracies and losses of each domain

Output: $j, k, h, \epsilon_{\mathcal{S}_j}(h \circ g) - \epsilon_{\mathcal{S}_k}(h \circ g), \epsilon_{\mathcal{S}_j}(\widehat{h}^*), \epsilon_{\mathcal{S}_k}(\widehat{h}^*)$

We can thus design an algorithm to evaluate the transferability in Section 4.1. By computing the lower bound in (13), we can disprove the transferability as in Prop. 5 and Prop. 11. Computing the lower bound in (13) can be regarded as an attack method: there is an adversary trying to show that \mathcal{S}^g is not transferable to \mathcal{T}^g . For this attack, we could also design a defence method aiming to minimize the lower bound and learn more transferable features.

4.1 Algorithm for evaluating transferability

In domain generalization we have one target domain and more than one source domains. To ease the presentation, we denote $\mathcal{S}_0 = \mathcal{T}$ (and thus $\mathcal{S}_0^g = \mathcal{T}^g$) and extend the index set to be $\{0, 1, \dots, n\}$. We need to evaluate the transferability (13) between all pairs of \mathcal{S}_i^g and \mathcal{S}_j^g . Algorithm 1 gives an efficient method to compute the worst-case gap $\sup_{\|\theta - \widehat{\theta}^*\| \leq \delta} \epsilon_{\mathcal{S}_i^g}(h) - \epsilon_{\mathcal{S}_j^g}(h)$ among all pairs of (i, j) . Essentially, it finds the worst pair of (i, j) at each step such that the gap $\epsilon_{\mathcal{S}_i^g}(h) - \epsilon_{\mathcal{S}_j^g}(h)$ takes the largest value, and then maximize this gap over parameter θ through gradient ascent.

Note that the computation of (13) also depends on the information from the target domain. This is valid since we are only *evaluating* but not *training* over these domains.

4.2 Algorithm for improving transferability

The evaluation sub-procedure provides us a way to pick a pair of non-transferable domains $(\mathcal{S}_i^g, \mathcal{S}_j^g)$, which in turn could be used to improve the transferability among all source domains by updating the feature embedding g such that the gap $\sup_{\|\theta - \widehat{\theta}^*\| \leq \delta} \epsilon_{\mathcal{S}_i^g}(h) - \epsilon_{\mathcal{S}_j^g}(h)$ for $(i, j) \in [n] \times [n]$. Simultaneously, we also require that the feature embedding g preserves information for the target task of interest. With the parametrization $h = q(\theta, \cdot)$, $h' = q(\theta', \cdot)$, the overall optimization problem can be formulated as:

$$\min_{g, h} \max_{\|\theta' - \theta\| \leq \delta} \frac{1}{n} \sum_{i=1}^n \epsilon_{\mathcal{S}_i}(h \circ g) + (\max_i \epsilon_{\mathcal{S}_i}(h' \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h' \circ g)). \quad (14)$$

Intuitively, we want to learn a common feature embedding and a classifier such that all source errors are small and the pairwise transferability between source domains is also small. If the optimization problem is properly solved, then we have the following guarantee:

Theorem 12 (optimization guarantee). *Assume that the function $q(\cdot, x)$ is L_θ Lipschitz continuous for any x . Suppose we have learned a feature embedding g and a classifier h such that the loss functional $\epsilon_{\mathcal{S}_i^g} : \mathcal{H} \rightarrow \mathbb{R}$ is L_ℓ Lipschitz continuous w.r.t. distribution \mathcal{S}_i^g for $i \in [n]$ and*

$$\max_{\|\theta' - \theta\| \leq \delta} \frac{1}{n} \sum_{i=1}^n \epsilon_{\mathcal{S}_i}(h \circ g) + (\max_i \epsilon_{\mathcal{S}_i}(h' \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h' \circ g)) \leq \eta, \quad (15)$$

where θ, θ' are parameters of h and h' . Then for any $h' \in \Gamma = \{q(\theta', \cdot) : \|\theta - \theta'\| \leq \delta\}$, we have:

$$\mathbb{T}_\Gamma^{\mathcal{T}_1^g, \mathcal{T}_2^g} \leq \eta, \quad \epsilon_{\mathcal{S}_i}(h' \circ g) \leq \eta + L_\ell L_\theta \delta, \quad \epsilon_{\mathcal{T}}(h' \circ g) \leq 2\eta + L_\ell L_\theta \delta, \quad (16)$$

for any $\mathcal{T}_1^g, \mathcal{T}_2^g, \mathcal{T}^g \in \text{conv}(\mathcal{S}_1^g, \dots, \mathcal{S}_n^g)$ and any $i \in [n]$.

The Lipschitzness assumption for $\epsilon_{\mathcal{S}_i^g}$ is mild and can be satisfied for cross entropy loss (c.f. Appendix B.4.1). Here $\text{conv}(\cdot)$ denotes the convex hull in the same sense as Albuquerque et al. [2], i.e., each element is a mixture of source distributions. Thm 12 tells us that if we can solve the optimization problem (14) properly, we can guarantee transferability on a neighborhood of the classifier, as an approximation of the δ -minimal set. We thus propose Algorithm 2, which shares similarity with existing frameworks, such as DANN [16] and Distributional Robust Optimization [43, 45], in the sense that they all involve adversarial training and minimax optimization. However, the objective in our case is different and we provide a more detailed comparison with existing methods in Appendix B.5.

Algorithm 2: Transfer algorithm for domain generalization

Input: samples sets of source domains $\mathcal{S}_1, \dots, \mathcal{S}_n$, feature embedding g , classifier $h = q(\theta, \cdot)$, adversarial classifier $h' = q(\theta', \cdot)$, surrogate loss $\epsilon_{\mathcal{D}}$, adversarial radius δ , ascent optimizer, descent optimizer, weight parameter λ , number of epochs T

for t in $1 \dots T$ **do**

Compute $\max_i \epsilon_{\mathcal{S}_i}(h \circ g)$ and $\min_i \epsilon_{\mathcal{S}_i}(h \circ g)$

Initialization $h' = h$ (or $\theta' = \theta$)

for k in $1 \dots N$ **do**

Run the ascent optimizer on h' to maximize $\max_i \epsilon_{\mathcal{S}_i}(h' \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h' \circ g)$ fixing g

Project θ' onto the Euclidean ball $\|\theta' - \theta\| \leq \delta$

Fixing h' , run the descent optimizer on g, h to minimize

error $= \frac{1}{n} \sum_i \epsilon_{\mathcal{S}_i}(h \circ g) + (\max_i \epsilon_{\mathcal{S}_i}(h' \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h' \circ g))$

Output: feature embedding g , classifier h

5 Experiments

Gulrajani and Lopez-Paz [20] did extensive experiments on comparing DG algorithms, using the same neural architecture and data split. Specifically, they show that with data augmentation, ERM perform relatively well among a large array of algorithms. Our experiments are based on their settings. We run Algorithm 1 on standard benchmarks, including RotatedMNIST [18], PACS [28], Office-Home [51] and WILDS-FMoW [23] (c.f. Appendix C.1). Specifically, WILDS-FMoW is a large dataset with nearly half a million images. Detailed experimental settings can be seen at Appendix C.

Evaluating transferability From Figure 3 it can be seen that at a neighborhood of the learned classifier, there exists a classifier such that the target accuracy is degraded significantly, whereas some source domain still has high accuracy. This poses questions to whether current popular algorithms such as ERM [50], DANN [17] and Mixup [53, 54] are really learning invariant and transferable features. If so, the target accuracy should be high given a high source accuracy. However, for the PACS dataset and Mixup model (the second column of Figure 3), the target accuracy decreases by more than 30% while the source accuracy remains roughly at the same level. We can also, e.g., read from the first column that with a small decrease of the source (test) accuracy by $\sim 2\%$ (at $\delta = 2$), the target accuracy of DANN drops by $\sim 10\%$.

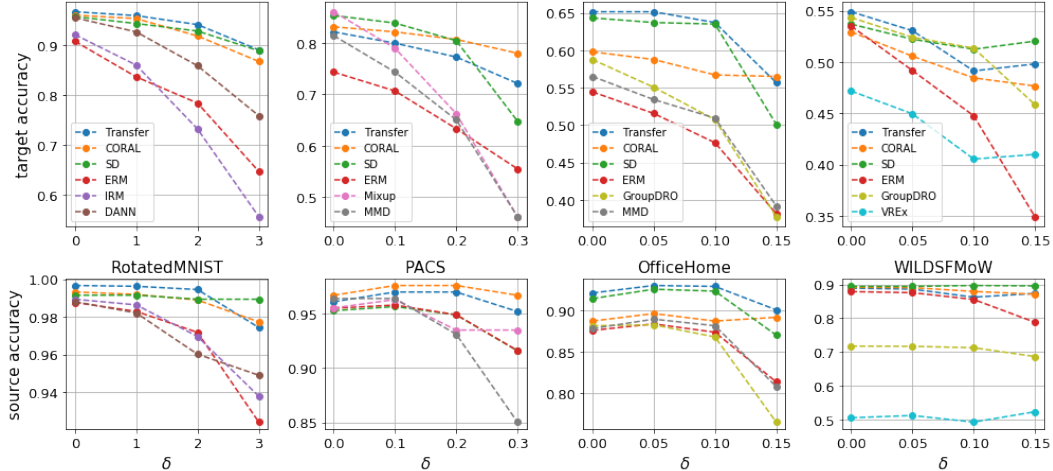


Figure 3: **Top row**: test accuracy of the target domain; **bottom row**: test accuracy of one of the source domains. Each column is for a given dataset with the name in the middle, and the legends on the bottom row are the same as those on the top row. δ is the parameter in Algorithm 1.

From Figure 3 we can also see that Correlation Alignment [CORAL, 47] and Spectral Decomposition [SD, 40] have better transferability than other algorithms. In some sense, they are in fact learning *robust classifiers*, i.e., all the classifiers on the neighborhood of the learned classifier can achieve good accuracies. With this robust classifier, the target accuracy does not decrease much even if the classifier is perturbed.

Improving transferability Algorithm 2 has good performance among all four datasets that we tried, comparable to CORAL and SD. Note that CORAL and SD do not always perform well, such as in the Office-Home and WILDS-FMoW datasets, but our Transfer algorithm does. However, in our experiments we find there are two limitations of Algorithm 2: **(1)** we need a large number of inner maximization steps to compute the gap, which needs more training time. This is similar to adversarial robustness [33] which is slower than usual training. In order to overcome this difficulty we used pretraining from other algorithms in the experiments on Office-Home and WILDS-FMoW; **(2)** Moderate hyper-parameter tuning is needed. For example, we need to tune N in Algorithm 2, the learning rate (lr) of SGA and the choice of δ . We find that taking $N = 20$ or 30 is usually a good choice, and δ can be quite large such that the projection step is not taken. We take $\text{lr} = 0.01$ for RotatedMNIST and $\text{lr} = 0.001$ for other datasets.

Label shift In order to show the difference with the well-known \mathcal{H} -divergence [8], we compute the label shifts in the PACS dataset. As shown in Zhao et al. [59], the optimal joint error $\epsilon_{\mathcal{S}}(h^*) + \epsilon_{\mathcal{T}}(h^*)$ (h^* is the optimal classifier that minimizes $\epsilon_{\mathcal{S}}(h) + \epsilon_{\mathcal{T}}(h)$) can be large under the shift of label distributions. We follow [59] and compute the label shift between pairs of domains in the PACS dataset, measured by total variation. From Table 1 we can see that the label shift is large in this case, and thus the \mathcal{H} -divergence bound [8] can be quite loose. Comparably, our transfer measure bound Prop. 3 is tighter (c.f. Prop. 27) and therefore still useful in practice.

Table 1: Label shift between pairs of domains in the PACS dataset. **TV**: total variation; **A**: art painting; **C**: cartoon; **P**: photo; **S**: sketch. The total variation is always between zero and one.

| TV | A | C | P | S |
|-----------|----------|----------|----------|----------|
| A | 0.0 | 0.12 | 0.11 | 0.3 |
| C | 0.12 | 0.0 | 0.18 | 0.24 |
| P | 0.11 | 0.18 | 0.0 | 0.37 |
| S | 0.3 | 0.24 | 0.37 | 0.0 |

6 Related Work

Multi-task learning Multi-task learning (MTL) [56] is related to but different from DG. In MTL, there are several tasks, and one hopes to improve the performance of each task by jointly training all the tasks simultaneously, utilizing the relationships between them. This is different from DG in the sense that in DG the target domain is unknown a priori, whereas in MTL the focus is more on better generalization on existing tasks that appear in training. Hence, there is no distribution shift in MTL per se. Furthermore, for MTL, the output spaces of different tasks are not necessarily the same.

Zero-shot learning / Few-shot learning / Meta-learning DG is different from zero-shot learning [27]. In zero-shot learning, one has labeled training data and the goal is to make predictions on a new unseen label set. However, in DG the label set remains the same for the source and the target domains. On the other hand, the focus of few-shot learning is on fast adaptation, in the sense that the test distribution remains the same as the training distribution, but the learner can only have access to a few labeled samples. Domain generalization also shares similarity with meta-learning. However, in meta-learning, the learner is allowed to fine-tune over the target domain. In other words, the protocol of meta-learning allows access to a small amount of labeled data from future unseen domains. Meta-learning is more or less one specific method that is used to tackle few-shot learning. Because of the similarity, some meta-learning algorithms can be applied to DG [29].

Self-supervised learning Self-supervised learning (SSL) is a popular unsupervised feature learning approach [13, 19, 21]. The goal of SSL is to learn invariant representations w.r.t. different views of the same image. Although it is a promising feature learning method, it differs from our DG settings in the sense that no labels are used in SSL.

Domain generalization There have been a lot of old and new algorithms proposed for domain generalization. The simplest one is Empirical Risk Minimization (ERM), where we simply minimize the empirical risk of (the sum of) all source domains. In Blanchard et al. [10], Muandet et al. [35], kernel methods for DG were proposed. Arjovsky et al. [3] proposed Invariant Risk Minimization (IRM) which aims to learn invariant predictors across source domains, and follow-up discussions can be found in [25, 41]. Another approach is called distributional robustness [43, 52], where the model is optimized over a worst-case distribution under the constraint that this distribution is generated from a small perturbation around the source distributions. In Albuquerque et al. [2], a DG scheme based on distribution matching was proposed. Moreover, many domain adaptation algorithms can be directly adapted to the task of domain generalization, such as CORAL [47] and DANN [16]. Last but not least, we mention a concurrent work [55] on the theory of domain generalization, which focuses more on proposing a model selection rule based on accuracy and variation.

Adversarial robustness Our evaluation and training methods in §4 are reminiscent of the adversarial training method [33] in the literature of adversarial robustness. Perturbing the classifier in our case corresponds to perturbing the input data in adversarial robustness. From this perspective, our Transfer algorithm is parallel to the adversarial training method. It would be interesting to design certified robust feature embeddings, by analogy with certified robust classifiers [15].

7 Conclusions

In this paper we formally define the notion of *transferability* that we can quantify, estimate and compute. Our transfer measures can be understood as a special class of IPMs. They are weaker than total variation and even very dissimilar distributions could be transferable to each other. Our definition of transferability can also be naturally used to derive a generalization bound for prediction error on the target domain. Based on our theory, we propose algorithms to evaluate and improve the transferability by learning feature representations. Experiments show that, somewhat surprisingly, many existing algorithms are not quite learning transferable features. From this perspective, our transfer measures offer a novel way to evaluate the features learned from different DG algorithms. We hope that our proposal of transferability could draw the community’s attention to further investigate and better understand the fundamental quantity that allows robust models under distribution shifts.

Broader Impact Reliable domain generalization models are important for practice use. Our work points out the reliability issue of DG algorithms. It is worth mentioning that our evaluation method can only disprove the transferability and survival of our attack method should not be treated as a warranty. Misunderstanding of it could lead to potential harm in practical applications.

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References

- [1] Kartik Ahuja, Karthikeyan Shanmugam, Kush Varshney, and Amit Dhurandhar. Invariant risk minimization games. In *International Conference on Machine Learning*, pages 145–155. PMLR, 2020.
- [2] Isabela Albuquerque, João Monteiro, Mohammad Darvishi, Tiago H Falk, and Ioannis Mitliagkas. Generalizing to unseen domains via distribution matching. *arXiv preprint arXiv:1911.00804*, 2019.
- [3] Martin Arjovsky, Léon Bottou, Ishaan Gulrajani, and David Lopez-Paz. Invariant risk minimization. *arXiv preprint arXiv:1907.02893*, 2019.
- [4] Sanjeev Arora, Rong Ge, Yingyu Liang, Tengyu Ma, and Yi Zhang. Generalization and equilibrium in generative adversarial nets (GANs). In *International Conference on Machine Learning*, pages 224–232. PMLR, 2017.
- [5] Peter L Bartlett and Shahar Mendelson. Rademacher and gaussian complexities: Risk bounds and structural results. *Journal of Machine Learning Research*, 3(Nov):463–482, 2002.
- [6] Peter L Bartlett, Michael I Jordan, and Jon D McAuliffe. Convexity, classification, and risk bounds. *Journal of the American Statistical Association*, 101(473):138–156, 2006.
- [7] Peter L Bartlett, Nick Harvey, Christopher Liaw, and Abbas Mehrabian. Nearly-tight VC-dimension and pseudodimension bounds for piecewise linear neural networks. *J. Mach. Learn. Res.*, 20(63):1–17, 2019.
- [8] Shai Ben-David, John Blitzer, Koby Crammer, and Fernando Pereira. Analysis of representations for domain adaptation. In *Advances in neural information processing systems*, pages 137–144, 2007.
- [9] Shai Ben-David, John Blitzer, Koby Crammer, Alex Kulesza, Fernando Pereira, and Jennifer Wortman Vaughan. A theory of learning from different domains. *Machine learning*, 79(1-2):151–175, 2010.
- [10] Gilles Blanchard, Gyemin Lee, and Clayton Scott. Generalizing from several related classification tasks to a new unlabeled sample. *Advances in neural information processing systems*, 24: 2178–2186, 2011.
- [11] Gilles Blanchard, Aniket Anand Deshmukh, Urun Dogan, Gyemin Lee, and Clayton Scott. Domain generalization by marginal transfer learning. *Journal of Machine Learning Research*, 22(2):1–55, 2021.
- [12] John Blitzer, Koby Crammer, Alex Kulesza, Fernando Pereira, and Jennifer Wortman. Learning bounds for domain adaptation. In *Advances in neural information processing systems*, 2007.
- [13] Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. In *Proceedings of the 37th International Conference on Machine Learning*, pages 1597–1607, 2020. URL <http://proceedings.mlr.press/v119/chen20j.html>.

- [14] Gordon Christie, Neil Fendley, James Wilson, and Ryan Mukherjee. Functional map of the world. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 6172–6180, 2018.
- [15] Jeremy Cohen, Elan Rosenfeld, and Zico Kolter. Certified adversarial robustness via randomized smoothing. In *International Conference on Machine Learning*, pages 1310–1320. PMLR, 2019.
- [16] Yaroslav Ganin and Victor Lempitsky. Unsupervised domain adaptation by backpropagation. In *International conference on machine learning*, pages 1180–1189. PMLR, 2015.
- [17] Yaroslav Ganin, Evgeniya Ustinova, Hana Ajakan, Pascal Germain, Hugo Larochelle, François Laviolette, Mario Marchand, and Victor Lempitsky. Domain-adversarial training of neural networks. *The Journal of Machine Learning Research*, 17(1):2096–2030, 2016.
- [18] Muhammad Ghifary, W Bastiaan Kleijn, Mengjie Zhang, and David Balduzzi. Domain generalization for object recognition with multi-task autoencoders. In *Proceedings of the IEEE international conference on computer vision*, pages 2551–2559, 2015.
- [19] Jean-Bastien Grill, Florian Strub, Florent Altché, Corentin Tallec, Pierre H. Richemond, Elena Buchatskaya, Carl Doersch, Bernardo Ávila Pires, Zhaohan Guo, Mohammad Gheshlaghi Azar, Bilal Piot, Koray Kavukcuoglu, Rémi Munos, and Michal Valko. Bootstrap your own latent - a new approach to self-supervised learning. In *NeurIPS*, 2020. URL <https://proceedings.neurips.cc/paper/2020/hash/f3ada80d5c4ee70142b17b8192b2958e-Abstract.html>.
- [20] Ishaan Gulrajani and David Lopez-Paz. In search of lost domain generalization. *arXiv preprint arXiv:2007.01434*, 2020.
- [21] Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross Girshick. Momentum contrast for unsupervised visual representation learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 9729–9738, 2020.
- [22] Zeyi Huang, Haohan Wang, Eric P. Xing, and Dong Huang. Self-challenging improves cross-domain generalization. In *ECCV*, 2020.
- [23] Pang Wei Koh, Shiori Sagawa, Henrik Marklund, Sang Michael Xie, Marvin Zhang, Akshay Balsubramani, Weihua Hu, Michihiro Yasunaga, Richard Lanus Phillips, Irena Gao, et al. WILDS: A benchmark of in-the-wild distribution shifts. *arXiv preprint arXiv:2012.07421*, 2020.
- [24] Vladimir Koltchinskii. Rademacher complexities and bounding the excess risk in active learning. *The Journal of Machine Learning Research*, 11:2457–2485, 2010.
- [25] Masanori Koyama and Shoichiro Yamaguchi. When is invariance useful in an out-of-distribution generalization problem?, 2021.
- [26] David Krueger, Ethan Caballero, Joern-Henrik Jacobsen, Amy Zhang, Jonathan Binas, Dinghuai Zhang, Remi Le Priol, and Aaron Courville. Out-of-distribution generalization via risk extrapolation (Rex). *arXiv preprint arXiv:2003.00688*, 2020.
- [27] Christoph H Lampert, Hannes Nickisch, and Stefan Harmeling. Learning to detect unseen object classes by between-class attribute transfer. In *2009 IEEE Conference on Computer Vision and Pattern Recognition*, pages 951–958. IEEE, 2009.
- [28] Da Li, Yongxin Yang, Yi-Zhe Song, and Timothy M Hospedales. Deeper, broader and artier domain generalization. In *Proceedings of the IEEE international conference on computer vision*, pages 5542–5550, 2017.
- [29] Da Li, Yongxin Yang, Yi-Zhe Song, and Timothy Hospedales. Learning to generalize: Meta-learning for domain generalization. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32, 2018.
- [30] Haoliang Li, Sinno Jialin Pan, Shiqi Wang, and Alex C Kot. Domain generalization with adversarial feature learning. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 5400–5409, 2018.

- [31] Ya Li, Xinmei Tian, Mingming Gong, Yajing Liu, Tongliang Liu, Kun Zhang, and Dacheng Tao. Deep domain generalization via conditional invariant adversarial networks. In *Proceedings of the European Conference on Computer Vision (ECCV)*, pages 624–639, 2018.
- [32] Mingsheng Long, Han Zhu, Jianmin Wang, and Michael I Jordan. Deep transfer learning with joint adaptation networks. In *International conference on machine learning*, pages 2208–2217. PMLR, 2017.
- [33] Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu. Towards deep learning models resistant to adversarial attacks. In *International Conference on Learning Representations*, 2018.
- [34] Mehryar Mohri, Afshin Rostamizadeh, and Ameet Talwalkar. *Foundations of machine learning*. MIT press, 2018.
- [35] Krikamol Muandet, David Balduzzi, and Bernhard Schölkopf. Domain generalization via invariant feature representation. In *International Conference on Machine Learning*, pages 10–18. PMLR, 2013.
- [36] Alfred Müller. Integral probability metrics and their generating classes of functions. *Advances in Applied Probability*, pages 429–443, 1997.
- [37] Hyeonseob Nam, HyunJae Lee, Jongchan Park, Wonjun Yoon, and Donggeun Yoo. Reducing domain gap via style-agnostic networks. *arXiv preprint arXiv:1910.11645*, 2019.
- [38] Balas K Natarajan. On learning sets and functions. *Machine Learning*, 4(1):67–97, 1989.
- [39] Jonas Peters, Peter Bühlmann, and Nicolai Meinshausen. Causal inference by using invariant prediction: identification and confidence intervals. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)*, pages 947–1012, 2016.
- [40] Mohammad Pezeshki, Sékou-Oumar Kaba, Yoshua Bengio, Aaron Courville, Doina Precup, and Guillaume Lajoie. Gradient starvation: A learning proclivity in neural networks. *arXiv preprint arXiv:2011.09468*, 2020.
- [41] Elan Rosenfeld, Pradeep Kumar Ravikumar, and Andrej Risteski. The risks of invariant risk minimization. In *International Conference on Learning Representations*, 2021. URL <https://openreview.net/forum?id=BbNIbVPJ-42>.
- [42] Walter Rudin. *Real and complex analysis*. McGraw-Hill Education, 1987.
- [43] Shiori Sagawa*, Pang Wei Koh*, Tatsunori B. Hashimoto, and Percy Liang. Distributionally robust neural networks. In *International Conference on Learning Representations*, 2020. URL <https://openreview.net/forum?id=ryxGuJrFvS>.
- [44] Shai Shalev-Shwartz and Shai Ben-David. *Understanding machine learning: From theory to algorithms*. Cambridge university press, 2014.
- [45] Aman Sinha, Hongseok Namkoong, Riccardo Volpi, and John Duchi. Certifying some distributional robustness with principled adversarial training. *arXiv preprint arXiv:1710.10571*, 2017.
- [46] Bharath K Sriperumbudur, Kenji Fukumizu, Arthur Gretton, Bernhard Schölkopf, Gert RG Lanckriet, et al. On the empirical estimation of integral probability metrics. *Electronic Journal of Statistics*, 6:1550–1599, 2012.
- [47] Baochen Sun and Kate Saenko. Deep CORAL: Correlation alignment for deep domain adaptation. In *European conference on computer vision*, pages 443–450. Springer, 2016.
- [48] Remi Tachet des Combes, Han Zhao, Yu-Xiang Wang, and Geoffrey J Gordon. Domain adaptation with conditional distribution matching and generalized label shift. *Advances in Neural Information Processing Systems*, 33, 2020.

- [49] Eric Tzeng, Judy Hoffman, Kate Saenko, and Trevor Darrell. Adversarial discriminative domain adaptation. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 7167–7176, 2017.
- [50] Vladimir Vapnik. Principles of risk minimization for learning theory. In *Advances in neural information processing systems*, pages 831–838, 1992.
- [51] Hemanth Venkateswara, Jose Eusebio, Shayok Chakraborty, and Sethuraman Panchanathan. Deep hashing network for unsupervised domain adaptation. In *(IEEE) Conference on Computer Vision and Pattern Recognition (CVPR)*, 2017.
- [52] Riccardo Volpi, Hongseok Namkoong, Ozan Sener, John C Duchi, Vittorio Murino, and Silvio Savarese. Generalizing to unseen domains via adversarial data augmentation. In *NeurIPS*, 2018.
- [53] Minghao Xu, Jian Zhang, Bingbing Ni, Teng Li, Chengjie Wang, Qi Tian, and Wenjun Zhang. Adversarial domain adaptation with domain mixup. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pages 6502–6509, 2020.
- [54] Shen Yan, Huan Song, Nanxiang Li, Lincan Zou, and Liu Ren. Improve unsupervised domain adaptation with mixup training. *arXiv preprint arXiv:2001.00677*, 2020.
- [55] Haotian Ye, Chuanlong Xie, Tianle Cai, Ruichen Li, Zhenguo Li, and Liwei Wang. Towards a theoretical framework of out-of-distribution generalization, 2021.
- [56] Yu Zhang and Qiang Yang. A survey on multi-task learning. *IEEE Transactions on Knowledge and Data Engineering*, pages 1–1, 2021. doi: 10.1109/TKDE.2021.3070203.
- [57] Yuchen Zhang, Tianle Liu, Mingsheng Long, and Michael Jordan. Bridging theory and algorithm for domain adaptation. In *International Conference on Machine Learning*, pages 7404–7413. PMLR, 2019.
- [58] Han Zhao, Shanghang Zhang, Guanhang Wu, José MF Moura, Joao P Costeira, and Geoffrey J Gordon. Adversarial multiple source domain adaptation. *Advances in neural information processing systems*, 31:8559–8570, 2018.
- [59] Han Zhao, Remi Tachet Des Combes, Kun Zhang, and Geoffrey Gordon. On learning invariant representations for domain adaptation. In *International Conference on Machine Learning*, pages 7523–7532. PMLR, 2019.

Checklist

1. For all authors...
 - (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
 - (b) Did you describe the limitations of your work? [Yes]
 - (c) Did you discuss any potential negative societal impacts of your work? [Yes] See the Conclusion section.
 - (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
 - (a) Did you state the full set of assumptions of all theoretical results? [Yes]
 - (b) Did you include complete proofs of all theoretical results? [Yes] See Appendix A.
3. If you ran experiments...
 - (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Appendix C.
 - (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Appendix C.2.
 - (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [N/A] We did try different random seeds, but we chose the worst case scenario.
 - (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Appendix C.2.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
 - (a) If your work uses existing assets, did you cite the creators? [Yes]
 - (b) Did you mention the license of the assets? [Yes]
 - (c) Did you include any new assets either in the supplemental material or as a URL? [Yes]
 - (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes] The license issue is discussed in Appendix C.1.
 - (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [Yes] We are not aware of any personally identifiable information or offensive content in the datasets we use. See Appendix C.1.
5. If you used crowdsourcing or conducted research with human subjects...
 - (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
 - (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
 - (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

A Proofs

In this appendix, we present proofs of our theoretical results in the main paper.

Proposition 4. For $\Gamma \subseteq \mathcal{H}$ and domains \mathcal{S}, \mathcal{T} we have: $\mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq 2\mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T})$.

Proof. We first note that:

$$\begin{aligned} \mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) &= \sup_{h \in \Gamma} |(\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h) - (\epsilon_{\mathcal{S}}^* - \epsilon_{\mathcal{T}}^*))| \leq \sup_{h \in \Gamma} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h)| + |\epsilon_{\mathcal{S}}^* - \epsilon_{\mathcal{T}}^*| \\ &= \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) + |\epsilon_{\mathcal{S}}^* - \epsilon_{\mathcal{T}}^*|. \end{aligned} \quad (\text{A.1})$$

It suffices to prove that $|\epsilon_{\mathcal{S}}^* - \epsilon_{\mathcal{T}}^*| \leq \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T})$. Suppose $\mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) \leq \delta$, and $h_{\mathcal{S}}^* \in \operatorname{argmin}_{h \in \Gamma} \epsilon_{\mathcal{S}}$. Then $\epsilon_{\mathcal{S}}(h_{\mathcal{S}}^*) = \inf_{h \in \Gamma} \epsilon_{\mathcal{S}} = \epsilon_{\mathcal{S}}^*$ and we have:

$$\epsilon_{\mathcal{T}}^* - \delta \leq \epsilon_{\mathcal{T}}(h_{\mathcal{S}}^*) - \delta \leq \epsilon_{\mathcal{S}}(h_{\mathcal{S}}^*) = \epsilon_{\mathcal{S}}^*, \quad (\text{A.2})$$

where in the first inequality, we used $\epsilon_{\mathcal{T}}^* = \inf_{h \in \Gamma} \epsilon_{\mathcal{T}}(h)$, and in the second inequality, we used that for any $h \in \Gamma$, we have:

$$\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{S}}(h) \leq \sup_{h \in \Gamma} |\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{S}}(h)| = \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) \leq \delta. \quad (\text{A.3})$$

Hence, we have $\epsilon_{\mathcal{T}}^* - \epsilon_{\mathcal{S}}^* \leq \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T})$. Since $\mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T})$ is symmetric in \mathcal{T} and \mathcal{S} , we also have $\epsilon_{\mathcal{S}}^* - \epsilon_{\mathcal{T}}^* \leq \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T})$. Hence we have proved $|\epsilon_{\mathcal{S}}^* - \epsilon_{\mathcal{T}}^*| \leq \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T})$. \square

Proposition 5 (equivalence between transferability and transfer measures). Let $\delta_{\mathcal{S}} > 0$ and $\Gamma = \operatorname{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})$ and suppose $\inf_{h \in \Gamma} \epsilon_{\mathcal{T}}(h) = \inf_{h \in \mathcal{H}} \epsilon_{\mathcal{T}}(h)$. If $\mathsf{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \delta$ or $\mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq \delta$, then \mathcal{S} is $(\delta_{\mathcal{S}}, \delta + \delta_{\mathcal{S}})$ -transferable to \mathcal{T} . Furthermore, if \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{T}})$ -transferable to \mathcal{T} , then $\mathsf{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \delta_{\mathcal{T}}$ and $\mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq \max\{\delta_{\mathcal{S}}, \delta_{\mathcal{T}}\}$.

Proof. If $\mathsf{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) = \sup_{h \in \Gamma} \epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* - (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*) \leq \delta$, then for any $h \in \Gamma = \operatorname{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})$ we have $\epsilon_{\mathcal{S}}(h) \leq \epsilon_{\mathcal{S}}^* + \delta_{\mathcal{S}}$ and

$$\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* \leq \epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^* + \delta \leq \delta_{\mathcal{S}} + \delta. \quad (\text{A.4})$$

Since we assume $\epsilon_{\mathcal{T}}^* = \inf_{h \in \Gamma} \epsilon_{\mathcal{T}}(h) = \inf_{h \in \mathcal{H}} \epsilon_{\mathcal{T}}(h)$, we obtain that \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{S}} + \delta)$ -transferable to \mathcal{T} . If $\mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq \delta$, then $\mathsf{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \delta$, and \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{S}} + \delta)$ -transferable to \mathcal{T} .

If \mathcal{S} is $(\delta_{\mathcal{S}}, \delta_{\mathcal{T}})$ -transferable to \mathcal{T} , then for any $h \in \operatorname{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})$, we have:

$$\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* - (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*) \leq \epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* \leq \delta_{\mathcal{T}}. \quad (\text{A.5})$$

We also have $\mathsf{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \delta_{\mathcal{T}}$ from (A.5). Moreover, we can derive that:

$$\mathsf{T}_\Gamma(\mathcal{T} \parallel \mathcal{S}) = \sup_{h \in \Gamma} (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*) - (\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^*) \leq \sup_{h \in \Gamma} (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*) \leq \delta_{\mathcal{S}}, \quad (\text{A.6})$$

and thus $\mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq \max\{\delta_{\mathcal{S}}, \delta_{\mathcal{T}}\}$ from the definition. \square

Proposition 6 (pseudo-metric). For a general loss $\epsilon_{\mathcal{D}}$ as in (1), $\mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T})$ is a pseudo-metric, i.e., for any distributions $\mathcal{S}, \mathcal{T}, \mathcal{P}$ on the same underlying space, we have $\mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{S}) = 0$, $\mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) = \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{T}, \mathcal{S})$ (symmetry), and $\mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) \leq \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{P}) + \mathsf{T}_\Gamma^\mathbb{F}(\mathcal{P}, \mathcal{T})$ (triangle inequality).

Proof. $\mathsf{T}_\Gamma(\mathcal{S}, \mathcal{S}) = 0$ and $\mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) = \mathsf{T}_\Gamma(\mathcal{T}, \mathcal{S})$ follow from the definition. Denote the excess risk $\operatorname{exc}_{\mathcal{S}}(h) = \epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*$ (we could change the letter \mathcal{S} here). The triangle inequality can be derived as:

$$\begin{aligned} \mathsf{T}_\Gamma(\mathcal{S}, \mathcal{T}) &= \sup_{h \in \Gamma} |\operatorname{exc}_{\mathcal{S}}(h) - \operatorname{exc}_{\mathcal{T}}(h)| \\ &= \sup_{h \in \Gamma} |\operatorname{exc}_{\mathcal{S}}(h) - \operatorname{exc}_{\mathcal{P}}(h) + \operatorname{exc}_{\mathcal{P}}(h) - \operatorname{exc}_{\mathcal{T}}(h)| \\ &\leq \sup_{h \in \Gamma} |\operatorname{exc}_{\mathcal{S}}(h) - \operatorname{exc}_{\mathcal{P}}(h)| + \sup_{h \in \Gamma} |\operatorname{exc}_{\mathcal{P}}(h) - \operatorname{exc}_{\mathcal{T}}(h)| \\ &= \mathsf{T}_\Gamma(\mathcal{S}, \mathcal{P}) + \mathsf{T}_\Gamma(\mathcal{P}, \mathcal{T}). \end{aligned} \quad (\text{A.7})$$

Similarly, we can derive $\mathsf{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \mathsf{T}_\Gamma(\mathcal{S} \parallel \mathcal{P}) + \mathsf{T}_\Gamma(\mathcal{P} \parallel \mathcal{T})$. \square

Proposition 7 (equivalence with total variation). For binary classification with labels $\{-1, 1\}$, given the 0-1 loss $\epsilon_{\mathcal{D}} = \epsilon_{\mathcal{D}}^{0-1}$, we have $\mathbb{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) \leq d_{\text{TV}}(\mathcal{S}, \mathcal{T})$ for domains \mathcal{S}, \mathcal{T} and any $\Gamma \subseteq \mathcal{H}$. Denote \mathcal{H}_t to be the set of all binary classifiers. Then we have $d_{\text{TV}}(\mathcal{S}, \mathcal{T}) \leq 4\mathbb{T}_{\mathcal{H}_t}^{\mathbb{F}}(\mathcal{S}, \mathcal{T})$.

Proof. Let us first recall the definition of IPMs:

$$d_{\mathcal{F}}(\mathcal{S}, \mathcal{T}) = \sup_{f \in \mathcal{F}} \left| \sum_y \int f(x, y)(p_{\mathcal{S}}(x, y) - p_{\mathcal{T}}(x, y))dx \right|. \quad (\text{A.8})$$

The symmetric transfer measure $\mathbb{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T})$ and the total variation can be represented as:

$$\mathbb{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) = d_{\mathcal{F}_{\Gamma}}(\mathcal{S}, \mathcal{T}), \quad d_{\text{TV}}(\mathcal{S}, \mathcal{T}) = d_{\mathcal{F}_{\text{TV}}}(\mathcal{S}, \mathcal{T}), \quad (\text{A.9})$$

with $\mathcal{F}_{\Gamma} := \{(x, y) \mapsto \mathbb{1}(h(x) \neq y), h \in \Gamma\}$, $\mathcal{F}_{\text{TV}} = \{f : \|f\|_{\infty} \leq 1\}$ (see also Appendix B.2). The first sentence follows from $\mathcal{F}_{\Gamma} \subseteq \mathcal{F}_{\text{TV}}$, and the definition of IPM.

Now let us prove the case when $\Gamma = \mathcal{H}_t$ is unconstrained. Suppose $\mathbb{T}_{\mathcal{H}_t}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) \leq \delta$, then for any binary classifier h , we have $|\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h)| \leq \delta$. For simplicity, denote the difference of the two distributions as:

$$d(x, y) := p_{\mathcal{S}}(x, y) - p_{\mathcal{T}}(x, y). \quad (\text{A.10})$$

Take h_+ to be the following (note that we allow the classifier to take a garbage value 0):

$$h_+(x) = \begin{cases} 0 & \text{if } x \in \mathcal{B}_{>>} := \{x \in \mathcal{X} : d(x, 1) \geq 0 \text{ and } d(x, -1) \geq 0\} \\ -1 & \text{if } x \in \mathcal{B}_{><} := \{x \in \mathcal{X} : d(x, 1) \geq 0, d(x, -1) < 0\} \\ 1 & \text{if } x \in \mathcal{B}_{<>} := \{x \in \mathcal{X} : d(x, 1) < 0, d(x, -1) \geq 0\} \\ 1 & \text{if } x \in \mathcal{B}_{<<}^- := \{x \in \mathcal{X} : d(x, 1) < d(x, -1) < 0\} \\ -1 & \text{if } x \in \mathcal{B}_{<<}^+ := \{x \in \mathcal{X} : 0 > d(x, 1) \geq d(x, -1)\} \end{cases}, \quad (\text{A.11})$$

and denote $\mathcal{B}_{<<} := \mathcal{B}_{<<}^- \cup \mathcal{B}_{<<}^+$. Then we have from the definition:

$$\begin{aligned} \epsilon_{\mathcal{S}}(h_+) - \epsilon_{\mathcal{T}}(h_+) &= \sum_y \int (p_{\mathcal{S}}(x, y) - p_{\mathcal{T}}(x, y)) \mathbb{1}(h_+(x) \neq y) dx \\ &= \int d(x, 1) \mathbb{1}(h_+(x) \neq 1) + d(x, -1) \mathbb{1}(h_+(x) \neq -1) dx \\ &= \int_{\mathcal{B}_{>>}} d(x, 1) + d(x, -1) dx + \int_{\mathcal{B}_{><}} d(x, 1) dx + \int_{\mathcal{B}_{<>}} d(x, -1) dx \\ &\quad - \int_{\mathcal{B}_{<<}} \min\{-d(x, 1), -d(x, -1)\} dx. \end{aligned} \quad (\text{A.12})$$

Moreover, one can verify that $\epsilon_{\mathcal{S}}(h_+) - \epsilon_{\mathcal{T}}(h_+) = \sup_{h \in \mathcal{H}_t} \epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h)$. Similarly, let us define h_- to be:

$$h_-(x) = \begin{cases} 0 & \text{if } x \in \mathcal{B}_{<<} := \{x \in \mathcal{X} : d(x, 1) < 0 \text{ and } d(x, -1) < 0\} \\ -1 & \text{if } x \in \mathcal{B}_{<>} := \{x \in \mathcal{X} : d(x, 1) < 0, d(x, -1) \geq 0\} \\ 1 & \text{if } x \in \mathcal{B}_{><} := \{x \in \mathcal{X} : d(x, 1) \geq 0, d(x, -1) < 0\} \\ -1 & \text{if } x \in \mathcal{B}_{>>}^- := \{x \in \mathcal{X} : 0 \leq d(x, 1) < d(x, -1)\} \\ 1 & \text{if } x \in \mathcal{B}_{>>}^+ := \{x \in \mathcal{X} : d(x, 1) \geq d(x, -1) \geq 0\} \end{cases}. \quad (\text{A.13})$$

Then we have from the definition:

$$\begin{aligned} \epsilon_{\mathcal{T}}(h_-) - \epsilon_{\mathcal{S}}(h_-) &= - \sum_y \int (p_{\mathcal{S}}(x, y) - p_{\mathcal{T}}(x, y)) \mathbb{1}(h_-(x) \neq y) dx \\ &= \int -d(x, 1) \mathbb{1}(h_-(x) \neq 1) - d(x, -1) \mathbb{1}(h_-(x) \neq -1) dx \\ &= \int_{\mathcal{B}_{<<}} -d(x, 1) - d(x, -1) dx + \int_{\mathcal{B}_{><}} -d(x, -1) dx + \int_{\mathcal{B}_{<>}} -d(x, 1) dx \\ &\quad - \int_{\mathcal{B}_{>>}} \min\{d(x, 1), d(x, -1)\} dx. \end{aligned} \quad (\text{A.14})$$

Moreover, $\epsilon_{\mathcal{T}}(h_-) - \epsilon_{\mathcal{S}}(h_-) = \sup_{h \in \mathcal{H}_t} \epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{S}}(h)$. Summing over (A.12) and (A.14) we have:

$$\begin{aligned}
2 \sup_{h \in \mathcal{H}_t} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h)| &\geq |\epsilon_{\mathcal{S}}(h_+) - \epsilon_{\mathcal{T}}(h_+)| + |\epsilon_{\mathcal{T}}(h_-) - \epsilon_{\mathcal{S}}(h_-)| \\
&\geq \epsilon_{\mathcal{S}}(h_+) - \epsilon_{\mathcal{T}}(h_+) + \epsilon_{\mathcal{T}}(h_-) - \epsilon_{\mathcal{S}}(h_-) \\
&= \int_{\mathcal{B}_{>>}} \max\{d(x, 1), d(x, -1)\} dx + \int_{\mathcal{B}_{><}} d(x, 1) - d(x, -1) dx \\
&\quad + \int_{\mathcal{B}_{<>}} -d(x, 1) + d(x, -1) dx + \int_{\mathcal{B}_{<<}} \max\{-d(x, 1), -d(x, -1)\} dx.
\end{aligned} \tag{A.15}$$

On the other hand, we can compute the total variation between \mathcal{S} and \mathcal{T} :

$$\begin{aligned}
d_{\text{TV}}(\mathcal{S}, \mathcal{T}) &= \sum_y \int |p_{\mathcal{S}}(x, y) - p_{\mathcal{T}}(x, y)| dx \\
&= \int |d(x, 1)| + |d(x, -1)| dx \\
&= \int_{\mathcal{B}_{>>}} d(x, 1) + d(x, -1) dx + \int_{\mathcal{B}_{><}} d(x, 1) - d(x, -1) dx \\
&\quad + \int_{\mathcal{B}_{<>}} -d(x, 1) + d(x, -1) dx + \int_{\mathcal{B}_{<<}} -d(x, 1) - d(x, -1) dx \\
&\leq 2 \int_{\mathcal{B}_{>>}} \max\{d(x, 1), d(x, -1)\} dx + 2 \int_{\mathcal{B}_{><}} d(x, 1) - d(x, -1) dx \\
&\quad + 2 \int_{\mathcal{B}_{<>}} -d(x, 1) + d(x, -1) dx + \int_{\mathcal{B}_{<<}} 2 \max\{-d(x, 1), -d(x, -1)\} dx \\
&\leq 4 \sup_{h \in \mathcal{H}_t} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h)| = 4\mathbb{T}_{\mathcal{H}_t}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}),
\end{aligned} \tag{A.16}$$

where in the last line we used (A.15). \square

In the proof above, we assumed a classifier $h \in \Gamma$ is allowed to take a garbage value 0 if it is not sure which label to choose. This is a mild assumption that can hold in practice.

Lemma 9' (reduction of estimation error). *Suppose $\widehat{\mathcal{S}}$ and $\widehat{\mathcal{T}}$ are i.i.d. sample distributions drawn from distributions of \mathcal{S} and \mathcal{T} , then for any $\Gamma \subseteq \mathcal{H}$ we have:*

$$\mathbb{T}_{\Gamma}(\mathcal{S} \| \mathcal{T}) \leq \mathbb{T}_{\Gamma}(\widehat{\mathcal{S}} \| \widehat{\mathcal{T}}) + 2\text{est}_{\Gamma}(\mathcal{S}) + 2\text{est}_{\Gamma}(\mathcal{T}), \tag{A.17}$$

$$\mathbb{T}_{\Gamma}(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_{\Gamma}(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + 2\text{est}_{\Gamma}(\mathcal{S}) + 2\text{est}_{\Gamma}(\mathcal{T}), \tag{A.18}$$

$$\mathbb{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_{\Gamma}^{\mathbb{F}}(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + \text{est}_{\Gamma}(\mathcal{S}) + \text{est}_{\Gamma}(\mathcal{T}), \tag{A.19}$$

where we define

$$\text{est}_{\Gamma}(\mathcal{S}) = \sup_{h \in \Gamma} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\widehat{\mathcal{S}}}(h)|, \quad \text{est}_{\Gamma}(\mathcal{T}) = \sup_{h \in \Gamma} |\epsilon_{\mathcal{T}}(h) - \epsilon_{\widehat{\mathcal{T}}}(h)|. \tag{A.20}$$

Proof. We prove the first inequality for example and others follow similarly. Note that:

$$\begin{aligned}
\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* - \epsilon_{\mathcal{S}}(h) + \epsilon_{\mathcal{S}}^* &= \epsilon_{\mathcal{T}}(h) - \epsilon_{\widehat{\mathcal{T}}}(h) + \epsilon_{\widehat{\mathcal{T}}}(h) - \epsilon_{\mathcal{T}}^* - \epsilon_{\widehat{\mathcal{T}}}^* + \epsilon_{\widehat{\mathcal{T}}}^* - \epsilon_{\mathcal{S}}(h) - \epsilon_{\widehat{\mathcal{S}}}(h) + \epsilon_{\widehat{\mathcal{S}}}(h) + \\
&\quad + \epsilon_{\mathcal{S}}^* - \epsilon_{\widehat{\mathcal{S}}}^* + \epsilon_{\widehat{\mathcal{S}}}^* \\
&= (\epsilon_{\widehat{\mathcal{T}}}(h) - \epsilon_{\widehat{\mathcal{T}}}^* - \epsilon_{\widehat{\mathcal{S}}}(h) + \epsilon_{\widehat{\mathcal{S}}}^*) + (\epsilon_{\mathcal{T}}(h) - \epsilon_{\widehat{\mathcal{T}}}(h)) + (\epsilon_{\widehat{\mathcal{T}}}^* - \epsilon_{\mathcal{T}}^*) + \\
&\quad + (\epsilon_{\widehat{\mathcal{S}}}(h) - \epsilon_{\mathcal{S}}(h)) + (\epsilon_{\mathcal{S}}^* - \epsilon_{\widehat{\mathcal{S}}}^*).
\end{aligned} \tag{A.21}$$

Taking the supremum on both sides we have:

$$\mathbb{T}_{\Gamma}(\mathcal{S} \| \mathcal{T}) \leq \mathbb{T}_{\Gamma}(\widehat{\mathcal{S}} \| \widehat{\mathcal{T}}) + \sup_{h \in \Gamma} |\epsilon_{\mathcal{T}}(h) - \epsilon_{\widehat{\mathcal{T}}}(h)| + \epsilon_{\widehat{\mathcal{T}}}^* - \epsilon_{\mathcal{T}}^* + \sup_{h \in \Gamma} |\epsilon_{\widehat{\mathcal{S}}}(h) - \epsilon_{\mathcal{S}}(h)| + \epsilon_{\mathcal{S}}^* - \epsilon_{\widehat{\mathcal{S}}}^*. \tag{A.22}$$

Take $h_{\mathcal{T}}^* \in \operatorname{argmin}_{h \in \Gamma} \epsilon_{\mathcal{T}}(h)$ to be an optimal classifier. We can derive:

$$\epsilon_{\mathcal{T}}^* \leq \epsilon_{\hat{\mathcal{T}}}(h_{\mathcal{T}}^*) \leq \epsilon_{\mathcal{T}}^*(h_{\mathcal{T}}^*) + \operatorname{est}_{\Gamma}(\mathcal{T}) = \epsilon_{\mathcal{T}}^* + \operatorname{est}_{\Gamma}(\mathcal{T}). \quad (\text{A.23})$$

Therefore, $\epsilon_{\hat{\mathcal{T}}}^* - \epsilon_{\mathcal{T}}^* \leq \operatorname{est}_{\Gamma}(\mathcal{T})$. Similarly, $\epsilon_{\hat{\mathcal{S}}}^* - \epsilon_{\mathcal{S}}^* \leq \operatorname{est}_{\Gamma}(\mathcal{S})$. Combining all those above we obtain (A.17). \square

Theorem 10' (estimation error with Rademacher complexity). *Given 0-1 loss $\epsilon_{\mathcal{D}} = \epsilon_{\mathcal{D}}^{0-1}$, suppose $\hat{\mathcal{S}}$ and $\hat{\mathcal{T}}$ are sample sets with m and k samples drawn i.i.d. from distributions \mathcal{S} and \mathcal{T} , respectively. For any $\Gamma \subseteq \mathcal{H}$ any of the following holds w.p. $1 - \delta$:*

$$\mathsf{T}_{\Gamma}(\mathcal{S} \parallel \mathcal{T}) \leq \mathsf{T}_{\Gamma}(\hat{\mathcal{S}} \parallel \hat{\mathcal{T}}) + 4\mathfrak{R}_m(\mathcal{F}_{\Gamma}) + 4\mathfrak{R}_k(\mathcal{F}_{\Gamma}) + 2\sqrt{\frac{\log(4/\delta)}{2m}} + 2\sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{A.24})$$

$$\mathsf{T}_{\Gamma}(\mathcal{S}, \mathcal{T}) \leq \mathsf{T}_{\Gamma}(\hat{\mathcal{S}}, \hat{\mathcal{T}}) + 4\mathfrak{R}_m(\mathcal{F}_{\Gamma}) + 4\mathfrak{R}_k(\mathcal{F}_{\Gamma}) + 2\sqrt{\frac{\log(4/\delta)}{2m}} + 2\sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{A.25})$$

$$\mathsf{T}_{\Gamma}^{\mathbb{F}}(\mathcal{S}, \mathcal{T}) \leq \mathsf{T}_{\Gamma}^{\mathbb{F}}(\hat{\mathcal{S}}, \hat{\mathcal{T}}) + 2\mathfrak{R}_m(\mathcal{F}_{\Gamma}) + 2\mathfrak{R}_k(\mathcal{F}_{\Gamma}) + \sqrt{\frac{\log(4/\delta)}{2m}} + \sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{A.26})$$

where $\mathcal{F}_{\Gamma} := \{(z, y) \mapsto \mathbb{1}(h(z) \neq y), h \in \Gamma\}$. If furthermore, Γ is a set of binary classifiers with labels $\{-1, 1\}$, then $2\mathfrak{R}_m(\mathcal{F}_{\Gamma}) = \mathfrak{R}_m(\Gamma)$, $2\mathfrak{R}_k(\mathcal{F}_{\Gamma}) = \mathfrak{R}_k(\Gamma)$.

Proof. We use the following lemma, which is a slight adaptation of Mohri et al. [34], Theorem 3.3:

Lemma 11. *Let \mathcal{F} be a family of functions from $\mathcal{X} \times \mathcal{Y}$ to $[0, 1]$. Then for any $\delta > 0$, with probability at least $1 - \delta$ over the draw from a distribution \mathcal{S} of an i.i.d. samples S of size m , $\{w_i\}_{i=1}^m$, the following holds for all $f \in \mathcal{F}$,*

$$\left| \mathbb{E}[f(w)] - \frac{1}{m} \sum_{i=1}^m f(w_i) \right| \leq 2\mathfrak{R}_m(\mathcal{F}) + \sqrt{\frac{\log(2/\delta)}{2m}}. \quad (\text{A.27})$$

Proof. From Mohri et al. [34], Theorem 3.3, we know with probability at least $1 - \delta/2$, the following holds

$$\mathbb{E}[f(w)] - \frac{1}{m} \sum_{i=1}^m f(w_i) \leq 2\mathfrak{R}_m(\mathcal{F}) + \sqrt{\frac{\log(2/\delta)}{2m}}. \quad (\text{A.28})$$

This result relies on applying McDiarmid's inequality on $\Phi(S) = \sup_{f \in \mathcal{F}} \mathbb{E}[f] - \frac{1}{m} \sum_{i=1}^m f(w_i)$. By repeating the same proof and applying McDiarmid's inequality on $\Phi'(S) = \sup_{f \in \mathcal{F}} \frac{1}{m} \sum_{i=1}^m f(w_i) - \mathbb{E}[f]$, we conclude that with probability at least $1 - \delta/2$, the following holds

$$\frac{1}{m} \sum_{i=1}^m f(w_i) - \mathbb{E}[f(w)] \leq 2\mathfrak{R}_m(\mathcal{F}) + \sqrt{\frac{\log(2/\delta)}{2m}}. \quad (\text{A.29})$$

Therefore, with union bound we obtain that with probability (w.p.) at least $1 - \delta$, we have (A.27). \square

Let us now go back to the proof of Theorem 10'. Taking $\mathcal{F}_{\Gamma} = \{(z, y) \mapsto \mathbb{1}(h(z) \neq y), h \in \Gamma\}$, we can derive from the theorem above that w.p. at least $1 - \delta$:

$$\operatorname{est}_{\Gamma}(\mathcal{S}) = \sup_{h \in \Gamma} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\hat{\mathcal{S}}}(h)| \leq 2\mathfrak{R}_m(\mathcal{F}_{\Gamma}) + \sqrt{\frac{\log(2/\delta)}{2m}}. \quad (\text{A.30})$$

With (A.30) we know that with probability at least $1 - \delta/2$:

$$\operatorname{est}_{\Gamma}(\mathcal{S}) = \sup_{h \in \Gamma} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\hat{\mathcal{S}}}(h)| \leq 2\mathfrak{R}_m(\mathcal{F}_{\Gamma}) + \sqrt{\frac{\log(4/\delta)}{2m}}, \quad (\text{A.31})$$

and w.p. at least $1 - \delta/2$:

$$\text{est}_\Gamma(\mathcal{T}) = \sup_{h \in \Gamma} |\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^*(h)| \leq 2\mathfrak{R}_k(\mathcal{F}_\Gamma) + \sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{A.32})$$

therefore from union bound w.p. at least $1 - \delta$ we have:

$$\text{est}_\Gamma(\mathcal{S}) + \text{est}_\Gamma(\mathcal{T}) \leq 2\mathfrak{R}_m(\mathcal{F}_\Gamma) + 2\mathfrak{R}_k(\mathcal{F}_\Gamma) + \sqrt{\frac{\log(4/\delta)}{2m}} + \sqrt{\frac{\log(4/\delta)}{2k}}. \quad (\text{A.33})$$

Moreover, from Lemma 3.4 of Mohri et al. [34] we have

$$2\mathfrak{R}_m(\mathcal{F}_\Gamma) = \mathfrak{R}_m(\Gamma), \quad 2\mathfrak{R}_k(\mathcal{F}_\Gamma) = \mathfrak{R}_k(\Gamma), \quad (\text{A.34})$$

for binary classification. The rest follows from Lemma 9'. \square

Proposition 11 (transfer measure with a surrogate loss). *Given surrogate loss $\epsilon_{\mathcal{D}} \geq \epsilon_{\mathcal{D}}^{0-1}$ on a general domain \mathcal{D} . Suppose $\Gamma = \text{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})$ and denote $\epsilon_{\mathcal{T}}^* = \inf_{h \in \Gamma} \epsilon_{\mathcal{T}}(h)$, $\epsilon_{\mathcal{S}}^* = \inf_{h \in \Gamma} \epsilon_{\mathcal{S}}(h)$, $(\epsilon_{\mathcal{T}}^{0-1})^* = \inf_{h \in \mathcal{H}} \epsilon_{\mathcal{T}}^{0-1}(h)$. If the following holds:*

$$\mathbb{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) = \sup_{h \in \Gamma} \epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{T}}^* - (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*) \leq \delta, \quad (8)$$

then we have $\text{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}}) \subseteq \text{argmin}(\epsilon_{\mathcal{T}}^{0-1}, \delta + \delta_{\mathcal{S}} + \epsilon_{\mathcal{T}}^* - (\epsilon_{\mathcal{T}}^{0-1})^*)$.

Proof. Suppose (8) holds and thus for any $h \in \text{argmin}(\epsilon_{\mathcal{S}}, \delta_{\mathcal{S}})$ we have:

$$\epsilon_{\mathcal{T}}^{0-1}(h) \leq \epsilon_{\mathcal{T}}(h) \leq (\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{S}}^*) + \delta + \epsilon_{\mathcal{T}}^* \leq \delta_{\mathcal{S}} + \delta + \epsilon_{\mathcal{T}}^*. \quad (\text{A.35})$$

The rest follows from definitions. \square

Proposition 12 (domain generalization guarantee). *Suppose we have n distributions $\mathcal{S}_1^g, \dots, \mathcal{S}_n^g$ which satisfy*

$$\sup_{h \in \Gamma} \max_i \epsilon_{\mathcal{S}_i^g}(h) - \min_j \epsilon_{\mathcal{S}_j^g}(h) \leq \delta. \quad (\text{A.36})$$

Then for any two distributions $\mathcal{T}_1^g, \mathcal{T}_2^g$ in $\text{conv}(\mathcal{S}_1^g, \dots, \mathcal{S}_n^g)$, we have $\mathbb{T}_\Gamma^g(\mathcal{T}_1^g, \mathcal{T}_2^g) \leq \delta$.

Proof. For the ease of notation we omit the superscript g in the proof. We treat distributions as probabilistic measures and thus for any $h \in \mathcal{H}$, $\epsilon_{\mathcal{D}}(h)$ is a linear function of \mathcal{D} , if we treat \mathcal{D} as a probability measure. It suffices to prove for a linear function f , we have:

$$|f(\sum_i \pi_i \mathcal{S}_i) - f(\sum_j \pi'_j \mathcal{S}_j)| \leq \max_i f(\mathcal{S}_i) - \min_j f(\mathcal{S}_j), \quad (\text{A.37})$$

where $\pi_i, \pi'_j \geq 0$ and $\sum_i \pi_i = \sum_j \pi'_j = 1$. This is because

$$\begin{aligned} |f(\sum_i \pi_i \mathcal{S}_i) - f(\sum_j \pi'_j \mathcal{S}_j)| &= |f(\sum_{i,j} \pi_i \pi'_j \mathcal{S}_i) - f(\sum_{i,j} \pi_i \pi'_j \mathcal{S}_j)| \\ &= |f(\sum_{i,j} \pi_i \pi'_j (\mathcal{S}_i - \mathcal{S}_j))| \\ &= |\sum_{i,j} \pi_i \pi'_j f(\mathcal{S}_i - \mathcal{S}_j)| \\ &\leq \sum_{i,j} \pi_i \pi'_j |f(\mathcal{S}_i - \mathcal{S}_j)| \\ &\leq \max_{i,j} |f(\mathcal{S}_i) - f(\mathcal{S}_j)| \\ &= \max_i f(\mathcal{S}_i) - \min_j f(\mathcal{S}_j). \end{aligned} \quad (\text{A.38})$$

The second and the third lines follow from the linearity of f and the fourth line follows from triangle inequality. Therefore, taking $f : \mathcal{D} \mapsto \epsilon_{\mathcal{D}}(h)$ for any $h \in \Gamma$, and $\mathcal{T}_1 = \sum_i \pi_i \mathcal{S}_i$, $\mathcal{T}_2 = \sum_j \pi'_j \mathcal{S}_j$, we can derive from (A.38) that:

$$|\epsilon_{\mathcal{T}_1}(h) - \epsilon_{\mathcal{T}_2}(h)| \leq \max_i \epsilon_{\mathcal{S}_i}(h) - \min_j \epsilon_{\mathcal{S}_j}(h), \quad (\text{A.39})$$

for any $h \in \Gamma$. Taking the supremum over h on both sides we finish the proof. \square

Theorem 12 (optimization guarantee). Assume that the function $q(\cdot, x)$ is L_θ Lipschitz continuous for any x . Suppose we have learned a feature embedding g and a classifier h such that the loss functional $\epsilon_{\mathcal{S}_i^g} : \mathcal{H} \rightarrow \mathbb{R}$ is L_ℓ Lipschitz continuous w.r.t. distribution \mathcal{S}_i^g for $i \in [n]$ and

$$\max_{\|\theta' - \theta\| \leq \delta} \frac{1}{n} \sum_{i=1}^n \epsilon_{\mathcal{S}_i}(h \circ g) + (\max_i \epsilon_{\mathcal{S}_i}(h' \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h' \circ g)) \leq \eta, \quad (15)$$

where θ, θ' are parameters of h and h' . Then for any $h' \in \Gamma = \{q(\theta', \cdot) : \|\theta - \theta'\| \leq \delta\}$, we have:

$$\mathbb{T}_\Gamma^{\mathcal{F}}(\mathcal{T}_1^g, \mathcal{T}_2^g) \leq \eta, \quad \epsilon_{\mathcal{S}_i}(h' \circ g) \leq \eta + L_\ell L_\theta \delta, \quad \epsilon_{\mathcal{T}}(h' \circ g) \leq 2\eta + L_\ell L_\theta \delta, \quad (16)$$

for any $\mathcal{T}_1^g, \mathcal{T}_2^g, \mathcal{T}^g \in \text{conv}(\mathcal{S}_1^g, \dots, \mathcal{S}_n^g)$ and any $i \in [n]$.

Proof. From (15) we know that:

$$\max_i \epsilon_{\mathcal{S}_i}(h' \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h' \circ g) \leq \eta, \quad (A.40)$$

for any $h' = q(\theta', \cdot)$ and $\|\theta' - \theta\|_2 \leq \delta$. Taking $h' = h$, we obtain that:

$$\begin{aligned} \max_i \epsilon_{\mathcal{S}_i}(h \circ g) &= \min_i \epsilon_{\mathcal{S}_i}(h \circ g) + \max_i \epsilon_{\mathcal{S}_i}(h \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h \circ g) \\ &\leq \frac{1}{n} \sum_{i=1}^n \epsilon_{\mathcal{S}_i}(h \circ g) + \max_i \epsilon_{\mathcal{S}_i}(h \circ g) - \min_i \epsilon_{\mathcal{S}_i}(h \circ g) \\ &\leq \eta. \end{aligned} \quad (A.41)$$

In other words, for any $i \in [n] = \{1, \dots, n\}$, $\epsilon_{\mathcal{S}_i}(h \circ g) \leq \eta$ holds. We have from Theorem 25 $\|h - h'\|_{1, \mathcal{D}} \leq L_\theta \delta$ for any probability measure \mathcal{D} . Using Definition 19 we know that $|\epsilon_{\mathcal{S}_i}(h' \circ g) - \epsilon_{\mathcal{S}_i}(h \circ g)| \leq L_\ell L_\theta \delta$. Therefore, for any $h' \in \Gamma$, we have:

$$\epsilon_{\mathcal{S}_i}(h' \circ g) \leq \epsilon_{\mathcal{S}_i}(h \circ g) + L_\ell L_\theta \delta \leq \eta + L_\ell L_\theta \delta. \quad (A.42)$$

From (A.40) and Prop. 12, for any $\mathcal{T} \in \text{conv}(\mathcal{S}_1, \dots, \mathcal{S}_n)$ and any \mathcal{S}_i , $\mathbb{T}_\Gamma^{\mathcal{F}}(\mathcal{T}, \mathcal{S}_i) \leq \eta$ holds, and thus from the definition of $\mathbb{T}_\Gamma^{\mathcal{F}}$ we have the third inequality of (16). The first inequality of (16) follows from Proposition 12. \square

B Additional theoretical results

In this appendix we present additional theoretical results as supplementary material.

B.1 Necessity of excess risks

We give an example where the realizable transfer measure is large but the source domain is transferable to the target domain.

Example 13. Consider two distributions:

$$p_{\mathcal{S}}(X, Y) = \begin{cases} 0.5 & Y = 1, -1 \leq X < 0, \\ 0.5 & Y = -1, 0 \leq X < 1 \end{cases}, \quad p_{\mathcal{T}}(X, Y) = \begin{cases} 0.2 & Y = 1, -1 \leq X < 0, \\ 0.2 & Y = -1, 0 \leq X < 1 \\ 0.3 & Y = 1, -1 \leq X < 1 \\ 0.3 & Y = -1, -1 \leq X < 1 \end{cases}, \quad (B.1)$$

and the hypothesis class \mathcal{H} to be the same as Example 8. Then \mathcal{S} is $(0.5\delta, 0.2\delta)$ -transferable (Definition 1) for small δ . However, for any Γ that includes the optimal (source and target) classifier h_0 we have

$$\mathbb{T}_\Gamma^{\mathcal{F}}(\mathcal{S}, \mathcal{T}) = \sup_{h \in \Gamma} |\epsilon_{\mathcal{S}}(h) - \epsilon_{\mathcal{T}}(h)| \geq |\epsilon_{\mathcal{S}}(h_0) - \epsilon_{\mathcal{T}}(h_0)| = 0.3. \quad (B.2)$$

The example above shows that when the optimal errors of two domains are dissimilar, simply measuring the difference of errors cannot fully describe the transferability. Instead, we should consider the difference of the *excess risks* as in Definition 1.

B.2 Other IPMs

Different choices the the function class in (6) could lead to various definitions [46]:

- maximum mean discrepancy (MMD): $\mathcal{F}_{\text{MMD}} = \{f : \|f\|_{\text{Hilbert}} \leq 1\}$ where the norm $\|f\|_{\text{Hilbert}}$ is defined on a reproducing kernel Hilbert space (RKHS).
- Wasserstein distance: $\mathcal{F}_{\text{Wasserstein}} = \{f : \|f\|_L \leq 1\}$ where $\|f\|_L = 1$ is the Lipschitz semi-norm of a real valued function f . It is also known as the Kantorovich metric.
- total variation metric: $\mathcal{F}_{\text{TV}} = \{\|f\|_\infty \leq 1\}$ where $\|f\|_\infty = \sup_x \{|f(x)|\}$ is the bound of f . This measures the total difference of the probability density functions (PDFs).
- Dudley metric: $\mathcal{F}_{\text{Dudley}} = \{\|f\|_\infty + \|f\|_L \leq 1\}$.
- Kolmogorov distance: $\mathcal{F}_{\text{Kolmogorov}} = \{x \mapsto \mathbb{1}(x \leq t), t \in \mathbb{R}^d\}$ where we have $x \in \mathbb{R}^d$ and $x \leq t$ means that for all components we have $x_i \leq t_i$. This measures the total difference of the cumulative density functions (CDFs).

B.3 Estimation of transfer measures with VC dimension and Natarajan dimension

In this section, we review Rademacher complexity and show that it can be upper bounded by VC dimension [e.g. 44]. We use $\text{VCdim}(\cdot)$ to represent the VC dimension of a function class. We also show that the estimation error in Lemma 9' can be upper bounded with Natarajan dimension.

Definition 14 (Rademacher complexity). *The Rademacher complexity of an i.i.d. drawn sample set $S = \{w_i\}_{i=1}^m$, over \mathcal{F} is defined as:*

$$\mathfrak{R}_m(\mathcal{F}) = \mathbb{E}_S \left[\mathbb{E}_{\sigma_i} \sup_{f \in \mathcal{F}} \frac{1}{m} \sum_{i=1}^m \sigma_i f(w_i) \right], \text{ where}$$

$$\{\sigma_i\}_{i=1}^m \text{ are independently drawn such that } \Pr(\sigma_i = 1) = \Pr(\sigma_i = -1) = \frac{1}{2}.$$

Lemma 15. *Denote $d = \text{VCdim}(\Gamma)$ where Γ is a set of functions taking values $\{-1, +1\}$. For any $m \in \mathbb{N}_+$, we have:*

$$\mathfrak{R}_m(\Gamma) \leq \sqrt{\frac{2}{m} \log \sum_{i=0}^d \binom{m}{i}}, \quad (\text{B.3})$$

if $m \geq d$, then

$$\mathfrak{R}_m(\Gamma) \leq \sqrt{\frac{2d}{m} \log \frac{em}{d}}. \quad (\text{B.4})$$

Proof. This lemma follows from Corollary 3.8, Theorem 3.17 and Corollary 3.18 of Mohri et al. [34]. \square

Combining Theorem 10' and Lemma 15, we obtain the following corollary:

Corollary 16. *Suppose $\widehat{\mathcal{S}}$ and $\widehat{\mathcal{T}}$ are sample distributions of \mathcal{S} and \mathcal{T} , with samples drawn i.i.d. Denote the sample numbers of $\widehat{\mathcal{S}}$ and $\widehat{\mathcal{T}}$ are separately m and k . If \mathcal{H} is a set of binary classifiers*

with labels $\{-1, 1\}$, then for any $\Gamma \subseteq \mathcal{H}$ with $d = \text{VCdim}(\Gamma)$, any of the following holds w.p. $1 - \delta$:

$$\mathbb{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \mathbb{T}_\Gamma(\widehat{\mathcal{S}} \parallel \widehat{\mathcal{T}}) + 2\sqrt{\frac{2}{m} \log \sum_{i=0}^d \binom{m}{i}} + 2\sqrt{\frac{2}{k} \log \sum_{i=0}^d \binom{k}{i}} + 2\sqrt{\frac{\log(4/\delta)}{2m}} + 2\sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{B.5})$$

$$\mathbb{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_\Gamma(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + 2\sqrt{\frac{2}{m} \log \sum_{i=0}^d \binom{m}{i}} + 2\sqrt{\frac{2}{k} \log \sum_{i=0}^d \binom{k}{i}} + 2\sqrt{\frac{\log(4/\delta)}{2m}} + 2\sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{B.6})$$

$$\mathbb{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_\Gamma^\mathbb{F}(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + \sqrt{\frac{2}{m} \log \sum_{i=0}^d \binom{m}{i}} + \sqrt{\frac{2}{k} \log \sum_{i=0}^d \binom{k}{i}} + \sqrt{\frac{\log(4/\delta)}{2m}} + \sqrt{\frac{\log(4/\delta)}{2k}}. \quad (\text{B.7})$$

If $m \geq d$ and $k \geq d$, then any of the following holds w.p. $1 - \delta$:

$$\mathbb{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \mathbb{T}_\Gamma(\widehat{\mathcal{S}} \parallel \widehat{\mathcal{T}}) + 2\sqrt{\frac{2d}{m} \log \frac{em}{d}} + 2\sqrt{\frac{2d}{k} \log \frac{ek}{d}} + 2\sqrt{\frac{\log(4/\delta)}{2m}} + 2\sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{B.8})$$

$$\mathbb{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_\Gamma(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + 2\sqrt{\frac{2d}{m} \log \frac{em}{d}} + 2\sqrt{\frac{2d}{k} \log \frac{ek}{d}} + 2\sqrt{\frac{\log(4/\delta)}{2m}} + 2\sqrt{\frac{\log(4/\delta)}{2k}}, \quad (\text{B.9})$$

$$\mathbb{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_\Gamma^\mathbb{F}(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + \sqrt{\frac{2d}{m} \log \frac{em}{d}} + \sqrt{\frac{2d}{k} \log \frac{ek}{d}} + \sqrt{\frac{\log(4/\delta)}{2m}} + \sqrt{\frac{\log(4/\delta)}{2k}}. \quad (\text{B.10})$$

Moreover, if the hypothesis class \mathcal{H} is the set of all possible functions that can be constructed through a fixed structure ReLU/LeakyReLU network, with W the number of parameters and L the number of layers, then there exists an absolute constant C such that $d \leq CWL \log W$ [7].

A generalization of VC dimension is called Natarajan dimension [38], which coincides with VC dimension when the classification task is binary. We have the following result [44, Theorem 29.3]:

Lemma 17. *Suppose the Natarajan dimension of Γ is d and the number of classes is K for multiclass classification. There exists absolute constant C such that for any domain \mathcal{D} , with probability $1 - \delta$ the following holds:*

$$\text{est}_\Gamma(\mathcal{D}) = \sup_{h \in \Gamma} |\epsilon_{\mathcal{D}}(h) - \epsilon_{\widehat{\mathcal{D}}}(h)| \leq C\sqrt{\frac{d \log K + \log(1/\delta)}{m}}. \quad (\text{B.11})$$

With this lemma we have the corollary:

Corollary 18. *Suppose the Natarajan dimension of Γ is d and the number of classes is K for multiclass classification. Suppose $\widehat{\mathcal{S}}$ and $\widehat{\mathcal{T}}$ are i.i.d. sample distributions drawn from distributions of \mathcal{S} and \mathcal{T} , with sample number m and k , then w.p. at least $1 - \delta$ we have:*

$$\mathbb{T}_\Gamma(\mathcal{S} \parallel \mathcal{T}) \leq \mathbb{T}_\Gamma(\widehat{\mathcal{S}} \parallel \widehat{\mathcal{T}}) + 2C\sqrt{\frac{d \log K + \log(2/\delta)}{m}} + 2C\sqrt{\frac{d \log K + \log(2/\delta)}{k}}, \quad (\text{B.12})$$

$$\mathbb{T}_\Gamma(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_\Gamma(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + 2C\sqrt{\frac{d \log K + \log(2/\delta)}{m}} + 2C\sqrt{\frac{d \log K + \log(2/\delta)}{k}}, \quad (\text{B.13})$$

$$\mathbb{T}_\Gamma^\mathbb{F}(\mathcal{S}, \mathcal{T}) \leq \mathbb{T}_\Gamma^\mathbb{F}(\widehat{\mathcal{S}}, \widehat{\mathcal{T}}) + C\sqrt{\frac{d \log K + \log(2/\delta)}{m}} + C\sqrt{\frac{d \log K + \log(2/\delta)}{k}}. \quad (\text{B.14})$$

Proof. This proof is similar to the proof of Theorem 10', using union bound as in (A.33). \square

Estimation of Natarajan dimension can be found in Natarajan [38], Shalev-Shwartz and Ben-David [44].

B.4 Functional point of view of surrogate loss

In this appendix we study the Lipschitzness and strong convexity of the surrogate loss, especially cross entropy. We use the terms distribution and measure interchangeably, since distributions can be treated as probability measures.

B.4.1 Lipschitz continuity of loss

Let define the L_p distance ($p \geq 1$) (e.g. Rudin [42]) between two functions:

$$\|h - h'\|_{p,\mu} = \left(\int \|h(x) - h'(x)\|_2^p d\mu \right)^{1/p}, \quad (\text{B.15})$$

where μ is a measure. We consider the following definition of Lipschitz functional:

Definition 19 (Lipschitz continuity). *A functional $h \mapsto f(h)$ that maps a function to a real number is f is Lipschitz continuous on \mathcal{H} w.r.t. measure μ if there exists an absolute constant L such that:*

$$|f(h) - f(h')| \leq L \|h - h'\|_{1,\mu} \quad (\text{B.16})$$

for all function $h, h' \in \mathcal{H}$.

One can show that the cross entropy loss is a Lipschitz continuous functional with mild assumptions:

Proposition 20. *For binary classification with labels $\{-1, +1\}$, suppose \mathcal{H} is a hypothesis class whose elements satisfy $h : \mathcal{X} \rightarrow (-1 + \delta, 1 - \delta)$ with $0 < \delta < 1$, then $\epsilon_{\mathcal{D}}^{\text{CE}}$ is $(\log 2)^{-1} \delta^{-1}$ Lipschitz continuous w.r.t. any distribution \mathcal{D} . Furthermore, for multi-class classification, suppose $\mathcal{Y} = \{1, 2, \dots, K\}$ and the prediction $h(x)$ is a K -dimensional probability vector on the simplex. If \mathcal{H} is a hypothesis class whose elements satisfy $h_i(x) \geq \delta$ for all $i \in \mathcal{Y}$ and $x \in \mathcal{X}$, then $\epsilon_{\mathcal{D}}^{\text{CE}}$ is $(\log 2)^{-1} \delta^{-1}$ Lipschitz continuous w.r.t. any distribution \mathcal{D} .*

Note that a simplex is defined as: $\{\pi \in \mathbb{R}^d : \mathbf{1}^\top \pi = 1, \pi_i \geq 0\}$, where π is called a probability vector. Before we move on to the proof, we can show that the assumption of h is often satisfied in practice. For binary classification, the widely used tanh/sigmoid function can guarantee that the value of h is never exactly -1 or 1 . For multiclass classification, the softmax function guarantees that $h_i(x) > 0$ for all i and $x \in \mathcal{X}$. If the input space is bounded and h is continuous, then $h_i(x) \geq \delta$ for all i and $x \in \mathcal{X}$.

Proof. For binary classification we have:

$$\begin{aligned} \epsilon_{\mathcal{D}}^{\text{CE}}(h) &= \int p_{\mathcal{D}}(x, 1) \ell^{\text{CE}}(h(x), 1) + p_{\mathcal{D}}(x, -1) \ell^{\text{CE}}(h(x), -1) dx \\ &= \int -p_{\mathcal{D}}(x, 1) \log_2 \frac{1+h(x)}{2} - p_{\mathcal{D}}(x, -1) \log_2 \frac{1-h(x)}{2} dx. \end{aligned} \quad (\text{B.17})$$

Therefore, with the mean value theorem we have:

$$\begin{aligned} |\epsilon_{\mathcal{D}}^{\text{CE}}(h) - \epsilon_{\mathcal{D}}^{\text{CE}}(h')| &= (\log 2)^{-1} \left| \int (h(x) - h'(x)) \left(\frac{-p_{\mathcal{D}}(x, 1)}{1+h_{\xi}(x)} + \frac{p_{\mathcal{D}}(x, -1)}{1-h_{\xi}(x)} \right) dx \right|, \\ &\leq (\log 2)^{-1} \int |h(x) - h'(x)| \left| \frac{-p_{\mathcal{D}}(x, 1)}{1+h_{\xi}(x)} + \frac{p_{\mathcal{D}}(x, -1)}{1-h_{\xi}(x)} \right| dx \\ &\leq (\log 2)^{-1} \int |h(x) - h'(x)| \left(\left| \frac{-p_{\mathcal{D}}(x, 1)}{1+h_{\xi}(x)} \right| + \left| \frac{p_{\mathcal{D}}(x, -1)}{1-h_{\xi}(x)} \right| \right) dx \\ &\leq (\log 2)^{-1} \int |h(x) - h'(x)| \delta^{-1} (p_{\mathcal{D}}(x, 1) + p_{\mathcal{D}}(x, -1)) dx \\ &= (\log 2)^{-1} \delta^{-1} \|h - h'\|_{1,\mathcal{D}}. \end{aligned} \quad (\text{B.18})$$

where in the first line $h_{\xi}(x) = (1 - \xi(x))h(x) + \xi(x)h'(x)$ is a (pointwise) convex combination of $h(x)$ and $h'(x)$ with $0 \leq \xi(x) \leq 1$; in the third line we used triangle inequality; in the fourth line we use the condition that the values of h, h' are in the region $(-1 + \delta, 1 - \delta)$.

Similarly, for multiclass classification with K classes, the ground truth y is a one-hot K -dimensional vector, and the prediction $h(x)$ is a K -dimensional vector on a simplex. The cross entropy loss is:

$$\epsilon_{\mathcal{D}}^{\text{CE}}(h) = \sum_y \int \ell^{\text{CE}}(h(x), y) p(x, y) dx = \sum_y \int -y \cdot \log_2 h(x) p(x, y) dx. \quad (\text{B.19})$$

Similarly, we have:

$$\begin{aligned} |\epsilon_{\mathcal{D}}^{\text{CE}}(h) - \epsilon_{\mathcal{D}}^{\text{CE}}(h')| &= (\log 2)^{-1} \left| \sum_y \int -y \cdot \frac{h(x) - h'(x)}{h_{\xi}(x)} p_{\mathcal{D}}(x, y) dx \right| \\ &\leq (\log 2)^{-1} \sum_y \int \left| -y \cdot \frac{h(x) - h'(x)}{h_{\xi}(x)} \right| p_{\mathcal{D}}(x, y) dx \\ &\leq (\log 2)^{-1} \delta^{-1} \sum_y \int \|y\|_2 \cdot \|h(x) - h'(x)\|_2 p_{\mathcal{D}}(x, y) dx \\ &= (\log 2)^{-1} \delta^{-1} \|h - h'\|_{1, \mathcal{D}}, \end{aligned} \quad (\text{B.20})$$

where in the first line we use the mean value theorem and $h_{\xi}(x) = (1 - \xi(x))h(x) + \xi(x)h'(x)$ is a (pointwise) convex combination of $h(x)$ and $h'(x)$ with $0 \leq \xi(x) \leq 1$; also in the first line we define $(h(x) - h'(x))/h_{\xi}(x)$ to be a vector with each component to be $(h_i(x) - h'_i(x))/h_{\xi}(x)_i$; in the third line we use Cauchy–Schwarz inequality and that $h_i(x) \geq \delta$, $h'_i(x) \geq \delta$ for any i and any $x \in \mathcal{X}$. \square

B.4.2 Strongly convex functional

So far, we have seen that for Lipschitz continuous loss, if the change of h is small, then the change of loss $\epsilon_{\mathcal{D}}(h)$ is also small. Now we ask if the converse is true. This is important to characterize the δ -minimal set (the set of approximately optimal classifiers). We first define strongly convex functional:

Definition 21. A functional $f : \mathcal{H} \rightarrow \mathbb{R}$ is λ -strongly convex on a convex set \mathcal{H} w.r.t. measure μ if for any $h, h' \in \mathcal{H}$ and $\alpha \in [0, 1]$, we have:

$$f(\alpha h + (1 - \alpha)h') \leq \alpha f(h) + (1 - \alpha)f(h') - \frac{\lambda}{2} \alpha(1 - \alpha) \|h - h'\|_{2, \mu}^2, \quad (\text{B.21})$$

where we defined the L_2 norm of a function:

$$\|h - h'\|_{2, \mu} := \left(\int \|h - h'\|_2^2 d\mu \right)^{1/2}. \quad (\text{B.22})$$

We use L_2 norm because it can translate the strong convexity of the loss functional to the strong convexity of the loss function $\ell(\cdot, y)$ easily:

Lemma 22. Given a convex hypothesis class \mathcal{H} , suppose that ℓ is λ -strongly convex in the first argument, i.e. for any $y \in \mathcal{Y}$, \hat{y}_1, \hat{y}_2 and $\alpha \in [0, 1]$ we have:

$$\ell(\alpha \hat{y}_1 + (1 - \alpha)\hat{y}_2, y) \leq \alpha \ell(\hat{y}_1, y) + (1 - \alpha)\ell(\hat{y}_2, y) - \frac{\lambda}{2} \alpha(1 - \alpha) \|\hat{y}_1 - \hat{y}_2\|_2^2, \quad (\text{B.23})$$

then the loss functional

$$\epsilon_{\mathcal{D}}(h) = \sum_y \int p_{\mathcal{D}}(x, y) \ell(h(x), y) dx \quad (\text{B.24})$$

is also λ -strongly convex w.r.t. measure \mathcal{D} .

Proof. Straightforward by plugging in Definition 21. \square

For cross entropy loss, we have the following:

Corollary 23. For binary classification, cross entropy risk functional $\epsilon_{\mathcal{D}}^{\text{CE}}$ is $(4 \log 2)^{-1}$ -strongly convex on \mathcal{D} and $(\log 2)^{-1}$ -strongly convex on \mathcal{D} for multiclass classification.

Proof. For binary classification, we have:

$$\ell^{\text{CE}}(\hat{y}, 1) = -\log_2 \frac{1 + \hat{y}}{2}, \quad \ell^{\text{CE}}(\hat{y}, -1) = -\log_2 \frac{1 - \hat{y}}{2}, \quad (\text{B.25})$$

which are both $(4 \log 2)^{-1}$ -strongly convex on $\hat{y} \in (-1, 1)$. For multiclass classification, we have:

$$\ell^{\text{CE}}(\hat{y}, y) = -\log_2 \hat{y}_i, \quad (\text{B.26})$$

for any unit one-hot vector $y = e_i$ (e_i is the i^{th} element of standard basis in \mathbb{R}^K). This is $(\log 2)^{-1}$ -strongly convex for $\hat{y}_i \in (0, 1)$. The rest follows from Lemma 22. \square

From the strongly convexity we can derive the uniqueness of the function (up to L_2 norm) and relate δ -minimal set to an L_2 neighborhood of an optimal classifier.

Theorem 24. *For any λ -strongly convex functional f on a convex hypothesis class \mathcal{H} w.r.t. measure μ , the minimizer is almost surely unique, in the sense that if h_1^*, h_2^* are both minimizers, then*

$$\|h_1^* - h_2^*\|_{2,\mu} = 0, \quad (\text{B.27})$$

and thus h_1^*, h_2^* only differ by a measure zero set. Suppose $h^* \in \text{argmin } f(h)$. If $f(h) \leq f^* + \epsilon$ with f^* the optimal value, then

$$\|h - h^*\|_{2,\mu} \leq \sqrt{\frac{2}{\lambda}} \epsilon. \quad (\text{B.28})$$

Proof. It suffices to prove the second claim only. From the definition of strong convexity, for $\alpha \in [0, 1]$ we have:

$$\begin{aligned} f^* &\leq f(\alpha h^* + (1 - \alpha)h) \leq \alpha f(h^*) + (1 - \alpha)f(h) - \frac{\lambda}{2} \alpha(1 - \alpha) \|h^* - h\|_{2,\mu}^2 \\ &\leq (1 - \alpha)\epsilon + f^* - \frac{\lambda}{2} \alpha(1 - \alpha) \|h^* - h\|_{2,\mu}^2, \end{aligned} \quad (\text{B.29})$$

where we use $h^* \in \text{argmin } f(h)$ and $f(h) \leq f^* + \epsilon$. From this inequality we obtain that:

$$\|h - h^*\|_{2,\mu}^2 \leq \frac{2\epsilon}{\alpha\lambda}. \quad (\text{B.30})$$

By taking $\alpha \rightarrow 1$ we obtain (B.28). \square

With this theorem we can characterize the δ -minimal set $\text{argmin}(\epsilon_{\mathcal{D}}, \delta)$ as some neighborhood of the unique optimal classifier h^* , if the functional $\epsilon_{\mathcal{D}}$ is strongly convex and Lipschitz continuous. Symbolically, it can be represented as:

$$\mathcal{B}_2(h^*) \subseteq \text{argmin}(\epsilon_{\mathcal{D}}, \delta) \subseteq \mathcal{B}_1(h^*), \quad (\text{B.31})$$

where $\mathcal{B}_p(h^*)$ is some L_p norm ball with the center h^* .

B.4.3 Parametric formulation of classifier

We discussed the L_p distance between functions in previous subsections. In practice the functions are often parametrized:

$$h(x) = q(\theta, x). \quad (\text{B.32})$$

One can show that L_p distances between two functions $h = q(\theta, \cdot)$ and $h' = q(\theta', \cdot)$ on the function space can be upper bounded:

Theorem 25. *Suppose $h = q(\theta, \cdot)$ is parameterized by θ and for any $x \in \mathcal{X}$, $q(\cdot, x)$ is L -Lipschitz continuous (w.r.t. ℓ_2 norm), then for any $1 \leq p < \infty$ and probability measure μ we have:*

$$\|h - h'\|_{p,\mu} \leq L \|\theta - \theta'\|_2. \quad (\text{B.33})$$

Proof. From the Lipschitz continuity we can derive:

$$\begin{aligned}
\|h - h'\|_{p,\mu} &= \left(\int \|h(x) - h'(x)\|_2^p d\mu \right)^{1/p} \\
&= \left(\int \|q(\theta, x) - q(\theta', x)\|_2^p d\mu \right)^{1/p} \\
&\leq \left(\int (L\|\theta - \theta'\|_2)^p d\mu \right)^{1/p} \\
&= L\|\theta - \theta'\|_2.
\end{aligned} \tag{B.34}$$

□

The theorem above tells us that in parametrized models the closeness in terms of parameters can imply the closeness in terms of the model function. However, the converse may not be true. For example, we can permute hidden neurons of the same layer in a neural network and obtain the same function, but the parametrization can be drastically different.

B.5 Comparison with other frameworks

We compare our Algorithm 2 with existing adversarial training frameworks.

Distributional robustness optimization (DRO) Sinha et al. [45] proposed a distributional robustness framework for generalizing to unseen domains. In this framework, the following minimax problem is proposed:

$$\min_{g,h} \max_{S': W(S', \mathcal{S}) \leq \delta} \epsilon'_S(h \circ g), \tag{B.35}$$

which says that the classification error is small for any distribution \mathcal{S}' close to our original source distribution \mathcal{S} . Here $W(\cdot, \cdot)$ denotes the Wasserstein metric. As we have discussed in Example 8, transferability does not necessarily mean that the distributions have to be close.

DANN The Domain Adversarial Neural Network (DANN) formulation [16] solves the following minimax optimization problem:

$$\min_{g,h} \max_{h'} \epsilon_S(h \circ g) + \mathbb{E}_{x \sim p_S|x} [\log(h' \circ g)(x)] + \mathbb{E}_{x \sim p_T|x} [\log(1 - (h' \circ g)(x))], \tag{B.36}$$

where g is a feature embedding, h is a classifier and h' is a domain discriminator. If we can solve the inner maximization problem exactly, then we obtain the Jensen–Shannon divergence between the push-forwards of the input distributions $g\#p_S|x$ and $g\#p_T|x$. In other words, we want to obtain a feature embedding g and a classifier h such that:

$$\epsilon_S(h \circ g) + D_{\text{JS}}((g\#p_S|x) \parallel (g\#p_T|x)), \tag{B.37}$$

is minimized, with D_{JS} denoting the Jensen–Shannon divergence. On the one hand, we need to have small classification error given the feature embedding g . On the other hand, the feature embedding between source and target should be similar. Our framework is similar to DANN in the sense that they both solve minimax problems. The difference is that we minimize the transfer measure which is weaker than the similarity between distributions (Example 8).

$\mathcal{H}\Delta\mathcal{H}$ -divergence Finally we prove that our transfer measure is tighter than $\mathcal{H}\Delta\mathcal{H}$ -divergence [12]. We rewrite the theoretical result regarding $\mathcal{H}\Delta\mathcal{H}$ -divergence:

Theorem 26 (Theorem 1, [12]). *Let $\lambda^* = \operatorname{argmin}_{h \in \mathcal{H}} (\epsilon_{\mathcal{T}}(h) + \epsilon_{\mathcal{S}}(h))$, and the $\mathcal{H}\Delta\mathcal{H}$ -divergence between the input marginal distributions $\mathcal{S}|_x$ and $\mathcal{T}|_x$ to be $d_{\mathcal{H}\Delta\mathcal{H}}(\mathcal{S}|_x, \mathcal{T}|_x)$, then for binary classification and for any $h \in \mathcal{H}$ we have:*

$$\epsilon_{\mathcal{T}}(h) \leq \epsilon_{\mathcal{S}}(h) + \lambda^* + \frac{1}{2} d_{\mathcal{H}\Delta\mathcal{H}}(\mathcal{S}|_x, \mathcal{T}|_x). \tag{B.38}$$

Now let us prove that our Proposition 3 is tighter than Theorem 26:

Proposition 27. *The target error bound with our transfer measure $T_\Gamma(\mathcal{S}||\mathcal{T})$ is tighter than the target error bound with $\mathcal{H}\Delta\mathcal{H}$ -divergence, i.e., for any $h \in \Gamma$ we have:*

$$\epsilon_{\mathcal{T}}(h) \leq \epsilon_{\mathcal{S}}(h) + \epsilon_{\mathcal{T}}^* - \epsilon_{\mathcal{S}}^* + T_\Gamma(\mathcal{S}||\mathcal{T}) \leq \epsilon_{\mathcal{S}}(h) + \lambda^* + \frac{1}{2}d_{\mathcal{H}\Delta\mathcal{H}}(\mathcal{S}|_x, \mathcal{T}|_x). \quad (\text{B.39})$$

Proof. Note that from Definition 2 we can rewrite the middle of (B.39) as $\sup_{h \in \Gamma}(\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{S}}(h))$. Suppose $h^* \in \operatorname{argmax}_{h \in \Gamma}(\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{S}}(h))$, then from Theorem 26 we have:

$$\epsilon_{\mathcal{T}}(h^*) \leq \epsilon_{\mathcal{S}}(h^*) + \lambda^* + \frac{1}{2}d_{\mathcal{H}\Delta\mathcal{H}}(\mathcal{S}|_x, \mathcal{T}|_x), \quad (\text{B.40})$$

and thus:

$$\epsilon_{\mathcal{T}}^* - \epsilon_{\mathcal{S}}^* + T_\Gamma(\mathcal{S}||\mathcal{T}) = \sup_{h \in \Gamma}(\epsilon_{\mathcal{T}}(h) - \epsilon_{\mathcal{S}}(h)) = \epsilon_{\mathcal{T}}(h^*) - \epsilon_{\mathcal{S}}(h^*) \leq \lambda^* + \frac{1}{2}d_{\mathcal{H}\Delta\mathcal{H}}(\mathcal{S}|_x, \mathcal{T}|_x). \quad (\text{B.41})$$

□

C Additional Experiments

We present additional experimental details in this section.

C.1 Datasets

The four datasets in this paper are RotatedMNIST [18], PACS [28], Office-Home [51] and WILDS-FMoW [23]. Here is a short description:

- **RotatedMNIST:** this dataset is an adaptation of MNIST. It has six domains, and each domain rotates the images in MNIST with a different angle. The angles are $\{0^\circ, 15^\circ, 30^\circ, 45^\circ, 60^\circ, 75^\circ\}$. We choose the domain with 0° to be the target domain and the rest to be the source domains. Each image is grayscale and has 28×28 pixels. The label set is $\{0, 1, \dots, 9\}$. The numbers of images of each domain are 11667, 11667, 11667, 11667, 11666, 11666. The total is 70000.
- **PACS:** this dataset has four domains: photo (P), art painting (A), cartoon (C) and sketch (S). Each image is RGB colored and has 224×224 pixels. There are 7 categories in total and 9991 images. The number of images of each domain: A: 2048; C: 2344; P: 1670; S: 3929. We choose the art painting domain to be the target domain and the rest to be the source domains.
- **Office-Home:** this dataset has four domains: Art, Clipart, Product, Real-World. Each image is RGB colored and has 224×224 pixels. There are 65 categories and 15588 images in total. The numbers of images of each domain: Art: 2427, Clipart: 4365, Product: 4439, Real-World: 4357. We choose the Art domain to be the target domain and the rest to be the source domains.
- **WILDS-FMoW:** WILDS [23] is a benchmark for domain generalization including several datasets. The Functional Map of the World (FMoW) is one of them, which is a variant of Christie et al. [14]. Each image is RGB colored and has 224×224 pixels. There are 62 categories and 469835 images in total. There six domains in total and we choose five of them, since the last domain has too few images. The numbers of images of each domain are 103299, 162333, 33239, 157711, 13253, and we choose the last domain as the target domain. The rest are source domains. The license can be found at <https://wilds.stanford.edu/datasets/>.

C.2 Experimental settings

We introduce the experimental settings in this subsection. The code is modified from <https://github.com/facebookresearch/DomainBed>, with the license in <https://github.com/facebookresearch/DomainBed/blob/master/LICENSE>.

- Hardware: Our experiments are run on a cluster of GPUs, including NVIDIA RTX6000, T4 and P100.
- Datasplit: we use the same data split as in Gulrajani and Lopez-Paz [20] except the WILDS-FMoW dataset, where we throw away the last region because it has only very few samples (201 samples). For all datasets we use data augmentation.
- Batch size: for all experiments on RotatedMNIST we choose batch size 64, for Office-Home and PACS we choose batch size 32 (for our Transfer algorithm and PACS we choose batch size 16), and for WILDS-FMoW we choose batch size 16. In each epoch, we go through k steps, where k is the smallest number of samples among domains, divided by the batch size.
- Optimization: for the training of all other algorithms different from our Transfer Algorithm, we use the default setting from Gulrajani and Lopez-Paz [20]. We choose Adam as the default optimizer for training, with learning rate $1e-3$ for RotatedMNIST, and learning rate $5e-5$ for other datasets. For RotatedMNIST, PACS and Office-Home we run for 5000 steps; For WILDS-FMoW we run for 50000 steps.
- Neural Architecture: we use the same neural architecture as in Gulrajani and Lopez-Paz [20]. For each dataset, the feature embedding and classifier architectures for all algorithms are the same. Specifically, all classifiers are linear layers. For RotatedMNIST the feature embedding is CNN with batch normalization and for other datasets the feature embedding is ResNet50.
- Algorithm 1: we choose Adam optimizer with projection. The learning rates are the same as the training algorithms: for RotatedMNIST we choose $1e-3$, and we choose $5e-5$ for others. We run the algorithm for 10 epochs and for three independent trials. Among the three trials, we choose the accuracies with the largest gap between the target domain and one of the source domains. The source domain is chosen in such a way that the gap is the largest among all source domains.
- Algorithm 2 optimization: for RotatedMNIST we run Adam for minimization with learning rate 0.01 and Stochastic Gradient Ascent (SGA) for maximization with learning rate 0.01. We choose the ascent steps to be 30 for each inner loop and the projection radius to be $\delta = 10.0$; for PACS we run Adam for minimization with learning rate $5e-5$ and Stochastic Gradient Ascent (SGA) for maximization with learning rate 0.001. We choose the ascent steps to be 30 for each inner loop and the projection radius to be $\delta = 0.3$; for Office-Home dataset we load the pretrained model from SD, and run Stochastic Gradient Descent Ascent with learning rate 0.001 and $\delta = 0.3$, i.e., each inner loop takes only one step of SGA and each outer loop takes one step of SGD; for WILDS-FMoW dataset we loaded the pretrained model from ERM, and run SGA for 20 steps in each inner loop, with learning rate 0.001 and $\delta = 0.5$, for each outer loop we run SGD with $\text{lr} = 0.001$.
- Step number for Algorithm 2: for RotatedMNIST and PACS we train for 8000 outer steps with each outer step including 30 inner steps. For Office-Home we train for 5000 outer steps with each outer step including one inner step; for WILDS-FMoW we train for 5000 outer loops with each outer step including 20 inner steps.

C.3 Additional results

We present additional experiments on RotatedMNIST [18], PACS [28] and Office-Home [51]. Thanks to the suite from Gulrajani and Lopez-Paz [20], we are able to compare a wide array of algorithms under the same settings. The algorithms that we compare include

- Empirical Risk Minimization [ERM, 50]
- Invariant Risk Minimization [IRM, 3]
- Domain Adversarial Neural Network [DANN, 16]
- Conditional DANN [CDANN, 31]
- Correlation Alignment [CORAL, 47]
- Maximum Mean Discrepancy [MMD, 30]
- Variance Risk Extrapolation [VREx, 26]

- Marginal Transfer Learning [MTL, 11]
- Spectral Decoupling [SD, 40]
- Meta Learning Domain Generalization [MLDG, 29]
- Mixup [53, 54]
- Representation Self-Challenging [RSC, 22]
- Group Distributionally Robust Optimization [GroupDRO, 43]
- Style-Agnostic Network [SagNet, 37]

C.3.1 RotatedMNIST

In Figure 4 we show the performance of various algorithms on RotatedMNIST, including ERM, IRM, DANN, CORAL, MMD, VREx, MTL, SD and our Transfer algorithm. It can be seen that many algorithms fail our attack. For instance, based on the learned features, MTL classifies a source domain with $\sim 95\%$ (at $\delta = 3.0$) but the target accuracy drops by $\sim 20\%$.

We also compare our Transfer algorithm (Algorithm 2) with different hyperparameters. From Figure 5 we can see that for RotatedMNIST, taking more inner steps (per outer step) has better performance.

Finally, we present results from Algorithm 1 with information about losses and accuracies, for a wide array of algorithms in Table 2.

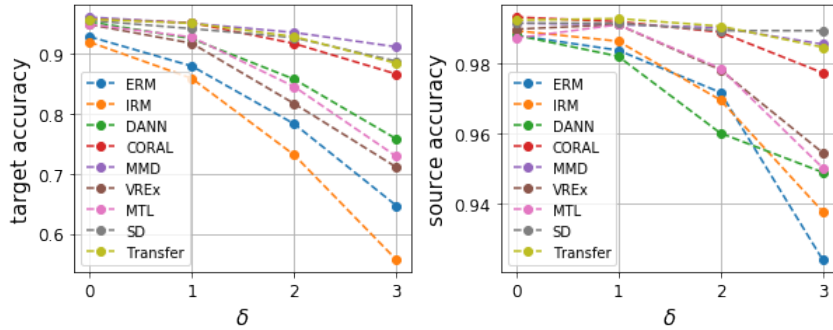


Figure 4: Measuring the transferability of various algorithms for domain generalization on RotatedMNIST. For the Transfer algorithm we take $\delta = 10.0$ and the number of ascent steps to be 30.

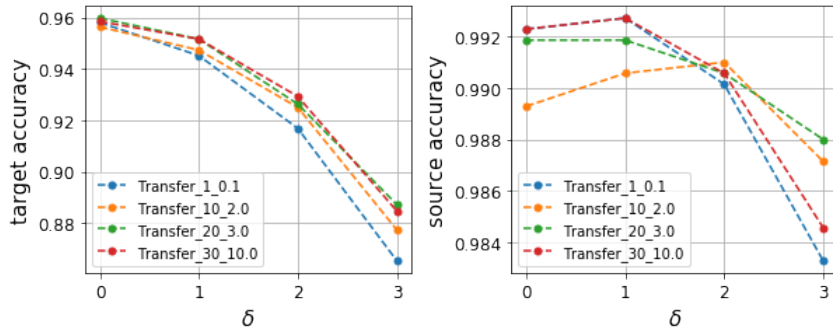


Figure 5: Evaluation of transferability of popular algorithms for domain generalization on Transfer algorithm with different hyperparameters. The dataset is RotatedMNIST. For the ascent method we use SGD with learning rate 0.01, and the descent method to be Adam with learning rate 10^{-3} . “Transfer_ d _ δ ” means the inner loop takes d steps with the radius δ .

Table 2: Evaluation of transferability of popular algorithms for domain generalization on RotatedMNIST. **algorithm**: the model that we evaluate; δ : the adversarial radius δ we choose in Algorithm 1; **max/min index**: the index of the domain with the maximal/minimal (test) classification errors (w.r.t. 0-1 loss), and index 0 denotes the target domain; **max/min loss**: the largest/smallest loss among domains (including the target domain); **worst/best acc**: the smallest/largest classification test accuracies among domains (including the target domain). All the algorithms are using the same architectures for the feature embedding and the classifier.

| algorithm | δ | max index | min index | max loss | min loss | worst acc | best acc |
|-----------|----------|-----------|-----------|----------|----------|-----------|----------|
| ERM | 0.0 | 0 | 4 | 0.229 | 0.003 | 92.93% | 98.80% |
| ERM | 2.0 | 0 | 4 | 0.975 | 0.083 | 78.61% | 97.17% |
| GroupDRO | 0.0 | 0 | 4 | 0.136 | 0.000 | 95.76% | 99.27% |
| GroupDRO | 2.0 | 0 | 4 | 0.370 | 0.015 | 84.48% | 98.07% |
| SagNet | 0.0 | 0 | 4 | 0.109 | 0.000 | 96.61% | 99.36% |
| SagNet | 2.0 | 0 | 4 | 0.222 | 0.008 | 91.30% | 98.67% |
| IRM | 0.0 | 0 | 4 | 0.578 | 0.263 | 81.87% | 92.20% |
| IRM | 2.0 | 0 | 4 | 1.759 | 0.637 | 46.29% | 86.76% |
| DANN | 0.0 | 0 | 5 | 0.136 | 0.014 | 95.41% | 98.29% |
| DANN | 2.0 | 0 | 5 | 0.441 | 0.098 | 85.81% | 96.19% |
| ARM | 0.0 | 0 | 4 | 0.145 | 0.002 | 95.76% | 99.10% |
| ARM | 2.0 | 0 | 4 | 0.523 | 0.047 | 84.23% | 98.54% |
| Mixup | 0.0 | 0 | 4 | 0.175 | 0.009 | 94.98% | 99.36% |
| Mixup | 2.0 | 0 | 4 | 0.701 | 0.035 | 73.98% | 98.71% |
| CORAL | 0.0 | 0 | 4 | 0.119 | 0.001 | 95.93% | 99.31% |
| CORAL | 2.0 | 0 | 4 | 0.230 | 0.005 | 91.77% | 98.89% |
| CORAL | 3.0 | 0 | 4 | 0.372 | 0.056 | 86.67% | 97.73% |
| MMD | 0.0 | 0 | 3 | 0.125 | 0.005 | 96.19% | 99.14% |
| MMD | 2.0 | 0 | 3 | 0.199 | 0.014 | 93.61% | 99.01% |
| MMD | 3.5 | 0 | 3 | 0.300 | 0.036 | 89.54% | 97.86% |
| RSC | 0.0 | 0 | 4 | 0.146 | 0.000 | 95.46% | 99.31% |
| RSC | 1.0 | 0 | 4 | 0.360 | 0.007 | 89.33% | 98.71% |
| RSC | 2.0 | 0 | 4 | 1.343 | 0.289 | 72.01% | 92.11% |
| VREx | 0.0 | 0 | 5 | 0.137 | 0.003 | 94.94% | 98.97% |
| VREx | 2.0 | 0 | 5 | 0.551 | 0.082 | 81.74% | 97.81% |
| CDANN | 0.0 | 0 | 5 | 0.121 | 0.010 | 95.97% | 98.76% |
| CDANN | 2.0 | 0 | 5 | 0.410 | 0.079 | 84.78% | 95.67% |
| MLDG | 0.0 | 0 | 5 | 0.151 | 0.000 | 95.63% | 98.89% |
| MLDG | 2.0 | 0 | 5 | 0.351 | 0.006 | 88.90% | 98.76% |
| MTL | 0.0 | 0 | 4 | 0.150 | 0.000 | 94.98% | 99.44% |
| MTL | 2.0 | 0 | 4 | 0.417 | 0.014 | 84.57% | 98.20% |
| SD | 0.0 | 0 | 2 | 0.250 | 0.092 | 95.63% | 99.01% |
| SD | 2.0 | 0 | 2 | 0.630 | 0.490 | 92.76% | 98.97% |
| SD | 3.0 | 0 | 2 | 1.070 | 0.937 | 88.81% | 98.33% |

C.3.2 PACS

We implement similar experiments on PACS. Figure 6 and Table 3 show the results of Algorithm 1. Figure 7 shows that taking more inner steps has better performance.

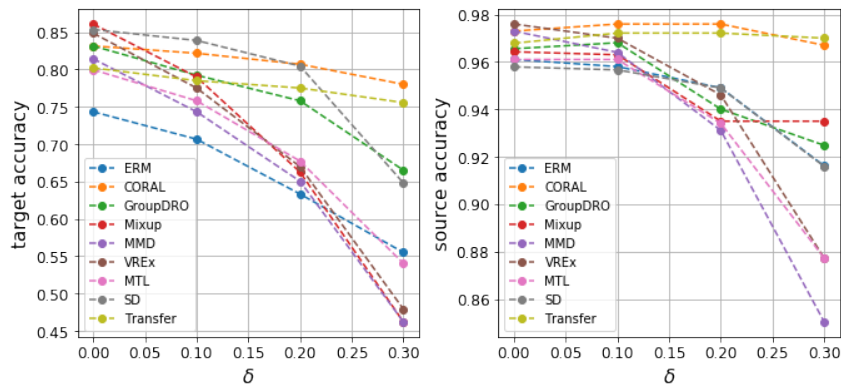


Figure 6: Measuring the transferability of various algorithms for domain generalization on PACS dataset. For the Transfer algorithm we choose $\delta = 0.3$, batch size 16, the number of ascent steps to be 30 using SGD with learning rate 0.001.

C.3.3 Office-Home

We present results from Algorithm 1 with information about losses and accuracies, for a wide array of algorithms in Table 4 for Office-Home. It can be seen that CORAL and SD learn more robust classifiers while other algorithms are not quite transferable: with a small decrease of source accuracy the target accuracy drops significantly.

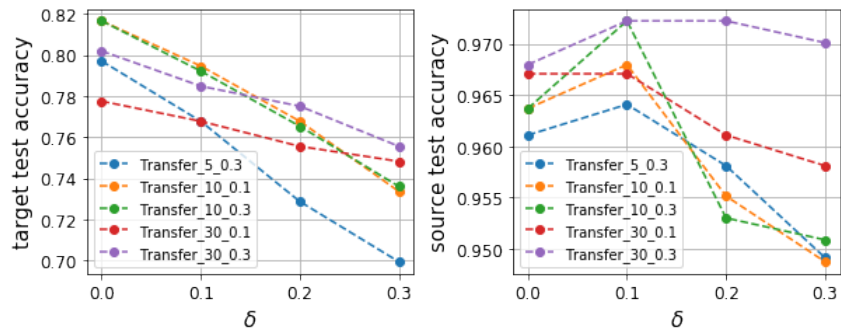


Figure 7: Evaluation of transferability of popular algorithms for domain generalization on Transfer algorithm with different hyperparameters. The dataset is PACS. One can see that if the number of inner steps is large and δ is large, then the classifier is more robust. “Transfer_ d _ δ ” means the inner loop takes d steps with the radius δ .

Table 3: Evaluation of transferability of popular algorithms for domain generalization on PACS. **algorithm**: the model that we evaluate; δ : the adversarial radius δ we choose in Algorithm 1; **max/min index**: the index of the domain with the maximal/minimal (test) classification errors (w.r.t. 0-1 loss); **max/min loss**: the largest/smallest loss among domains (including the target domain); **worst/best acc**: the smallest/largest classification test accuracies among domains (including the target domain).

| algorithm | δ | max index | min index | max loss | min loss | worst acc | best acc |
|-----------|----------|-----------|-----------|----------|----------|-----------|----------|
| ERM | 0.0 | 0 | 2 | 1.327 | 0.011 | 74.33% | 96.11% |
| ERM | 0.2 | 0 | 2 | 2.449 | 0.064 | 63.33% | 94.91% |
| GroupDRO | 0.0 | 0 | 2 | 0.820 | 0.012 | 83.13% | 97.60% |
| GroupDRO | 0.2 | 0 | 2 | 1.509 | 0.052 | 75.79% | 95.81% |
| SagNet | 0.0 | 0 | 2 | 0.919 | 0.002 | 77.51% | 99.10% |
| SagNet | 0.1 | 0 | 2 | 1.409 | 0.014 | 71.39% | 97.01% |
| SagNet | 0.2 | 0 | 2 | 2.002 | 0.094 | 60.64% | 94.31% |
| Mixup | 0.0 | 0 | 2 | 0.471 | 0.009 | 86.06% | 99.70% |
| Mixup | 0.1 | 0 | 2 | 0.681 | 0.016 | 78.97% | 98.80% |
| Mixup | 0.2 | 0 | 2 | 0.974 | 0.067 | 66.26% | 96.41% |
| CORAL | 0.0 | 0 | 2 | 0.743 | 0.006 | 83.13% | 97.31% |
| CORAL | 0.2 | 0 | 2 | 0.954 | 0.008 | 80.68% | 97.60% |
| CORAL | 0.3 | 0 | 2 | 1.147 | 0.012 | 78.00% | 96.71% |
| MMD | 0.0 | 0 | 2 | 0.776 | 0.005 | 81.42% | 97.31% |
| MMD | 0.1 | 0 | 2 | 1.203 | 0.006 | 74.33% | 96.41% |
| MMD | 0.2 | 0 | 2 | 1.832 | 0.066 | 65.04% | 93.11% |
| RSC | 0.0 | 0 | 2 | 1.089 | 0.003 | 77.75% | 95.81% |
| RSC | 0.1 | 0 | 2 | 2.535 | 0.129 | 63.81% | 93.41% |
| RSC | 0.2 | 0 | 2 | 4.732 | 0.560 | 43.52% | 82.63% |
| VREx | 0.0 | 0 | 2 | 0.593 | 0.002 | 84.84% | 97.60% |
| VREx | 0.1 | 0 | 2 | 0.912 | 0.009 | 77.51% | 97.01% |
| VREx | 0.2 | 0 | 2 | 1.518 | 0.049 | 66.99% | 94.61% |
| MTL | 0.0 | 0 | 2 | 1.269 | 0.001 | 79.95% | 96.11% |
| MTL | 0.2 | 0 | 2 | 2.477 | 0.060 | 67.73% | 93.41% |
| SD | 0.0 | 0 | 2 | 0.589 | 0.113 | 85.33% | 98.20% |
| SD | 0.2 | 0 | 2 | 0.930 | 0.262 | 80.44% | 97.60% |
| SD | 0.3 | 0 | 2 | 1.191 | 0.454 | 73.35% | 96.11% |

Table 4: Evaluation of transferability of popular algorithms for domain generalization on Office-Home. **algorithm**: the model that we evaluate; δ : the adversarial radius δ we choose in Algorithm 1; **max/min index**: the index of the domain with the maximal/minimal (test) classification errors (w.r.t. 0-1 loss); **max/min loss**: the largest/smallest loss among domains (including the target domain); **worst/best acc**: the smallest/largest classification test accuracies among domains (including the target domain).

| algorithm | δ | max index | min index | max loss | min loss | worst acc | best acc |
|-----------|----------|-----------|-----------|----------|----------|-----------|----------|
| ERM | 0.0 | 0 | 2 | 2.688 | 0.054 | 54.43% | 88.16% |
| ERM | 0.1 | 0 | 2 | 3.701 | 0.098 | 47.63% | 87.37% |
| GroupDRO | 0.0 | 0 | 2 | 2.940 | 0.072 | 58.76% | 88.61% |
| GroupDRO | 0.1 | 0 | 2 | 4.042 | 0.147 | 50.72% | 86.81% |
| SagNet | 0.0 | 0 | 2 | 2.030 | 0.055 | 56.08% | 87.94% |
| SagNet | 0.1 | 0 | 2 | 2.316 | 0.071 | 54.02% | 88.05% |
| Mixup | 0.0 | 0 | 2 | 1.657 | 0.051 | 60.62% | 90.76% |
| Mixup | 0.1 | 0 | 2 | 2.074 | 0.075 | 53.40% | 90.08% |
| CORAL | 0.0 | 0 | 2 | 1.878 | 0.043 | 59.79% | 89.06% |
| CORAL | 0.1 | 0 | 2 | 2.111 | 0.053 | 56.70% | 88.73% |
| MMD | 0.0 | 0 | 2 | 2.201 | 0.037 | 56.49% | 89.74% |
| MMD | 0.1 | 0 | 2 | 2.860 | 0.060 | 50.93% | 88.16% |
| VREx | 0.0 | 0 | 2 | 1.926 | 0.207 | 55.46% | 85.46% |
| VREx | 0.1 | 0 | 2 | 2.414 | 0.245 | 49.28% | 84.89% |
| MTL | 0.0 | 0 | 2 | 2.736 | 0.047 | 52.58% | 87.71% |
| MTL | 0.1 | 0 | 2 | 3.921 | 0.109 | 42.06% | 85.12% |
| SD | 0.0 | 0 | 2 | 1.535 | 0.047 | 64.33% | 91.54% |
| SD | 0.1 | 0 | 2 | 1.717 | 0.049 | 63.51% | 92.33% |