ABSTRACT

Recent advances in domain adaptation establish that requiring a low risk on the source domain and equal feature marginals degrade the adaptation's performance. At the same time, empirical evidence shows that incorporating an unsupervised target domain term that pushes decision boundaries away from the high-density regions, along with relaxed alignment, improves adaptation. In this paper, we theoretically justify such observations via a new bound on the target risk, and we connect two notions of relaxation for divergence, namely $\beta$-relaxed divergences and localization. This connection allows us to incorporate the source domain’s categorical structure into the relaxation of the considered divergence, provably resulting in a better handling of the label shift case in particular.

1 Introduction

Supervised learning algorithms are prone to failure when the training and testing distributions are different. That arises in several real-world applications such as speech recognition and computer vision, due to changes in the data collection process for example. As solving this problem by collecting more data might be problematic due to the potential cost of the labeling process, the Domain Adaptation (DA) field (Pan and Yang, 2010; Weiss et al., 2016) has emerged to tackle the issue in attempt to transfer the knowledge acquired on the labeled training set, stemming from a source distribution, to a partially or totally unlabeled testing set, corresponding to a target distribution.

Over the last decade, DA has been the focus of several lines of work. On the theoretical level, in the context of tackling the distribution shift problem (Quinonero-Candela et al., 2008), one salient idea is to bound the risk on the target distribution by quantities reflecting the performance on the source domain along with its relatedness to the target (Ben-David et al., 2007; Mansour et al., 2009; Cortes and Mohri, 2011; Ben-David and Urner, 2014; Cortes and Mohri, 2014; Germain et al., 2013, 2016; Zhang et al., 2019). We refer the interested reader to Redko et al. (2020) for a more exhaustive account in this regard. On the algorithmic level, early approaches aim at aligning distributions on the feature level (Blitzer et al., 2007; Daumé III, 2009; Fernando et al., 2013) or at the instance level via reweighting (Shimodaira, 2000; Sugiyama et al., 2007; Huang et al., 2007; Cortes et al., 2010). The goal behind such an alignment is to reduce some dissimilarity measure between the domains, such as the Wasserstein distance (Courty et al., 2016, 2017), the Maximum Mean Discrepancy (Huang et al., 2007; Gong et al., 2013), or the distance between covariance matrices (Sun et al., 2016), to name a few. The recent reviews of Kouw and Loog (2019); Zhang (2019); Zhuang et al. (2020) provide an excellent overview of the different methods. More recently, the emergence of deep learning (Goodfellow et al., 2016) resulted in a family of methods looking for a feature representation that not only is discriminative for classes on the source domain, but that is also domain-agnostic (Ganin et al., 2016; Long et al., 2018; Shu et al., 2018).
Such approaches have proven their effectiveness especially for computer vision (Csurka et al., 2017). We refer the interested reader to Wang and Deng (2018); Wilson and Cook (2020) for reviews on deep DA.

Nevertheless, domain alignment imposes the cross-labeling risk, resulting in a correspondence between instances having different labels (Mehra et al., 2021). That happens, for example, when the label marginals vary between the two domains. Provably, this situation deteriorates the adaptation performance when combined with a good performance on the source domain (Zhao et al., 2019; Wu et al., 2019; Le et al., 2021). As a result, two directions to tackle this problem have been recently studied. On the one hand, some lines of work relax the requirement of equality of distribution when trying to align them (Johansson et al., 2019; Wu et al., 2019; Zhang et al., 2020; Tong et al., 2022), whereas other approaches jointly align the label and feature marginals in an attempt to circumvent the label shift problem (Redko et al., 2019; Tachet des Combes et al., 2020) and its generalizations (Rakotomamonjy et al., 2021; Kirchmeyer et al., 2022) allowing an additional shift in label-conditionals. These approaches, however, are disconnected and more understanding on their relations is needed. Moreover, they only handle the problem of strictness of the divergence, whereas the recent negative results we mentioned also point out to the role of requiring a good performance on the source domain. In this regard, recent deep learning approaches are increasingly using an unsupervised loss on the target domain to promote a more class-discriminative structure in addition to requiring a good performance on the source (Shu et al., 2018; Saito et al., 2019; Tan et al., 2020; Kirchmeyer et al., 2022; Tong et al., 2022). To the best of our knowledge, only a few papers, including Germain et al. (2016) and Morerio and Murino (2017), deliver theoretical evidence of the benefits of such terms.

Against this background, in this paper we provide the following contributions:

• We theoretically prove the utility of the minimizing the uncertainty of the considered scoring function in its predictions on the target domain while being guided by the predictions on the source domain. Our result tightens a broad class of previously established DA bounds in the sense that it only requires these bounds to involve a risk on the source domain.

• We introduce a new discrepancy between measures that generalizes Integral Probability Metrics (Zolotarev, 1984) when the compared measures do not have the same mass, and use it to connect two notions of relaxed dissimilarity between domains, namely localized discrepancies (Zhang et al., 2020) and $\beta$-admissible distances (Wu et al., 2019). We further harness our established link in order to incorporate the source domain’s observable categorical structure into the relaxation, leading to an additional connection to class re-weighting methods.

• Depending on the choice of the functional space defining our discrepancy measure, we revisit previously established results. In particular we theoretically justify approaches that rely on the extremely relaxed requirement of confusion of supports rather than of distributions.

• We illustrate the benefits of taking the categorical structure of the source into account when relaxing the discrepancy between distributions, via experiments on toy datasets in the particular case of Wasserstein distances.

Outline of the paper After introducing the problem setup and the notations in Section 2, we prove in Section 3 the theoretical interest of enforcing a scoring function at hand to be confident in its predictions. Then, we specialize our study to bounds involving a divergence term and a joint risk in Section 4, where we link previously introduced notions of relaxation, and we extend them by incorporating the source domain’s categorical structure. Section 6 is dedicated to revisiting previously established DA results in the light of our theoretical results. Finally, we illustrate the interest of incorporating the categorical structure over classic relaxation in Section 7.

2 Problem setup and notations

We consider a multi-class domain adaptation setting, where the feature space is $\mathcal{X}$, a compact subset of $\mathbb{R}^p$ ($p \in \mathbb{N}^*$) and the label space is $\mathcal{Y} = \{y_1, \cdots, y_K\}$, where the different classes are encoded as the basis vectors of $\mathbb{R}^K$ (one hot encoding), unless specified otherwise. The source and target domains correspond to two joint distributions $S$ and $T$ over $\mathcal{X} \times \mathcal{Y}$. For any probability distribution $D$ over $\mathcal{X} \times \mathcal{Y}$, we denote by $D_{X}, D_{Y}, D_{X|Y}, D_{Y|X}$ its feature- and label-marginals, and label- and feature- conditionals respectively, for $x \in \mathcal{X}, y \in \mathcal{Y}$. In particular, for the class conditional

1Vectors are denoted in bold lower case font.
distributions, by abuse of notation we will denote \( D_{X|Y} \) instead of \( D_{XY} \). When we refer to labeling functions \( f_S \) (resp. \( f_T \)) of the source (resp. target) domain, we mean a function that outputs a vector over the \( K \)-dimensional probability simplex, which can be degenerated to indicate only one class in the case of deterministic labeling. All of the measures we consider over \( X \) have densities, \textit{i.e.}, they are absolutely continuous with respect to the Lebesgues measure.

Concerning the performance of classification, we consider classifiers as functions in \( Y^X \) that are typically selected from a hypothesis space \( \mathbb{H} \subseteq Y^X \), and scoring functions as functions in \( (\mathbb{R}^K)^X \). A loss function is any function \( l : \mathbb{R}^K \times \mathbb{R}^K \to \mathbb{R}_+ \), typically taking a scoring function or a classifier for the first argument, and a classifier for the second, and verifying \( l(y, y) = 0 \) \( \forall y \in Y \). Given a scoring function \( g \), we denote its associated classifier as \( h_g \), \textit{i.e.} \( h_g(x) = y_k \) with \( k \in \text{argmax}_y g(x) \), and assume that for all the loss functions we consider, we have \( h_g(x) \in \text{argmin}_{y \in Y} l(g(x), y) \) for any \( x \) in \( X \). For the sake of conciseness, we consider that any classifier is also a scoring function, with \( h_g = g \). Finally, we define the \( l \)-risk of a scoring function \( g \) over a distribution \( D \) over \( X \times Y \) as \( \mathcal{L}_D(g) := \mathbb{E}_{(x,y) \sim D}[l(g(x), y)] \), and we extend it to the disagreement of \( g \) with a classifier \( h \) as \( \mathcal{L}_D(g, h) := \mathbb{E}_{x \sim D}[l(g(x), h(x))] \).

3 Role of the confidence of a scoring functions in its predictions on the target domain

Given a scoring function \( g : X \to \mathbb{R}^K \), one approach to measure its uncertainty in its predictions \( h_g \), using a loss function \( l \), is to compute the following quantity.

**Definition 1** (Uncertainty of a scoring function). Given a scoring function \( g \) with \( h_g \in \mathbb{H} \), we define its uncertainty in its predictions over a distribution \( D \) over \( X \times Y \) by

\[
\inf_{h \in \mathbb{H}} \mathcal{L}_D(g, h) = \mathcal{L}_D(g, h_g).
\]  

Below, we give two known examples of this quantity for different choices of the loss function \( l \).

**Example 2** (Cross entropy loss). In this case, \( g(x) \) is in the \( K \)-dimensional probability simplex (after applying the softmax function). We then have \( l(g(x), h_g(x)) = H_{\alpha}(g(x)) \),\(^2\) where \( H_{\alpha} \) denotes the Renyi entropy (Rényi, 1961) defined as \( H_{\alpha}(g(x)) = \frac{1}{\alpha - 1} \log \left( \sum_y (g(x))^\alpha \right) \), which is equal to the Shannon entropy when \( \alpha = 1 \). Since we have \( H_{\alpha}(g(x)) \leq H_{1}(g(x)) \) \( \forall \alpha \geq 0 \), having a small conditional entropy of \( g(x) \) in particular results in a small uncertainty of \( g(x) \). Minimizing the conditional entropy, borrowed from the semi-supervised learning literature (Grandvalet et al., 2005; Erkan and Altun, 2010), is now a standard approach in domain adaptation (Shu et al., 2018; Liang et al., 2021; Kirchmeyer et al., 2022).

**Example 3** (Hinge loss). The binary SVM (Boser et al., 1992; Cortes and Vapnik, 1995) problem can be written as minimizing the regularized hinge loss function \( l(g(x), y) = (1 - yg(x))^+ \), \( \text{where} \ g \ \text{is a linear classifier and} \ y \in \{-1, 1\} \). Computing the uncertainty of \( g \) at \( x \) yields \( (1 - |g|)^+ \), the latter being an unsupervised loss appearing in the transductive SVM formulation (Chapelle and Zien, 2005; Collobert et al., 2006). A smooth analogue of this quantity also appears in Germain et al. (2016). In the absence of labeled target data, the best one can hope for by obtaining a confident classifier is a clustering in which the scoring function identifies the classes up to a permutation. In what follows, we combine the previous quantity with supervision from the source domain to obtain a source-guided measure of uncertainty.

**Definition 4** (Source-guided uncertainty). Let \( \mathbb{H} \) be a hypothesis space, and let \( l^1 \) and \( l^2 \) be two loss functions with associated risks \( \mathcal{L}_S^1(\cdot) \) and \( \mathcal{L}_S^2(\cdot) \) for a distribution \( D \). The source-conditioned confidence of a function \( g \in Y^X \) associated to the two previous losses is:

\[
\mathcal{C}_{\mathbb{H}}^{1,2}(g) = \inf_{h \in \mathbb{H}} \mathcal{L}_S^1(g, h) + \mathcal{L}_S^2(h).
\]  

In the case where \( l^1 = l^2 = l \), we simply denote \( \mathcal{C}_{\mathbb{H}}(h) \), where \( l \) is clear from the context.

Compared with Definition 1, we have an additional term that can be thought of as a regularization forcing \( h \) to be compatible with the labels on the source domain. A second interpretation of the source-guided uncertainty is that when \( l^1 = l^2 = l \), it is equal to the ideal joint \( l \)-risk corresponding to the class of functions \( \mathbb{H} \), for a target domain

\(^2\)The proofs of all theoretical claims can be found in the appendix.
labeled by $g$. In particular, for $g = f_T$, it is equal to the ideal joint risk (Ben-David et al., 2010; Acuna et al., 2021; Zhong et al., 2021).

The next proposition formalizes some properties of the source-guided uncertainty and helps to understand when it is small.

**Proposition 5** (Properties of the source-guided uncertainty). The source-guided uncertainty of a scoring function verifies the following properties:

1. If $g$ is a scoring function and $h_g \in \mathbb{H}$, then $\mathcal{C}_{\mathbb{H}}^{1,2} (g) \leq \mathcal{L}_T^1 (g, h_g) + \mathcal{L}_S^2 (h_g)$. In particular, if $g \in \mathbb{H}$, then $\mathcal{C}_{\mathbb{H}}^{1,2} (g) \leq \mathcal{L}_S^2 (g)$.

2. If $\mathbb{H} \subseteq \tilde{\mathbb{H}} \subseteq \mathbb{Y}^X$, and if $l^1(a, a) = 0$, then $\inf_{g \in \mathbb{H}} \mathcal{C}_{\mathbb{H}}^{1,2} (g) = \inf_{h \in \mathbb{H}} \mathcal{L}_S^2 (h)$.

3. If $l = l^1 = l^2$ obeys the triangle inequality, then $\mathcal{L}_{\mathbb{H}} (h) = \mathcal{L}_S (h)$ for $h \in \{ h_S, h^* \}$, where $h_S \in \arg\min \mathcal{L}_S (h)$ and $h^* \in \arg\min \mathcal{L}_S (h)$.

In Proposition 5, the first point justifies the intuition that the source-guided uncertainty is small whenever the scoring function $g$ performs well on $S$ (in terms of the risk of $h_g$), while having a low uncertainty on $T$ (i.e., a low $\mathcal{L}_S^2 (g, h_g)$). And when specialized to the case where $g$ is a classifier in $\mathbb{H}$, it provides a lower bound for the risk on the source domain. The second point shows that when the space of scoring functions is rich enough to contain classifiers, the source-guided uncertainty coincides with the best achievable $l^2$-risk on the source domain. The last point states an interesting fact about the case of equality with the source risk, achieved for the ideal joint hypothesis that normally requires access to target labels, and for the best source hypothesis.

Our next result shows the role of the source-guided uncertainty in tightening any domain adaptation bound that comprises the risk of the considered classifier on the source domain.

**Proposition 6** (Tightening bounds on the target risk). Let $g$ be a scoring function, and let $l^1$ be a loss function, verifying $l^1(u, y_1) - l^2(y_2, y_1) \leq l^1(u, y_2) \forall u \in \mathbb{R}^K, y_1, y_2 \in \mathbb{Y}$. Then given a bound on the target risk of the following form:

$$\mathcal{L}_T^2 (h) \leq \mathcal{L}_S^2 (h) + A(T, S); \quad \forall h \in \mathbb{H},$$

where $A(T, S)$ reflects a relatedness between the domains’ joint distributions, we have for any scoring function $g$,

$$\mathcal{L}_T^1 (g) \leq \mathcal{C}_{\mathbb{H}}^{1,2} (g) + A(T, S).$$

The statement of Proposition 6 holds for a large class of domain adaptation bounds on the target risk, and according to point 1 of Proposition 5, when $g \in Hbb$, it theoretically shows that the source-guided uncertainty provides a bound that is tighter than classic bounds involving the risk on the source domain. For scoring functions, this tightness may justify the empirical effectiveness of the conditional entropy minimization (Example 2), as done in (Shu et al., 2018; Kirchmeyer et al., 2022). Beyond the case of $g \in \mathbb{H}$, we have a bound that holds even when space $\tilde{\mathbb{H}}$ is richer than the hypothesis space from which we select $g$. In the next section, we will use this fact to derive bounds with several families of divergences between the two domains, after we specialize $A(T, S)$ to the form of the sum of a divergence term and a joint minimum risk (Ben-David et al., 2010; Acuna et al., 2021). Concerning the assumption on the loss function, it reduces to the triangle inequality when both are equal. It also holds, for example, for $l^1$ and $l_2$ chosen as the cross-entropy loss and the $l^1$ loss up to a multiplicative factor.

### 4 Relating weak alignment and localization

So far, we theoretically justified the role of the source-guided uncertainty term on the target domain. Now we focus on a special class of bounds that assume low value of the ideal joint risk. Our results will involve relaxed divergences that do not require equality of the two distributions to be null, a property shared by the $\mathbb{H}\Delta\mathbb{H}$-distance (Ben-David et al., 2010) and its generalization the $l$—discrepancy (Mansour et al., 2009). They will also be asymmetric, as in the case of the recently introduced $\beta$—admissible distances (Wu et al., 2019) and localized discrepancies (Zhang et al., 2020). In order to proceed, we begin by the following definitions for localized sets.

**Definition 7** ($\mathcal{E}, \mathcal{S}_\mathcal{E}$)—localized space of nonnegative functions). Let $\mathbb{F}$ be a set of nonnegative functions. For $\epsilon \geq 0$, the ($\mathcal{E}, \mathcal{S}_\mathcal{E}$) localized subset of $\mathbb{F}$ is defined as

$$\mathbb{F}_\mathcal{E} = \{ f \in \mathbb{F}; \quad \mathbb{E}_{\mathcal{S}_\mathcal{E}} [f] \leq \epsilon \}$$

(5)
An instance of Definition 7 allows to define the localized discrepancy introduced in Zhang et al. (2020), by choosing \( \mathcal{F} = l(\mathcal{H}, f_S) := \{l(h, f_S); h \in \mathcal{H}\} \), where \( l \) is a loss function. As indicated in Zhang et al. (2020), the previous example is motivated by the following observation: If the ideal joint risk is \( \lambda = \text{localized discrepancy} \), an instance of Definition 7 allows to define the ideal joint risk \( \lambda \). If \( \mathcal{Q} \) is identically null, then \( \mathcal{Q} \) is rich enough (feature space \( \mathcal{X} \)) and the value will not change when restricting the choice of \( h \in \mathcal{H} \) to hypotheses achieving risk at most \( \lambda \) on the source domain. In other words, among all of the hypotheses that perform well on \( \mathcal{S} \), there is one that has a low risk on both domains.

In addition the previous notion of localization, we introduce a family of dissimilarities between measures over the feature space \( \mathcal{X} \) in the following definition.

**Definition 8** (Integral Measure Discrepancy). Let \( \mathcal{F} \) be a family of nonnegative functions over \( \mathcal{X} \), containing the null function. The Integral Measure Discrepancy (IMD) associated to \( \mathcal{F} \) between two nonnegative finite measures \( \mathcal{Q}_1 \) and \( \mathcal{Q}_2 \) over \( \mathcal{X} \) is

\[
\text{IMD}_\mathcal{F}(\mathcal{Q}_1, \mathcal{Q}_2) := \sup_{f \in \mathcal{F}} \int f \, d\mathcal{Q}_1 - \int f \, d\mathcal{Q}_2.
\]

The IMD is obviously a generalization of Integral Probability Metrics (IPM) (Zolotarev, 1984; Müller, 1997) to measures with possibly different masses. The interest in distances between measures with different masses is not new and has been the topic of Steerneman (1983) for the total variation distance and Hellinger distances, Benamou et al. (2015) to define Bregman projections and Chizat et al. (2018b,a); Liero et al. (2018); Fatras et al. (2021) for the unbalanced optimal transport problem, to name a few. Some of the IMD’s basic properties are given by the following proposition.

**Proposition 9** (Properties of the IMD). The IMD is nonnegative, satisfies the triangle inequality, and we have \( \text{IMD}_\mathcal{F}(\mathcal{Q}_1, \mathcal{Q}_2) = 0 \) if \( \mathcal{Q}_1 \leq \mathcal{Q}_2 \) (i.e., \( q_1 \leq q_2 \) when \( q_1 \) and \( q_2 \) are the densities of \( \mathcal{Q}_1 \) and \( \mathcal{Q}_2 \)). Moreover, for \( \mathcal{F} \) rich enough (i.e., containing the continuous functions or the indicator functions), we have \( \text{IMD}(\mathcal{Q}_1, \mathcal{Q}_2) = 0 \) only if \( \mathcal{Q}_2 \geq \mathcal{Q}_1 \).

In particular, Proposition 9 shows that the IMD is asymmetric. Indeed, it is sufficient to take a measure \( \mathcal{Q} \) that is nonidentically null, then \( \text{IMD}(\mathcal{Q}, 2\mathcal{Q}) = 0 \) while \( \text{IMD}(2\mathcal{Q}, \mathcal{Q}) > 0 \) whenever \( \mathcal{F} \) contains a function with \( \int f \, d\mathcal{Q} > 0 \).

With the previously introduced quantities, we are now ready to state our domain adaptation bound involving the IMD and localization.

**Proposition 10.** Let \( \mathcal{H} \) be a hypothesis space, \( g \) a scoring function not necessarily in \( \mathcal{H} \), and \( l \) a loss function verifying the triangle inequality. Assume that \( l(\mathcal{H}, \mathcal{H}) := \{l(h_1(\cdot), h_2(\cdot)); h_1, h_2 \in \mathcal{H}\} \subseteq \mathcal{F} \), where \( \mathcal{F} \) is a set of bounded nonnegative functions. Also, for any \( r \geq 0 \), we consider the localized hypothesis space \( \mathcal{H}^r := \{h \in \mathcal{H}; \mathcal{L}_r(h) \leq r\} \).

Then, for any \( r_1, r_2 \geq 0 \),

\[
\mathcal{L}_r(h) \leq \mathcal{C}_{\mathcal{H}^r_1}(g) + \text{IMD}_{\mathcal{F}_{r_1+r_2}}(\mathcal{T}_\mathcal{X}, \mathcal{S}_\mathcal{X}) + \inf_{h \in \mathcal{H}^r_2} \mathcal{L}_r(h) + \mathcal{L}_\mathcal{S}(h).
\]

Proposition 10 is a generalization of the ones in Ben-David et al. (2010); Zhang et al. (2019); Acuna et al. (2021), as it involves an ideal joint risk. It is based on localized hypothesis spaces that have been considered for DA in Zhang et al. (2020); however, our result extends the latter in the following aspects. First, as we pointed out in Section 3, the concerned hypothesis \( g \) does not have to be in \( \mathcal{H} \), and our bound is tighter than using a source loss whenever \( g \in \mathcal{H}^r \), a condition that is required in the analogous result of Zhang et al. (2020). Second, the space \( \mathcal{F} \) we consider to define the discrepancy term is more general as it includes the result of Zhang et al. (2020) for \( \mathcal{F} = \mathcal{H} \Delta \mathcal{H} \).

In the next proposition, we leverage the Lagrange duality to prove an upper bound for the localized IMD, that will hold tightly under mild conditions. It will be the key to establish the connection between localization (Zhang et al., 2020) and \( \beta \)-admissible distances (Wu et al., 2019).

**Proposition 11** (Duality for localized IMD). Assume \( \mathcal{F} \) is a space of nonnegative functions over \( \mathcal{X} \). Then

\[
\forall \varepsilon \geq 0, \quad \text{IMD}_{\mathcal{F}_{\varepsilon}}(\mathcal{T}_\mathcal{X}, \mathcal{S}_\mathcal{X}) \leq \inf_{\alpha \geq 0} \text{IMD}_{\mathcal{F}}(\mathcal{T}_\mathcal{X}, (1 + \alpha)\mathcal{S}_\mathcal{X}) + \varepsilon \alpha.
\]

Moreover, if \( \mathcal{F} \) is convex, \( \text{IMD}(\mathcal{T}_\mathcal{X}, \mathcal{S}_\mathcal{X}) \) is finite and \( \varepsilon > 0 \), then we have an equality, and the infimum at the right hand side is achieved for some \( \alpha^* \geq 0 \).

In spite of having a lower value than IPM’s (since \( \mathcal{F}_\varepsilon \subseteq \mathcal{F} \)), a localized IMD is null if and only if both distributions are identical whenever \( \mathcal{F} \) is rich enough as expressed in the following corollary.
Corollary 12. If $\mathbb{F}$ is rich enough, then for any $\epsilon > 0$, $\text{IMD}_{\mathbb{F}}(T_\mathcal{X}, S_\mathcal{X}) = 0$ if and only if $T_\mathcal{X} = S_\mathcal{X}$.

To guard against the drawbacks of strict alignment implying that $T_\mathcal{X} = S_\mathcal{X}$ (Zhao et al., 2019; Wu et al., 2019; Le et al., 2021), we apply Proposition 11 via bounding the infimum over the choice of $\alpha \geq 0$ by an arbitrary $\beta \geq 0$, thus leading to the following corollary.

Corollary 13. With the assumptions of Proposition 10, for a scoring function $g$, any $r_1, r_2, \beta \geq 0$, we have
\[
\mathcal{L}_T(g) \leq \mathcal{C}_{\mathbb{H}_r}(g) + \text{IMD}_{\mathbb{F}}(T_\mathcal{X}, (1 + \beta)S_\mathcal{X}) + \beta(r_1 + r_2) + \inf_{h \in \mathbb{H}_r^2} \mathcal{L}_T(h) + \mathcal{L}_S(h)
\]

(8)

Corollary 13 is reminiscent of the DA bound in Wu et al. (2019), and shows the interest of $\beta$–admissible distances through a different derivation. Indeed, we do not have a $(1 + \beta)$ factor multiplying the source risk of $g$ as in their work. Moreover, as implied by Proposition 9, the discrepancy $\text{IMD}_{\mathbb{F}}(T_\mathcal{X}, (1 + \beta)S_\mathcal{X})$ is always nonnegative and is null if and only if $t(x) \leq (1 + \beta)s(x)$ almost surely for $\mathbb{F}$ rich enough. The latter condition is the bounded ratio condition required to define $\beta$–admissible distances (Wu et al., 2019). However, when $\mathbb{F}$ is more restricted, it generalizes it in the same way that Integral Probability Metrics do not need the density ratio to be defined, compared to Csiszár divergences (Csiszár, 1967).

In the next section, we will utilize the link between localization and $\beta$–admissible in order to extend these notions by taking into account the categorical structure of the source domain.

5 Incorporating the source’s categorical structure

A limitation of the localization introduced Zhang et al. (2020) is that it is a global consideration of the performance on the source domain, without a finer look at the performance per class. In the following definition, we introduce a stricter notion of localization that requires the bound on the expectation to hold per class.

Definition 14 ($\epsilon, S_{\mathcal{X}|y}$–localized space of nonnegative functions). Let $\mathbb{F}$ be a set of nonnegative measurable functions over $\mathcal{X}$. For $\epsilon = (\epsilon_1, \ldots, \epsilon_K) \geq 0$, the $(\epsilon, S_{\mathcal{X}|y})$ localized subset of $\mathbb{F}$ is defined as
\[
\mathbb{F}_\epsilon = \{ f \in \mathbb{F}; \quad E_{S_{\mathcal{X}|k}}[f] \leq \epsilon_k \quad \forall 1 \leq k \leq K \}
\]

(9)

Choosing $\mathbb{F} = l(\mathbb{H}, f_S)$ corresponds to a stricter notion of localization than the one introduced in Zhang et al. (2020), as it requires the hypothesis to have a good performance for every class on the source domain. The intuition behind this requirement is that the considered hypothesis space must contain an ideal joint hypothesis with a performance that should not depend on the class proportions of the source domain. Requiring a low classification risk per class has already been theoretically considered in the definition of the Balanced Error Rate of Tachet des Combes et al. (2020), in which the authors use it to bound on the target risk.

From now on, we define $p := (S_{\mathcal{X}|[y = 1]}, \ldots, S_{\mathcal{X}|[y = k]}) \in \Delta_K$, the vector of class proportions for the source domain. Also, we will refer to localization considered in Definition 7 and 14 respectively as global and per-class localization. The two notions are linked as stated by the following proposition.

Proposition 15. If $\epsilon = (\epsilon_1, \ldots, \epsilon_K)^T \geq 0^3$, then $\mathbb{F}_\epsilon \subseteq \mathbb{F}_{p\epsilon}$. Conversely, if $\eta = (\eta_1, \ldots, \eta_K) \in \{ \mathbb{R}_+ \cup \{ \infty \} \}^K$ with $\eta_k = \frac{\epsilon}{S_{\mathcal{X}|[y = k]}}$ if $S_{\mathcal{X}|[y = k]} > 0$ and $\eta_k = \infty$ otherwise. Then $\mathbb{F}_\epsilon \subseteq \mathbb{F}_\eta$.

An interpretation for the first result of Proposition 15 is that a hypothesis having a risk at most $\epsilon$ per class will have a global risk at most $\epsilon$. For the second one, it shows that we can obtain localization per class at the price of losing in accuracy by dividing it by the class proportions. For example, on a class-balanced source domain, having an $l$–risk of at most $\epsilon > 0$ implies having a risk of at most $K\epsilon$ per class.

Of course, the reasoning we used to link global localization and $\beta$–admissible distances through Propositions 10,11 and Corollary 13 can be performed again for the per-class discrepancy, which leads to the following proposition.

Proposition 16. Let $\mathbb{H}$ be a hypothesis space, $g$ a scoring function, and $l$ a loss function verifying the triangle inequality. Assume that $l(\mathbb{H}, \mathbb{H}) \subseteq \mathbb{F}$, where $\mathbb{F}$ is a set of bounded nonnegative functions. Also, for any $r = (r_1, \ldots, r_K) \geq 0$, we consider the localized hypothesis space $\mathbb{H}^r := \{ h \in \mathbb{H}; \mathcal{L}^r_{S_{\mathcal{X}|k}}(h) \leq r_k \forall 1 \leq k \leq K \}$.

3We write $u \geq 0$ for $u \in \mathbb{R}_+^p$.  

6
Then for any $r_1, r_2, \beta \geq 0$, we have

$$\mathcal{L}_\mathcal{T}(g) \leq \mathcal{C}_{\mathbb{R}^r}(g) + \text{IMD}_\mathcal{F}\left(\mathcal{T}_\mathcal{X}, \mathcal{S}_\mathcal{X} + \sum_{k=1}^{K} \beta_k \mathcal{S}_{\mathcal{X}|k}\right) + \beta^T(r_1 + r_2) + \inf_{h \in \mathbb{R}^r} \mathcal{L}_\mathcal{T}(h) + \mathcal{L}_\mathcal{S}(h). \tag{10}$$

The latter result is a generalization of Corollary 13. Indeed, for $r_i = r_i \mathbf{1}, i \in \{1, 2\},$ and $\beta = \beta \mathbf{p}$, where $\beta > 0$ is a fixed parameter, we recover the global localization case. However, it requires $K$ parameters to fix (the components of $\beta$) instead of one scalar $\beta \geq 0$, which is impractical. One can overcome this drawback by noticing the following: The choice of $\beta \mathbf{p}$ can be thought of as a particular splitting of $\beta$’s value across different classes. This naturally hints towards a better splitting. We formalize this observation in the following corollary.

**Corollary 17.** With the assumptions of Proposition 16, let $r_1, r_2, \beta \geq 0$. Besides, let $r_1 = r_2 = r \mathbf{1}$. Then

$$\mathcal{L}_\mathcal{T}(g) \leq \mathcal{C}_{\mathbb{R}^r}(g) + \min_{\beta \geq 0} \text{IMD}_\mathcal{F}\left(\mathcal{T}_\mathcal{X}, \mathcal{S}_\mathcal{X} + \sum_{k=1}^{K} \beta_k \mathcal{S}_{\mathcal{X}|k}\right) + \beta^T(r + r) + \inf_{h \in \mathbb{R}^r} \mathcal{L}_\mathcal{T}(h) + \mathcal{L}_\mathcal{S}(h). \tag{11}$$

Moreover, the inequality in the constraint $\beta \mathbf{1} \leq 1$ can be replaced by an equality.

Corollary 17 shows the way to make the most of the per-class localization, while a priori fixing only one parameter $\beta$. Such an optimal splitting can be interpreted as a relaxed class reweighting. Indeed, denoting the $K$-dimensional probability simplex by $\Delta_K$, the minimization problem in Corollary 17 is equivalent to

$$\min_{\beta \in \Delta_K, \text{ (1+\beta)\mathbf{p} \geq \mathbf{p}}} \text{IMD}_\mathcal{F}\left(\mathcal{T}_\mathcal{X}, (1+\beta) \sum_{k=1}^{K} \beta_k S_{\mathcal{X}|k}\right), \tag{12}$$

which is a combination of $\beta$-relaxation (Wu et al., 2019) and re-weighting approaches (Redko et al., 2019; Tachet des Combes et al., 2020; Rakotomamonjy et al., 2021; Kirchmeyer et al., 2022), although the reweighting is taken over a proper subset of the $K$-dimensional probability simplex. However, to the best of our knowledge, our result is the first to involve a minimum over source class weights in a DA bound, in contrast with the previously mentioned contributions.

We now prove that for label shift, a special case considered in the DA literature (Zhang et al., 2013; Lipton et al., 2018; Redko et al., 2019) in which the distribution mismatch is due to a shift in the label marginals, the per-class localization is more beneficial than the global one.

**Proposition 18 (Case of label shift).** Assume that the source and target distributions verify $\mathcal{T}_{\mathcal{X}|y} = \mathcal{S}_{\mathcal{X}|y} = \mathcal{D}_{\mathcal{X}|y}$ for all $y \in \mathcal{Y}$. Let $(q_k)_{k=1}^{K}$ denote the target class proportions. Then

1. If $\min_{1 \leq k \leq K} p_k > 0$ and $\beta \geq \max_{1 \leq k \leq K} \left(\frac{q_k}{p_k} - 1\right)_+$, then $\text{IMD}_\mathcal{F}(\mathcal{T}_\mathcal{X}, (1+\beta)\mathcal{S}_\mathcal{X}) = 0$.

2. If $\beta_k \geq (q_k - p_k)_+ \forall 1 \leq k \leq K$, then $\text{IMD}_\mathcal{F}(\mathcal{T}_\mathcal{X}, \mathcal{S}_\mathcal{X} + \sum_{k=1}^{K} \beta_k \mathcal{S}_{\mathcal{X}|k}) = 0$.

Moreover, if $\mathcal{F}$ is rich enough, and if there exists a family $\{B_l\}_{l=1}^{K}$ of subsets of $\mathcal{X}$ such that $\mathcal{D}_{\mathcal{X}|k}(B_l) > 0$ if $k = l$ and $\mathcal{D}_{\mathcal{X}|k}(B_l) = 0$ otherwise, then the converses of the two previous statements holds.

Statements 1 and 2 of Proposition 18 show the existence of some $\beta \geq 0$ or $\beta \geq 0$ in the per-class localization case such that the relaxed IMD between $\mathcal{T}_\mathcal{X}$ and $\mathcal{S}_\mathcal{X}$ is null. However, in the first case, $\beta$ grows with the ratio $\frac{q_k}{p_k}$ which can go arbitrarily large depending on the class proportions on the source domain, whereas in the case of per class localization, the lower bound on components $\beta_k$ is less prohibitive as it can at most be equal to 1 (since $\sum_{k=1}^{K} (q_k - p_k)_+ \leq 1$). Hence, the range of $\beta$ to test when implementing the $\beta$-splitting minimization problem of Corollary 17 is bounded. The converse statement relies on the capacity of $\mathcal{F}$, and the existence of regions of $\mathcal{X}$ having only one label. This is a relaxation of the cluster structure assumption (Tachet des Combes et al., 2020; Kirchmeyer et al., 2022) as the family $\{B_l\}_{l=1}^{K}$ does not need to form a partition of $\mathcal{X}$. Whether the richness assumption can be relaxed (for example, for Lipschitz functions that define the Wasserstein distance) remains an open question.

---

4 $\mathbf{1}$ is the vector with all coordinates equal to 1.
6 Some implications for specific choices of \( F \)

In this section, we explore the consequences of some choices of \( F \) on the definition of the relaxed IMD. We will link this choice to that of \( H \), as we assume \( l(H, H) \subseteq F \). Before continuing, we denote the support of a probability \( D_X \) over \( X \) by \( \text{supp} \ D_X \). We will successively consider \( F \) as the space of all bounded measurable functions (infinite capacity), an arbitrary hypothesis space (typically with a finite VC dimension) and a space of 1–Lipschitz functions.

6.1 Bounded functions: revisiting total variation and reweighting

The following corollary revisits the total variation bound from Ben-David et al. (2010, Theorem 1).

**Proposition 19.** Assume \( l(H, H) \) is the space of all measurable functions bounded by 1 over \( X \). Denoting \( t \) and \( s \) the densities of \( T_X \) and \( S_X \) with respect to some dominating measure \( \mu \), we have for any scoring function \( g \)

\[
\mathcal{L}_T (g) \leq \mathcal{L}_T (g, h_g) + \int \min(s, t) l(h_g, f_s) + d_1(T_X, S_X) \leq \int \min(s, t) l(f_s, f_T)
\]

(13)

where \( d_1 \) denotes the total variation distance.

The first result (13) of Proposition 19 is a refinement of a result from Ben-David et al. (2010). Apart from the total variation, the remaining terms are smaller due to point 1 of Proposition 5 and the \( \min(s, t) \) term. The latter captures the unimportance of the covariate shift assumption outside of the overlap of the support of marginals (i.e., one can always extend \( f_g \) to be equal to \( f_T \) on \( \text{supp} \ T_X \setminus \text{supp} \ S_X \), and vice-versa for \( f_T \)). In the extreme case where both supports are disjoint, the \( \min(s, t) \) term is null, letting only the total variation distance and the \( \mathcal{L}_T (g, h_g) \) the uncertainty of \( g \) in its predictions (which disappears if \( g \) is a classifier). Bound (13) is also linked to Ben-David and Urner (2012), specifically to their Algorithm \( \mathcal{A} \) that considers an intersection between the source and target domains in terms of boxes of a grid defined over the \( d \)-dimensional unit cube. Our bound points out to the sufficiency of minimizing the source risk over the intersection of supports of both domains encoded by the \( \min(s, t) \) term. For the second bound (14), it corresponds to the extreme localization case from Proposition 10 for \( r_1 = r_2 = 0 \) or \( r_1 = r_2 = 0 \). It reduces to the importance-weighted risk on the source domain when the source support contains the target’s, and when the labeling functions are the same, i.e., in the classic covariate shift setting (Shimodaira, 2000; Huang et al., 2007; Sugiyama et al., 2007; Cortes et al., 2010). This latter result, which only requires the inclusion of the support of the target in the source’s, will have analogues that we will present in the next two sections.

6.2 Hypothesis symmetric differences: revisiting \( H \Delta H \)–distances

The seminal work of Ben-David et al. (2010) proves a bound on the target risk involving the \( H \Delta H \) distance, where \( H \Delta H := \{ x \mapsto [h_1(x) \neq h_2(x)]; h_1, h_2 \in H \} \) the space of disagreements between hypotheses in \( H \). Choosing \( F = H \Delta H \), corresponding to setting \( l \) to the \( 0 \rightarrow 1 \) loss, \( F \) is not convex and thus only the upper bound from from Proposition 11 holds. The global localization in this case was the topic of Zhang et al. (2020). The next corollary addresses its upper bound from Proposition 11.

**Corollary 20.** For any \( \beta \geq 0 \), \( \beta \geq 0 \), we have

\[
1 - \text{IMD}_{H \Delta H}(T_X, (1 + \beta)S_X) = \inf_{f \in H \Delta H} \mathbb{P}_{T_X}[f = 0] + (1 + \beta)\mathbb{P}_{S_X}[f = 1]
\]

(15)

\[
1 - \min_{\beta \geq 0} \text{IMD}_{H \Delta H}(T_X, S_X + \sum_{k=1}^{K} \beta_k S_{x|k}) = \max_{\beta \geq 0} \inf_{g \in H \Delta H} \mathbb{P}_{T_X}[f = 0] + \sum_{k=1}^{K} (r_k + \beta_k)\mathbb{P}_{S_{x|k}}[f = 1]
\]

(16)

For \( \beta = 0 \), the result of Equation (15) coincides with the seminal result from Ben-David et al. (2010) that links the \( H \Delta H \)–divergence and the binary classification problem of distinguishing the source from the target, and resulting in adversarial approaches (Ganin et al., 2016). Besides, it provides an additional justification to the deep DA approach proposed in Zhang et al. (2019), in which a hyperparameter \( \gamma \) multiplies the domain discriminator’s risk on the source domain. As for result (16), although it is not convex in \( h \), it can be approximated in practice using convex surrogate loss functions, thus leading to a convex-concave for which the minimax theorem (Sion, 1958) holds. Hence, it can be formulated as a binary classification that is robust to the choice of the \( \beta \) vector. A more rigorous link with the theory
in this case remains an open direction linked with variational representations of \( f \)-divergences (Keziou, 2003; Nguyen et al., 2009; Reid and Williamson, 2011).

The next proposition concerns the extreme case of localization with \( r_1 = r_2 = 0 \) (or \( r_1 = r_2 = 0 \)).

**Proposition 21.** **Given a hypothesis space** \( \mathbb{H} \), let \( \mathbb{H} \cdot \mathbb{H} := \{ x \mapsto [h_1(x) = h_2(x)]; h_1, h_2 \in \mathbb{H} \} \), and define the \( \mathbb{H} \cdot \mathbb{H} \)-support of \( S_X \) as

\[
\text{supp}_{\mathbb{H} \cdot \mathbb{H}} S_X := \bigcap_{h_1, h_2 \in \mathbb{H}} \{ h_1 = h_2 \}.
\]

Then

\[
\text{IMD}_{\mathbb{H} \Delta \mathbb{H}} (T_X, S_X) \leq 1 - T_X (\text{supp}_{\mathbb{H} \cdot \mathbb{H}} S_X).
\]

The inequality (18) is a weakening of the result from bound (14), in the same way that the \( \mathbb{H} \Delta \mathbb{H} \)-divergence generalizes the bound relying on the total variation by restricting the family of sets defining the supremum (Ben-David et al., 2010). Indeed, while the support of \( S_X \) is the intersection of all the closed sets with \( S_X \)-probability equal to 1, the \( \mathbb{H} \cdot \mathbb{H} \)-support restricts the family of sets defining the intersection. For example, if the preimages of 1 by hypotheses of \( \mathbb{H} \cdot \mathbb{H} \) are convex sets, then \( \text{supp}_{\mathbb{H} \Delta \mathbb{H}} (S_X) \) is necessarily convex, while \( \text{supp} S_X \) does not need to be convex.

Whether such a restriction improves the estimation of the \( \text{IMD}_{\mathbb{H} \Delta \mathbb{H}} \)-bound depends on the rest of the \( \mathbb{H} \Delta \mathbb{H} \)-based DA bound from Ben-David et al. (2010). Our results from Proposition 10 and 16 overcome this limitation. Moreover, by Proposition 21, we show that their algorithm moves the target data to the structured support of the source, not the classic one.

### 6.3 Lipschitz functions: revisiting Optimal Transport for Domain Adaptation

One of the most common assumptions about labeling functions is their Lipschitzness, as it represents an inductive bias allowing to propagate the label of an instance to its neighbors. Lipschitzness of labeling functions and large margin separation between classes representing high density clusters are two equivalent notions as noted in (Ben-David and Urner, 2014). Relying on the Lipschitzness for the considered hypothesis space, several works in the literature establish bounds on the target risk involving the Wasserstein distance (Redko et al., 2017; Courty et al., 2014). Relying on the Lipschitzness for the considered hypothesis space, several works in the literature establish bounds on the target risk involving the Wasserstein distance (Redko et al., 2017; Courty et al., 2014). Relying on the Lipschitzness for the considered hypothesis space, several works in the literature establish bounds on the target risk involving the Wasserstein distance (Redko et al., 2017; Courty et al., 2014).

The per-class formulation provides a new partial optimal transport problem in which the maximum mass received by the source depends on the different class-conditional predictions.
In the case $\epsilon = 0$, we can show that $IMD_{\bar{\tau}_S}(T_S, S_T) = \mathbb{E}_{T_S}[d(x, \text{supp} S_T)]$, hence providing a first theoretical justification for the use of the Symmetric Support Divergence (SSD) (Tong et al., 2022) in domain adaptation via incorporating it in a bound on the target risk. Indeed, the SSD is an upper bound on $\mathbb{E}_{T_S}[d(x, \text{supp} S_T)]$.

7 Some empirical illustrations

7.1 Experiment description

Toy dataset generation: For the source domain, we generate $n_s = 300$ points from a mixture of 2-dimensional $K$ Gaussians, i.e. $S_X = \sum_{k=1}^{K} p_k N(\mu_k, \sigma I_2)$ and each component corresponds to a class. We obtain the centers $\mu_k$ by rotating the vector $(0, 1)$ by an angle $\frac{2k\pi}{K}$. The label marginal distribution is $p_k \propto e^{\eta k}$, where $\eta > 0$ captures the intensity of the imbalance. We generate the target domain by rotating the source by an angle $\theta$ around the origin. Its label proportions follow from sorting those of the source domain in the descending order, to accentuate the shift between $S_Y$ and $T_Y$. Hence, $\theta = 0$ or $\theta > 0$ respectively correspond to the label shift- and the generalized label shift cases.

Comparing per-class vs global relaxation: We consider the special case of Section 6.3. For a given $\beta > 0$, we compute the corresponding transport plan for global (Wu et al., 2019) and per-class (minimization problem in Corollary 17), where computing the IMD is done by solving Problem (19). To assess whether the obtained transport plan respects the class information, we compute the accuracy of a labeling that results from the propagation of the source labels as proposed in Redko et al. (2019). More precisely, given a transport plan $P \in \mathbb{R}^{n_t \times n_s}$ and the source labels matrix $Y_s \in \mathbb{R}^{n_s \times K}$, we estimate the target labels $\tilde{Y}_t \in \mathbb{R}^{n_t}$ at $x_t$ as $\tilde{y}_t = \arg\max_s (PY_s)$: the label of a target point is a majority vote of the labels of the source instances to which its mass is transported. After computing the difference in accuracy between per-class and global relaxation over 50 draws of source and target data, we report the median, the maximum, and the minimum of these draws. When not mentioned on the figures, different parameters are fixed as $K = 3, \beta = 0.5,$ and $\eta = 1$.

7.2 Results

Label shift case

For $\theta = 0^\circ$, Figure 1 illustrates Proposition 18. Recall that the proposition guarantees the existence of some $\beta \in [0, 1]$ that makes the IMD null for the per-class relaxation, whereas it is not the case for the global case (Wu et al., 2019). In fact, solving the per-class relaxed optimal transport problem results in a transportation plan without cross-labeling, whereas this latter issue persists with global localization. Figure 2 also shows this advantage by examining the difference in accuracy between the per-class and global localization. In particular, it shows that the difference grows larger as the number of classes or the imbalance intensity $\eta$ grows for the same sample size.

Generalized label shift case

For $\theta = 30^\circ$, we carry out the same experiments as in the label shift case. We do not have a theoretical guarantee on the value of $\beta$ for the per-class relaxation, but we notice a similar phenomenon when $\beta$ is allowed to grow greater than 1, as illustrated in Figure 3: less connections between instances of different label are present as $\beta$ increases. However, on Figure 4, we no longer have the same trend when varying the class numbers, whereas a similar trend is observed for different imbalance intensities $\eta$. The change in trend observed in Figure 4a can be explained as follows: When the number of classes grows, instances of different classes get closer to each other. As a result, the difficulty of the adaptation outweighs the benefit of per-class localization.

8 Related Work

Confident predictions The idea of promoting the confidence of a classifier in its predictions appears in the semi-supervised learning literature, where the goal is to encourage the cluster assumption. It implies that no high density region is crossed by decision boundaries (Grandvalet et al., 2005). Some early domain adaptation approaches relied purely on this assumption without aligning the domains (Bruzzone and Marconcini, 2010). Newer methods encourage
it via conditional entropy minimization along with domain alignment and source performance optimization (Shu et al., 2018; Kirchmeyer et al., 2022; Tong et al., 2022), or rely on it to define pseudo-labels when the considered approach requires some supervision on the target domain (Kang et al., 2019). In Ben-David and Urner (2012, 2014), the authors studied the cluster assumption for its impact on the sample complexity of some DA algorithms, where it concerns the labeling function, not the learned classifier as in our case. More recently, the contributions of Germain et al. (2016); Morerio and Murino (2017) addressed this problem theoretically. The former leverages the PAC-Bayesian theory (McAllester, 1999; Catoni, 2007) to prove a theoretical bound that is a combination of the source risk and an unsupervised target risk in a binary classification setting. The latter shows a relation between the alignment of covariance matrices (Sun et al., 2016; Sun and Saenko, 2016) and conditional entropy minimization on the target domain. Our work, however, provides justification in a more general multi-class setting, and is an improvement over a general class of bounds.

**Asymmetry in the relation between domains** Relaxing the requirement of equality of the distribution marginals is not new and has been considered in the definition of the $\Delta H$—distance (Ben-David et al., 2010) and the $l$—discrepancy (Mansour et al., 2009). In both cases, the restriction of the supremum over the considered hypothesis space makes the divergence null even when distributions are not equal. In contrast, the interest in asymmetric divergences is more recent (Zhang et al., 2019; Wu et al., 2019; Zhang et al., 2020; Kpotufe and Martinet, 2021). In particular, Zhang et al. (2020); Hanneke and Kpotufe (2019); Kpotufe and Martinet (2021) advocated the interest of
Figure 3: Illustration of the transport plan obtained by solving the problem with global vs per-class relaxation. Circles and triangles correspond to the source and target domains respectively.

Figure 4: Difference in accuracy due to label propagation as a function of $\beta$.

asymmetry to capture the easiness of adaptation depending on its direction, and showed the benefit of asymmetry in reducing the sample complexity at the source level. Although we did not study sample complexity, our IMD notion can be considered complementary to these approaches. In fact, it relates to several previously considered IPM’s that led to the implementations of DA algorithms.

9 Conclusion and future perspectives

In this work, we provided several refinements to domain adaptation theory on two main aspects. On the one hand, we highlighted the role of the certainty of the considered scoring function in its predictions on the target domain while being guided by the source labels. Our result in this regard spans over a large class of domain adaptation theoretical bounds. On the other hand, we connected two families of relaxations of divergences between probabilities and we extended them by utilizing the source domain’s categorical information.

The future perspectives of this work are many. Indeed, whether a prior on target marginal class distribution will lead to other forms of divergence relaxation is an open direction. Also, other specializations of our divergence term such as considering universal kernels are to consider. And apart from IPM’s, variational representations of $f$—divergences would link our analysis to adversarial deep learning methods. Finally, providing generalization rates in the same way
as in Zhang et al. (2020) would be informative about the role of localization depending on the choice of $\mathcal{F}$ and whether it is performed per class.

10 Acknowledgements

We thank Ievgen Redko for the fruitful discussions and the valuable feedback.
References

D. Acuna, G. Zhang, M. T. Law, and S. Fidler. f-domain adversarial learning: Theory and algorithms. In Proceedings of the 38th International Conference on Machine Learning, pages 66–75. PMLR, 2021.

S. Ben-David and R. Urner. On the Hardness of Domain Adaptation and the Utility of Unlabeled Target Samples. In Algorithmic Learning Theory, Lecture Notes in Computer Science, pages 139–153, 2012.

S. Ben-David and R. Urner. Domain adaptation–can quantity compensate for quality? Annals of Mathematics and Artificial Intelligence, 70(3):185–202, 2014.

S. Ben-David, J. Blitzer, K. Crammer, A. Kulesza, and F. Pereira. Analysis of Representations for Domain Adaptation. In Advances in Neural Information Processing Systems 19, pages 137–144, 2007.

S. Ben-David, J. Blitzer, K. Crammer, A. Kulesza, F. Pereira, and J. W. Vaughan. A theory of learning from different domains. Mach. Learn., 79(1-2):151–175, 2010.

J.-D. Benamou. Numerical resolution of an “unbalanced” mass transport problem. ESAIM: Mathematical Modelling and Numerical Analysis, 37(5):851–868, 2003.

J.-D. Benamou, G. Carlier, M. Cuturi, L. Nenna, and G. Peyré. Iterative bregman projections for regularized transportation problems. SIAM Journal on Scientific Computing, 37(2):A1111–A1138, 2015.

J. Blitzer, M. Dredze, and F. Pereira. Biographies, bollywood, boomboxes and blenders: Domain adaptation for sentiment classification. In In ACL, pages 187–205, 2007.

B. E. Boser, I. M. Guyon, and V. N. Vapnik. A Training Algorithm for Optimal Margin Classifiers. In Proceedings of the 5th Annual ACM Workshop on Computational Learning Theory, pages 144–152, 1992.

L. Bruzzone and M. Marconcini. Domain Adaptation Problems: A DASVM Classification Technique and a Circular Validation Strategy. IEEE Transactions on Pattern Analysis and Machine Intelligence, 32(5):770–787, 2010.

L. A. Caffarelli and R. J. McCann. Free boundaries in optimal transport and monge-ampere obstacle problems. Annals of Mathematics, pages 673–730, 2010.

O. Catoni. Pac-bayesian supervised classification: the thermodynamics of statistical learning. arXiv preprint arXiv:0712.0248, 2007.

O. Chapelle and A. Zien. Semi-supervised classification by low density separation. In International workshop on artificial intelligence and statistics, pages 57–64. PMLR, 2005.

L. Chizat, G. Peyré, B. Schmitzer, and F.-X. Vialard. Scaling algorithms for unbalanced optimal transport problems. Mathematics of Computation, 87(314):2563–2609, 2018a.

L. Chizat, G. Peyré, B. Schmitzer, and F.-X. Vialard. Unbalanced optimal transport: Dynamic and kantorovich formulations. Journal of Functional Analysis, 274(11):3090–3123, 2018b.

R. Collobert, F. Sinz, J. Weston, L. Bottou, and T. Joachims. Large scale transductive svms. Journal of Machine Learning Research, 7(8), 2006.

C. Cortes and M. Mohri. Domain adaptation in regression. In ALT, 2011.

C. Cortes and M. Mohri. Domain adaptation and sample bias correction theory and algorithm for regression. Theoretical Computer Science, 519:103–126, 2014.

C. Cortes and V. Vapnik. Support-Vector Networks. Machine Learning, 20(3):273–297, 1995.

C. Cortes, Y. Mansour, and M. Mohri. Learning bounds for importance weighting. In Advances in Neural Information Processing Systems, volume 23, 2010.

N. Courty, R. Flamary, D. Tuia, and A. Rakotomamonjy. Optimal Transport for Domain Adaptation. IEEE Transactions on Pattern Analysis and Machine Intelligence, 39(9):1853–1865, 2016.
N. Courty, R. Flamary, A. Habrard, and A. Rakotomamonjy. Joint distribution optimal transportation for domain adaptation. In Advances in Neural Information Processing Systems, pages 3730–3739, 2017.

I. Csiszár. Information-type measures of difference of probability distributions and indirect observation. studia scientiarum Mathematicarum Hungarica, 2:229–318, 1967.

G. Csurka et al. Domain adaptation in computer vision applications. Springer, 2017.

H. Daumé III. Frustratingly Easy Domain Adaptation. arXiv:0907.1815 [cs], 2009.

A. Erkan and Y. Altun. Semi-supervised learning via generalized maximum entropy. In Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, pages 209–216. JMLR Workshop and Conference Proceedings, 2010.

K. Fatras, T. Séjourné, R. Flamary, and N. Courty. Unbalanced minibatch optimal transport; applications to domain adaptation. In International Conference on Machine Learning, pages 3186–3197. PMLR, 2021.

B. Fernando, A. Habrard, M. Sebban, and T. Tuytelaars. Unsupervised Visual Domain Adaptation Using Subspace Alignment. In ICCV 2013, pages 2960–2967, Sydney, Australia, 2013.

A. Figalli. The optimal partial transport problem. Archive for rational mechanics and analysis, 195(2):533–560, 2010.

Y. Ganin, E. Ustinova, H. Ajakan, P. Germain, H. Larochelle, F. Laviolette, M. March, and V. Lempitsky. Domain-Adversarial Training of Neural Networks. Journal of Machine Learning Research, 17(59):1–35, 2016.

P. Germain, A. Habrard, F. Laviolette, and E. Morvant. A PAC-Bayesian Approach for Domain Adaptation with Specialization to Linear Classifiers. In International Conference on Machine Learning, pages 738–746, 2013.

P. Germain, A. Habrard, F. Laviolette, and E. Morvant. A New PAC-Bayesian Perspective on Domain Adaptation. In International Conference on Machine Learning, pages 859–868, 2016.

B. Gong, K. Grauman, and F. Sha. Connecting the Dots with Landmarks: Discriminatively Learning Domain-Invariant Features for Unsupervised Domain Adaptation. In International Conference on Machine Learning, pages 222–230, 2013.

I. Goodfellow, Y. Bengio, and A. Courville. Deep learning. MIT press, 2016.

Y. Grandvalet, Y. Bengio, et al. Semi-supervised learning by entropy minimization. CAP, 367:281–296, 2005.

S. Hanneke and S. Kpotufe. On the value of target data in transfer learning. 32, 2019.

J. Huang, A. Gretton, K. Borgwardt, K. Schölkopf, and A. J. Smola. Correcting sample selection bias by unlabeled data. In Advances in neural information processing systems, pages 601–608, 2007.

F. D. Johansson, D. Sontag, and R. Ranganath. Support and Invertibility in Domain-Invariant Representations. In The 22nd International Conference on Artificial Intelligence and Statistics, pages 527–536, 2019.

G. Kang, L. Jiang, Y. Yang, and A. G. Hauptmann. Contrastive Adaptation Network for Unsupervised Domain Adaptation. In 2019 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), pages 4888–4897, 2019.

A. Keziou. Dual representation of ϕ-divergences and applications. Comptes rendus mathématique, 336(10):857–862, 2003.

M. Kirchmeyer, A. Rakotomamonjy, E. de Bezenac, and Patrick Gallinari. Mapping conditional distributions for domain adaptation under generalized target shift. In International Conference on Learning Representations, 2022. URL https://openreview.net/forum?id=spF2Pi87BZ.

W. M. Kouw and M. Loog. A review of single-source unsupervised domain adaptation. arXiv:1901.05335 [cs, stat], 2019.
S. Kpotufe and G. Martinet. Marginal singularity and the benefits of labels in covariate-shift. *The Annals of Statistics*, 49(6):3299–3323, 2021.

T. Le, T. Nguyen, N. Ho, H. Bui, and D. Phung. Lamda: Label matching deep domain adaptation. In *International Conference on Machine Learning*, pages 6043–6054. PMLR, 2021.

J. Liang, D. Hu, Y. Wang, R. He, and J. Feng. Source data-absent unsupervised domain adaptation through hypothesis transfer and labeling transfer. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2021.

M. Liero, A. Mielke, and G. Savaré. Optimal entropy-transport problems and a new hellinger–kantorovich distance between positive measures. *Inventiones mathematicae*, 211(3):969–1117, 2018.

Z. Lipton, Y.-X. Wang, and A. Smola. Detecting and correcting for label shift with black box predictors. In *International conference on machine learning*, pages 3122–3130. PMLR, 2018.

M. Long, Z. CAO, J. Wang, and M. I. Jordan. Conditional adversarial domain adaptation. In S. Bengio, H. Wallach, H. Larochelle, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 31. Curran Associates, Inc., 2018.

D. G. Luenberger. *Optimization by vector space methods*. John Wiley & Sons, 1997.

Y. Mansour, M. Mohri, and A. Rostamizadeh. Domain adaptation: Learning bounds and algorithms. In *COLT 2009 - The 22nd Conference on Learning Theory, Montreal, Quebec, Canada, June 18-21, 2009*, 2009.

D. A. McAllester. Some pac-bayesian theorems. *Machine Learning*, 37(3):355–363, 1999.

A. Mehra, B. Kailkhura, P.-Y. Chen, and J. Hamm. Understanding the limits of unsupervised domain adaptation via data poisoning. *arXiv preprint arXiv:2107.03919*, 2021.

P. Morerio and V. Murino. Correlation Alignment by Riemannian Metric for Domain Adaptation. *arXiv:1705.08180 [cs]*, 2017.

A. Müller. Integral Probability Metrics and Their Generating Classes of Functions. *Advances in Applied Probability*, 29(2):429–443, 1997.

X. Nguyen, M. J. Wainwright, and M. I. Jordan. On surrogate loss functions and f-divergences. *The Annals of Statistics*, 37(2):876–904, 2009.

S. J. Pan and Q. Yang. A Survey on Transfer Learning. *IEEE Transactions on Knowledge and Data Engineering*, 22(10):1345–1359, 2010.

J. Quiñonero-Candela, M. Sugiyama, A. Schwaighofer, and N. D. Lawrence. *Dataset shift in machine learning*. Mit Press, 2008.

A. Rakotomamonjy, R. Flamary, G. Gasso, M. E. Alaya, M. Berar, and N. Courty. Optimal transport for conditional domain matching and label shift. *Machine Learning*, pages 1–20, 2021.

I. Redko, A. Habrard, and M. Sebban. Theoretical analysis of domain adaptation with optimal transport. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pages 737–753. Springer, 2017.

I. Redko, N. Courty, R. Flamary, and D. Tuia. Optimal transport for multi-source domain adaptation under target shift. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 849–858. PMLR, 2019.

I. Redko, E. Morvant, A. Habrard, M. Sebban, and Y. Bennani. A survey on domain adaptation theory. *CoRR*, abs/2004.11829, 2020.

M. D. Reid and R. C. Williamson. Information, divergence and risk for binary experiments. *Journal of Machine Learning Research*, 12:731–817, 2011.
A. Rényi. On measures of entropy and information. In *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Contributions to the Theory of Statistics*, pages 547–561. University of California Press, 1961.

H. L. Royden and P. Fitzpatrick. *Real analysis*, volume 32. Macmillan New York, 1988.

K. Saito, K. Watanabe, Y. Ushiku, and T. Harada. Maximum Classifier Discrepancy for Unsupervised Domain Adaptation. *arXiv:1712.02560 [cs]*, 2017.

K. Saito, D. Kim, S. Sclaroff, T. Darrell, and K. Saenko. Semi-supervised Domain Adaptation via Minimax Entropy. *arXiv:1904.06487 [cs]*, 2019.

F. Santambrogio. Optimal transport for applied mathematicians. *Birkhäuser, NY*, 55(58-63):94, 2015.

J. Shen, Y. Qu, W. Zhang, and Y. Yu. Wasserstein distance guided representation learning for domain adaptation. In *Thirty-Second AAAI Conference on Artificial Intelligence*, 2018.

H. Shimodaira. Improving predictive inference under covariate shift by weighting the log-likelihood function. *Journal of Statistical Planning and Inference*, 90(2):227–244, 2000.

R. Shu, H. H. Bui, H. Narui, and S. Ermon. A DIRT-T Approach to Unsupervised Domain Adaptation. *arXiv:1802.08735 [cs, stat]*, 2018.

M. Sion. On general minimax theorems. *Pacific J. Math.*, 8(1):171–176, 1958.

T. Steerneman. On the total variation and hellinger distance between signed measures; an application to product measures. *Proceedings of the American Mathematical Society*, 88(4):684–688, 1983.

M. Sugiyama, M. Krauledat, and K.-R. Müller. Covariate Shift Adaptation by Importance Weighted Cross Validation. *Journal of Machine Learning Research*, 8(May):985–1005, 2007.

B. Sun and K. Saenko. Deep CORAL: Correlation Alignment for Deep Domain Adaptation. *arXiv:1607.01719 [cs]*, 2016.

B. Sun, J. Feng, and K. Saenko. Return of frustratingly easy domain adaptation. In *Proceedings of the Thirtieth AAAI Conference on Artificial Intelligence*, AAAI’16, page 2058–2065, 2016.

R. Tachet des Combes, H. Zhao, Y.-X. Wang, and G. J. Gordon. Domain adaptation with conditional distribution matching and generalized label shift. In *Advances in Neural Information Processing Systems*, volume 33, pages 19276–19289, 2020.

S. Tan, X. Peng, and K. Saenko. Class-imbalanced domain adaptation: an empirical odyssey. In *European Conference on Computer Vision*, pages 585–602. Springer, 2020.

S. Tong, T. Garipov, Y. Zhang, S. Chang, and T. S. Jaakkola. Adversarial support alignment. In *International Conference on Learning Representations*, 2022. URL https://openreview.net/forum?id=26gkg6x-ie.

M. Wang and W. Deng. Deep visual domain adaptation: A survey. *Neurocomputing*, 312:135–153, 2018.

K. Weiss, T. M. Khoshgoftaar, and D. Wang. A survey of transfer learning. *Journal of Big Data*, 3(1):9, 2016.

G. Wilson and D. J. Cook. A survey of unsupervised deep domain adaptation. *ACM Transactions on Intelligent Systems and Technology (TIST)*, 11(5):1–46, 2020.

Y. Wu, E. Winston, D. Kaushik, and Z. Lipton. Domain adaptation with asymmetrically-relaxed distribution alignment. In *International Conference on Machine Learning*, pages 6872–6881. PMLR, 2019.

K. Zhang, B. Schölkopf, K. Muandet, and Z. Wang. Domain Adaptation under Target and Conditional Shift. In *International Conference on Machine Learning*, pages 819–827, 2013.

L. Zhang. Transfer Adaptation Learning: A Decade Survey. *arXiv:1903.04687 [cs]*, 2019.
Y. Zhang, T. Liu, M. Long, and M. Jordan. Bridging Theory and Algorithm for Domain Adaptation. In *International Conference on Machine Learning*, pages 7404–7413, 2019.

Y. Zhang, M. Long, J. Wang, and M. I. Jordan. On localized discrepancy for domain adaptation. *arXiv preprint arXiv:2008.06242*, 2020.

H. Zhao, R. T. D. Combes, K. Zhang, and G. Gordon. On Learning Invariant Representations for Domain Adaptation. In *International Conference on Machine Learning*, pages 7523–7532, 2019.

L. Zhong, Z. Fang, F. Liu, J. Lu, B. Yuan, and G. Zhang. How does the combined risk affect the performance of unsupervised domain adaptation approaches? In *Proceedings of the 35th AAAI Conference on Artificial Intelligence*, 2021.

F. Zhuang, Z. Qi, K. Duan, D. Xi, Y. Zhu, H. Zhu, H. Xiong, and Q. He. A comprehensive survey on transfer learning. *Proceedings of the IEEE*, 109(1):43–76, 2020.

V. M. Zolotarev. Probability metrics. *Theory of Probability & Its Applications*, 28(2):278–302, 1984.
A Proofs for the different claims

In this appendix, we provide proofs for the different claims made in the manuscript. We denote the indicator function of a set $A$ using the Iverson Bracket, i.e., $[x \in A] = 1$ if $x \in A$ and 0 otherwise.

**Example 2** (Cross entropy loss). In this case, $g(x)$ is in the $K$-dimensional probability simplex (after applying the softmax function). We then have $l(g(x), h_g(x)) = H_\infty(g(x)),^5$ where $H_\infty$ denotes the Renyi entropy (Renyi, 1961) defined as $H_\alpha(g(x)) = \frac{1}{1-\alpha} \log (\sum_i (g(x)_i)^\alpha)$, which is equal to the Shannon entropy when $\alpha = 1$. Since we have $H_\infty(g(x)) \leq H_\alpha(g(x)) \forall \alpha \geq 0$, having a small conditional entropy of $g(x)$ in particular results in a small uncertainty of $g(x)$. Minimizing the conditional entropy, borrowed from the semi-supervised learning literature (Grandvalet et al., 2005; Erkan and Altun, 2010), is now a standard approach in domain adaptation (Shu et al., 2018; Liang et al., 2021; Kirchmeyer et al., 2022).

**Proof.** Given $g$ as a scoring function and a point $x \in \mathbb{X}$, we have
\[
l(g(x), h_g(x)) = \inf_{y \in \mathcal{Y}} - \sum_{i=1}^{K} y_i \log g(x)_i,
\]
\[
= - \max_i \log g(x)_i = H_\infty(g(x)) < H_\alpha(g(x)) \forall \alpha \geq 1.
\]

**Example 3** (Hinge loss). The binary SVM (Boser et al., 1992; Cortes and Vapnik, 1995) problem can be written as minimizing the regularized risk of the hinge loss function $l(g(x), y) = (1 - yg(x))_+$, where $g$ is a linear classifier and $y \in \{-1, 1\}$. Computing the uncertainty of $g$ at $x$ yields $(1 - |x|)_+$, the latter being an unsupervised loss appearing in the transductive SVM formulation (Chapelle and Zien, 2005; Collobert et al., 2006). A smooth analogue of this quantity also appears in Germain et al. (2016).

**Proof.** For a scoring function $g$ and a point $x \in \mathbb{X}$ we have
\[
(1 - \text{sgn}(g(x)) g(x))_+ = (1 - |g(x)|)_+ \leq (1 - yg(x)) \forall y \in \{-1, 1\}
\]
, where we used the the fact that the hinge loss is nonincreasing. The computation can be generalized to any loss function that is non-increasing and applied to $yg(x)$.

**Proposition 5** (Properties of the source-guided uncertainty). The source-guided uncertainty of a scoring function verifies the following properties:

1. If $g$ is a scoring function and $h_g \in \mathbb{H}$, then $C_{\mathbb{H}}^{1,2}(g) \leq \mathcal{L}_T^1(\mathcal{H}, h_g) + \mathcal{L}_S^2(h_g)$. In particular, if $g \in \mathbb{H}$, then $C_{\mathbb{H}}^{1,2}(g) \leq \mathcal{L}_S^2(g)$.

2. If $\mathbb{H} \subseteq \mathbb{H'} \subseteq \mathcal{Y}^\mathbb{X}$, and if $l^1(a, a) = 0$, then $\inf_{g \in \mathbb{H}} C_{\mathbb{H}}^{1,2}(g) = \inf_{h \in \mathbb{H}} \mathcal{L}_S^2(h)$.

3. If $l^1 = l^2$ obeys the triangle inequality, then $C_{\mathbb{H}}(h) = \mathcal{L}_S(h)$ for $h \in \{h_S, h^*\}$, where $h_S \in \text{argmin} \mathcal{L}_S(h)$ and $h^* \in \text{argmin} \mathcal{L}_T(h) + \mathcal{L}_S(h)$.

**Proof.**

**Point 1** follows from bounding the infimum over $h \in \mathbb{H}$ by the value for $h = h_g$, and that if $g$ is a classifier then $g = h_g$.

**Point 2**
\[
\inf_{h \in \mathbb{H}} C_{\mathbb{H}}^{1,2}(h) = \inf_{h \in \mathbb{H}} \inf_{h' \in \mathbb{H'}} (\mathcal{L}_T^1(h, h') + \mathcal{L}_S^2(h'))
\]
\[
= \inf_{h' \in \mathbb{H'}} \inf_{h \in \mathbb{H}} (\mathcal{L}_T^1(h, h') + \mathcal{L}_S^2(h'))
\]
\[
= \inf_{h' \in \mathbb{H'}} \mathcal{L}_S^2(h') \text{ using } \mathbb{H} \subseteq \mathbb{H'}
\]
where the last equality is obtained by setting $h$ to $h'$, which is possible since $\mathbb{H'} \subseteq \mathbb{H}$.

---

^5The proofs of all theoretical claims can be found in the appendix.
Proof. Let 

\[ L_T(h^*) + L_S(h^*) \geq L_T(h^*) + \mathfrak{C}_H(h^*) \quad \text{(from point 1)} \]

\[ = \inf_{h \in H} L_T(h^*) + L_T(h^*, h) + L_S(h) \]

\[ \geq \inf_{h \in H} L_T(h^*) + L_S(h^*) \quad \text{(triangle inequality)} \]

\[ = L_T(h^*) + L_S(h^*) . \]

Hence \( L_S(h^*) = \mathfrak{C}_H(h^*) \). For the second equality, we have

\[ L_S(h_S) = \inf_{h \in H} L_S(h) \quad \text{(by definition of } h_S \text{)} \]

\[ = \inf_{h \in H} \mathfrak{C}_H(h) \quad \text{(by point 2)} \]

\[ \leq \mathfrak{C}_H(h_S) \quad \text{(by point 1).} \]

\[ \Box \]

Proposition 6 (Tightening bounds on the target risk). Let \( g \) be a scoring function, and let \( l^1 \) be a loss function, verifying \( l^1(u, y_1) - l^2(y_2, y_1) \leq l^1(u, y_2) \forall u \in \mathbb{R}^K, y_1, y_2 \in \mathbb{Y} \). Then given a bound on the target risk of the following form:

\[ L^2_T(h) \leq L^2_S(h) + A(T, S); \quad \forall h \in H, \]

where \( A(T, S) \) reflects a relatedness between the domains’ joint distributions, we have for any scoring function \( g \)

\[ L^1_T(g) \leq \mathfrak{C}^{l^2}_{H} \left( g \right) + A(T, S). \]

Proof. Let \( g \in \mathbb{Y}^X \). We have

\[ \mathcal{L}^1_T(g) - \sup_{h \in H} \left( L^2_T(h) - L^2_S(h) \right) = \mathcal{L}^1_T(g) + \inf_{h \in H} \left( -L^2_T(h) + L^2_S(h) \right) \]

\[ = \inf_{h \in H} \mathcal{L}^1_T(g) - L^2_T(h) + L^2_S(h) \]

\[ \leq \inf_{h \in H} \mathcal{L}^1_T(g, h) + L^2_S(h) \quad \text{(by assumption on loss functions)} \]

On the other hand, by assumption, we have \( \sup_{h \in H} L^2_T(h) - L^2_S(h) \leq A(T, S) \). Summing the last two inequalities gives the result.

\[ \Box \]

Proof for choices of loss functions in Proposition 6

Case of the cross entropy loss Let \( l^1 \) be chosen as the cross-entropy loss. For \( y_1, y_2 \) we have two basis vectors of \( \mathbb{R}^K \):

\[ l^1(g(x), y_1) - l^1(g(x), y_2) = (y_2 - y_1)^T \log(g(x)) \leq \|y_2 - y_1\|_1 \|\log(g(x))\|_\infty \]

Assume \( g_i(x) = \frac{e^{a_i(x)}}{\sum_{k=1}^{e^{a_i(x)}}}, \) where \( g_i \) denotes the \( i \)-th component of \( g \). Then we have

\[ \|\log(g(x))\|_\infty = \max_{1 \leq k \leq K} |\log(g(x))| \]

\[ = \max_{1 \leq k \leq K} -\log(g(x)) \quad \text{(since } 0 \leq g(x) \leq 1) \]

\[ = \max_{1 \leq k \leq K} \log \left( \sum_{i=1}^{K} e^{a_i(x)} \right) - a_k(x) \]

\[ \leq \max_{1 \leq k, i \leq K} a_i(x) - a_k(x) + \log K \]

\[ \leq 2R + \log K \]

Hence, the condition on losses holds for \( l^1 \) being the cross entropy loss and \( L^2(\cdot, \cdot) = (2R + \log K)|\cdot - \cdot|_1 \).
**Proposition 9** (Properties of the IMD). The IMD is nonnegative, satisfies the triangle inequality, and we have $\text{IMD}_F(Q_1, Q_2) = 0$ if $Q_1 \leq Q_2$ (i.e., $q_1 \leq q_2$ when $q_1$ and $q_2$ are the densities of $Q_1$ and $Q_2$). Moreover, for $F$ rich enough (i.e., containing the continuous functions or the indicator functions), we have $\text{IMD}(Q_1, Q_2) = 0$ only if $Q_2 \geq Q_1$.

**Proof.** For nonnegativity, for any two finite measures $Q_1$ and $Q_2$, and since $F$ contains the null function, we have

$$\text{IMD}_F(Q_1, Q_2) = \sup_{f \in F} \int f \, dQ_1 - \int f \, dQ_2 \geq \int 0 \, dQ_1 - \int 0 \, dQ_2 = 0.$$ 

For the triangle inequality, for any three measures $Q_1, Q_2, Q_3$, we have:

$$\text{IMD}_F(Q_1, Q_3) = \sup_{f \in F} \int f \, dQ_1 - \int f \, dQ_3 = \sup_{f \in F} \int f \, dQ_1 - \int f \, dQ_2 + \int f \, dQ_2 - \int f \, dQ_3 \leq \sup_{f \in F} \int f \, dQ_1 - \int f \, dQ_2 + \sup_{f \in F} \int f \, dQ_2 - \int f \, dQ_3 \quad \text{(by sub-additivity of the supremum)},$$

hence the IMD satisfies the triangle inequality.

For the characterization of a null IMD, let $Q_1, Q_2$ be two measures. First, assume that $Q_2 \geq Q_1$. Then for any $f \in F$, since $F$ is nonnegative, we have $\int f \, dQ_1 \leq \int f \, dQ_2$. Hence $\text{IMD}_F(Q_1, Q_2) \leq 0$. Due to the nonnegativity of the IMD, we conclude that $\text{IMD}(Q_1, Q_2) = 0$. Conversely, assume that $\text{IMD}_F(Q_1, Q_2) = 0$, implying that $\forall f \in F$, $\int f \, d(Q_1 - Q_2) \leq 0$. We will examine two richness assumptions on $F$: containing the continuous functions over $X$ and containing indicators functions of measurable sets.

**Case when $F$ contains indicator functions** In this case, the choice $f = [\cdot \in A]$ where $A$ is a measurable set implies that $Q_2(A) \geq Q_1(A)$ for any set $A$ and allows to conclude.

**Case when $F$ contains the continuous functions** We will prove that for any compact set $K \subseteq X$, we have $Q_1(K) \leq Q_2(K)$, following the same proof of Royden and Fitzpatrick (1988, Chapter 21, Section 4, Proposition 11). Let $K \subseteq X$ be a compact set and let $\epsilon > 0$. The measures, $Q_1$ and $Q_2$ are Radon measures in our case, hence by outer regularity of $Q_2$, there is a neighborhood of $O$ of $K$ such that

$$Q_2(O \setminus K) \leq \epsilon. \quad (22)$$

By the compact extension property (Royden and Fitzpatrick, 1988, Chapter 21, Section 2, Theorem 7), there exists a continuous function $0 \leq f \leq 1$ over $X$ with compact support, such that

$$f(x) = 1 \quad \forall x \in K \quad (23)$$
$$f(x) = 0 \quad \forall x \in X \setminus O. \quad (24)$$

We have

$$Q_1(K) - Q_2(K) = \int_K f \, dQ_1 - \int_K f \, dQ_2 \quad \text{(by property (23))}$$

$$= \int f \, dQ_1 - \int f \, dQ_2 + \int_{X \setminus K} f \, dQ_2 - \int_{X \setminus K} f \, dQ_1$$

$$\leq \int_{X \setminus K} f \, dQ_2 - \int_{X \setminus K} f \, dQ_1 \quad \text{(since $f \in F$ and $\int f \, d(Q_1 - Q_2) \leq 0$)}$$

$$= \int_{O \setminus K} f \, dQ_2 - \int_{O \setminus K} f \, dQ_1 \quad \text{(by property (24))}$$

$$\leq \epsilon \quad \text{(by property (22) and since $0 \leq f \leq 1$)} \quad (25)$$

Hence, we have $Q_1(K) - Q_2(K) \leq \epsilon$ for an arbitrary $\epsilon > 0$, implying that $Q_1(K) \leq Q_2(K)$ and allowing to conclude.
Concerning the densities of $Q_2$ and $Q_1$, since $Q_2 - Q_1$ is absolutely continuous, it has a Radon-Nikodym derivative that we denote $q$. We have $Q_2 = Q_2 - Q_1 + Q_1$. By the linearity of the Radon-Nikodym derivative, we have $q = q + q_1$, implying that $q_2 \geq q_1$. □

**Proposition 10.** Let $\mathbb{H}$ be a hypothesis space, $g$ a scoring function not necessarily in $\mathbb{H}$, and $l$ a loss function verifying the triangle inequality. Assume that $l(\mathbb{H}, \mathbb{H}) := \{(l(h_1), l(h_2)); h_1, h_2 \in \mathbb{H}\} \subseteq \mathbb{F}$, where $\mathbb{F}$ is a set of bounded nonnegative functions. Also, for any $r \geq 0$, we consider the localized hypothesis space $\mathbb{H}^r := \{h \in \mathbb{H}; L_S(h) \leq r\}$. Then, for any $r_1, r_2 \geq 0,$

$$
\mathcal{L}_T(g) \leq \mathcal{L}_{\mathbb{H}^{r_1}}(g) + \text{IMD}_{r_1 + r_2}(T_X, S_X) + \inf_{h \in \mathbb{H}^{r_2}} \mathcal{L}_T(h) + \mathcal{L}_S(h).
$$

**Proof.** We first use a generalization of Zhang et al. (2020, Theorem). Let $h_1 \in \mathbb{H}^{r_1}, h_2 \in \mathbb{H}^{r_2}$. Then

$$
\mathcal{L}_T(h_1) \leq \mathcal{L}_T(h_1, h_2) + \mathcal{L}_T(h_2)
$$

$$
= \mathcal{L}_T(h_1, h_2) - \mathcal{L}_S(h_2) + \mathcal{L}_S(h_2) + \mathcal{L}_T(h_2)
$$

$$
\leq \mathcal{L}_S(h_1) + \mathcal{L}_T(h_1, h_2) - \mathcal{L}_S(h_1, h_2) + \mathcal{L}_S(h_2) + \mathcal{L}_T(h_2)
$$

$$
\leq \mathcal{L}_S(h_1) + \sup_{h_1 \in \mathbb{H}^{r_1}} \inf_{h_2 \in \mathbb{H}^{r_2}} (\mathcal{L}_S(h_2) + \mathcal{L}_T(h_2))
$$

$$
= \mathcal{L}_S(h_1) + \text{IMD}_{(\mathbb{H}^{r_1}, \mathbb{H}^{r_2})} + \inf_{h_2 \in \mathbb{H}^{r_2}} (\mathcal{L}_S(h_2) + \mathcal{L}_T(h_2)),
$$

where

$$
l(\mathbb{H}^{r_1}, \mathbb{H}^{r_2}) := \{(x, l(h_1, l(h_2(x)))); h_1 \in \mathbb{H}^{r_1}, h_2 \in \mathbb{H}^{r_2}\}
$$

Now we prove that $l(\mathbb{H}^{r_1}, \mathbb{H}^{r_2}) \subseteq \mathbb{F}_{r_1 + r_2}$. Given $h_i \in \mathbb{H}_{r_i}$, for $i \in \{1, 2\}$, we have

$$
\mathcal{L}_S(h_1, h_2) \leq \mathcal{L}_S(h_1) + \mathcal{L}_S(h_2) \quad \text{(triangle inequality)}
$$

$$
\leq r_1 + r_2 \quad \text{(definition of $\mathbb{H}^{r_1}, \mathbb{H}^{r_2}$)}.
$$

meaning that $l(h_1, h_2) \in \mathbb{F}_{r_1 + r_2}$. Since the last inequality holds for any $l(h_1, h_2) \in l(\mathbb{H}^{r_1}, \mathbb{H}^{r_2})$, we conclude that $l(\mathbb{H}^{r_1}, \mathbb{H}^{r_2}) \subseteq \mathbb{F}_{r_1 + r_2}$. Since the supremum taken over $\mathbb{F}_{r_1 + r_2}$ is at least equal to the supremum over its subset $l(\mathbb{H}^{r_1}, \mathbb{H}^{r_2})$, we have

$$
\mathcal{L}_T(h_1) \leq \mathcal{L}_S(h_1) + \text{IMD}_{r_1 + r_2} + \inf_{h \in \mathbb{H}^{r_2}} \mathcal{L}_T(h) + \mathcal{L}_S(h) \quad \forall h_1 \in \mathbb{H}^{r_1}.
$$

At this stage, we have bounds on the target domain that involve a source risk. Hence, applying our result from Proposition 6, allows to replace the source risk by the source-guided uncertainty and to conclude. □

**Proposition 11 (Duality for localized IMD).** Assume $\mathbb{F}$ is a space of nonnegative functions over $X$. Then

$$
\forall \epsilon \geq 0, \quad \text{IMD}_{\epsilon}(T_X, S_X) \leq \inf_{\alpha \geq 0} \text{IMD}_{\epsilon}(T_X, (1 + \alpha)S_X) + \epsilon\alpha.
$$

Moreover, if $\mathbb{F}$ is convex, $\text{IMD}_{\epsilon}(T_X, S_X)$ is finite and $\epsilon > 0$, then we have an equality, and the infimum at the right hand side is achieved for some $\alpha^* \geq 0$.

**Proof.** We have

$$
\text{IMD}_{\epsilon}(T_X, S_X) = \sup_{f \in \mathbb{F}} \inf_{\alpha \geq 0} \mathbb{E}_T[f] - \mathbb{E}_S[f] + \alpha(\epsilon - \mathbb{E}_S[f]).
$$

Applying the inf-sup inequality gives the first part of the result.

The result of equality for $\epsilon > 0$ is an application of Luenberger (1997, Chapter 8, Section 6, Theorem 1). We consider the optimization problem:

$$
\inf_{f \in \mathbb{F}} \mathbb{E}_S[f] - \mathbb{E}_T[f] \quad \text{s.t.} \quad \mathbb{E}_S[f] \leq \epsilon
$$

which is equivalent to our problem up to a minus sign. We have

- $\mathbb{F}$ is a convex subset the vector space of real valued functions taking an argument in $X$. 

22
• The value of the problem at the solution is finite since its unconstrained optimal value is finite by assumption (equal to $\text{IMD}_F (T_X, S_X)$).

• The null function $f_0 = 0 \in F$, and we have $\mathbb{E}_{S_X} [f_0] = 0 < \epsilon$.

• The objective function and constraints are all linear.

Hence, applying Luenberger (1997, Chapter 8, section 6, Theorem 1), the value of the constrained problem at the optimum is equal to $\max_{\alpha \geq 0} \inf_{f \in F} \mathbb{E}_{S_X} [f] - \mathbb{E}_{T_X} [f] + \alpha (\mathbb{E}_{S_X} [f] - \epsilon)$, i.e., the maximum is achieved for some $\alpha^* \geq 0$.

**Corollary 12.** If $F$ is rich enough, then for any $\epsilon > 0$, $\text{IMD}_F (T_X, S_X) = 0$ if and only if $T_X = S_X$.

**Proof.** Let $\epsilon > 0$, and assume $\text{IMD}_F$ is null. By Proposition 11, there exists $\alpha^* \geq 0$ such that for any $f \in F$, we have $\mathbb{E}_{T_X} [f] \leq (1 + \alpha^*) \mathbb{E}_{S_X} [f] - \epsilon \alpha^*$. That holds in particular for $f$ chosen as the null function, which would result a contradiction unless $\alpha^* = 0$. In that case, $\mathbb{E}_{T_X} [f] \leq \mathbb{E}_{S_X} [f]$ $\forall f \in F$. This means that $\text{IMD}(T_X, S_X) = 0$ and by Proposition 9, it implies that $S_X \geq T_X$. Since $S_X$ and $T_X$ are probability distributions, this implies that $T_X = S_X$. $\square$

**Proposition 16.** Let $H$ be a hypothesis space, $g$ a scoring function, and $l$ a loss function verifying the triangle inequality. Assume that $l(H, H) \subseteq F$, where $F$ is a set of bounded nonnegative functions. Also, for any $r = (r_1, \cdots, r_K) \geq 0$, we consider the localized hypothesis space $H^r = \{h \in H ; S_{\xi_k} (h) \leq r_k \forall 1 \leq k \leq K\}$.

Then for any $r_1, r_2, r_\beta \geq 0$, we have

$$\mathcal{L}_T (g) \leq \mathcal{C}_{H^r_1} (g) + \text{IMD}_F \left( T_X, S_X + \sum_{k=1}^K \beta_k S_{\xi_k} \right) + \mathcal{L}_T (r_1 + r_2) + \inf_{h \in H^r_2} \mathcal{L}_T (h) + \mathcal{L}_S (h).$$

**Proof.** The proof follows the same reasoning we had through Propositions 10, 11 and Corollary 13, through the following steps:

1. Adapting the proof of Proposition 10 to $F_{r_1}$ and $F_{r_2}$ instead of $F_{r_1}$ and $F_{r_2}$.

2. Adapting the proof of Proposition 11:

$$\text{IMD}_F (T_X, S_X) = \sup_{f \in F} \inf_{\alpha \in \mathbb{R}_+} \mathbb{E}_{T_X} [f] - \mathbb{E}_{S_X} [f] + \sum_{k=1}^K \alpha_k (\epsilon_k - S_{\xi_k} [f])$$

Then the inf-sup upper bound follows similarly. Again, we can apply the same strong duality argument if $\epsilon_k > 0$ for any $1 \leq k \leq K$.

3. The last step is to use the inf-sup upper bound to bound the IMD for an arbitrary $\beta \in \mathbb{R}_+^K$.

$\square$

**Corollary 17.** With the assumptions of Proposition 16, let $r_1, r_2, \beta \geq 0$. Besides, let $r_1 = r_2 = r_1$. Then

$$\mathcal{L}_T (g) \leq \mathcal{C}_{H^r_1} (g) + \min_{\beta \geq 0} \text{IMD}_F \left( T_X, S_X + \sum_{k=1}^K \beta_k S_{\xi_k} \right) + \beta (r_1 + r_2) + \inf_{h \in H^r_2} \mathcal{L}_T (h) + \mathcal{L}_S (h).$$

Moreover, the inequality in the constraint $\beta 1 \leq 1$ can be replaced by an equality.

**Proof.** Applying Proposition 16 with the specified choice of $r_1$ and $r_2$, and with $\beta$ verifying $\beta^T 1 \leq \beta$, we get

$$\text{IMD}_F \left( T_X, S_X + \sum_{k=1}^K \beta_k S_{\xi_k} \right) + \beta^T (r_1 + r_2) \leq \text{IMD}_F \left( T_X, S_X + \sum_{k=1}^K \beta_k S_{\xi_k} \right) + \beta (r_1 + r_2).$$

Since this inequality holds for any choice of $\beta^T 1 \leq \beta$, we can take the minimum which results in the DA bound (the minimum is achieved as the set $\{\beta \in \mathbb{R}_+^K : \beta^T 1 \leq \beta\}$ is compact).

As for the equality constraint, it is sufficient to notice that increasing any of the $\beta_k$ cannot increase the value of $\text{IMD}_F \left( T_X, S_X + \sum_{k=1}^K \beta_k S_{\xi_k} \right)$.

$\square$
Proof of the reweighting interpretation. Let $\beta \geq 0$ and $p$ be the vector of source class proportions. For $\beta \geq 0$ verifying $\beta^T 1 = \beta$, we have
\[
\sum_{k=1}^{K} \beta_k S_{X|k} = \sum_{k=1}^{K} (p_k + \beta_k) S_{X|k} = (1 + \beta) \sum_{k} p_k S_{X|k},
\]
where $\hat{p} = \frac{p + \beta}{1 + \beta}$. Conversely, for any $\hat{p} \in \Delta_K$ such that $(1 + \beta)\hat{p} \geq p$, letting $\beta = (1 + \beta)\hat{p} - p$, we have $\beta^T 1 = \beta$.

That results in the following set equality
\[
\left\{ \beta + p \left| \beta \geq 0; \beta^T 1 = \beta \right. \right\} = \{ \hat{p} \in \Delta_K; (1 + \beta)\hat{p} \geq p \},
\]
which allows to conclude.

Proposition 18 (Case of label shift). Assume that the source and target distributions verify $T_{X|y} = S_{X|y} = D_{X|y}$ for all $y \in \mathbb{Y}$. Let $\{q_k\}_{k=1}^{K}$ denote the target class proportions. Then
\begin{enumerate}
\item If $\min_{1 \leq k \leq K} p_k > 0$ and $\beta \geq \max_{1 \leq k \leq K} \left( \frac{q_k}{p_k} - 1 \right)_+$, then $\text{IMD}_F(T_X, (1 + \beta)S_X)$ is nonpositive for any $1 \leq k \leq K$.
\end{enumerate}

Furthermore, if $\mathbb{F}$ is rich enough, and if there exists a family $\{B_1\}_{l=1}^K$ of subsets of $\mathbb{X}$ such that $D_{X|k}(B_1) > 0$ if $k = l$ and $D_{X|k}(B_1) = 0$ otherwise, then the converses of the two previous statements holds.

Proof. Let $D_{X|y} = T_{X|y} = S_X$. Then
\[
\text{IMD}_F(T_X, (1 + \beta)S_X) = \sup_{f \in \mathbb{F}} \mathbb{E}_{T_X}[f] - \mathbb{E}_{S_X}[f]
\]
\[
= \sup_{f \in \mathbb{F}} \sum_{k=1}^{K} (q_k - (1 + \beta)p_k) \mathbb{E}_{D_{X|k}}[f].
\]
Choosing $\beta \geq \max_k \left( \frac{q_k}{p_k} - 1 \right)_+$ will guarantee that the quantity $(q_k - (1 + \beta)p_k)$ is nonpositive for any $1 \leq k \leq K$. In this case, $f = 0$ achieves the supremum and the IMD is null.

Likewise, we have
\[
\text{IMD}_F \left( T_X, \sum_{k=1}^{K} (p_k + \beta_k)S_{X|k} \right) = \sup_{f \in \mathbb{F}} \mathbb{E}_{T_X}[f] - \sum_{k=1}^{K} (p_k + \beta_k) \mathbb{E}_{S_{X|k}}[f]
\]
\[
= \sup_{f \in \mathbb{F}} \sum_{k} (q_k - p_k - \beta_k) \mathbb{E}_{D_{X|k}}[f]
\]
Choosing $\beta_k \geq (q_k - p_k)_+$ will guarantee that the quantity $(q_k - p_k - \beta_k)$ is nonpositive for any $1 \leq k \leq K$. The rest follows as in the first case.

For the converse, assume that $\mathbb{F}$ is rich enough, then by Proposition 9, having $\text{IPM}(T_X, (1 + \beta)S_X) = 0$ implies that $\sum_{k} (q_k - p_k - \beta p_k) D_{X|k} \leq 0$. By the assumption made on the family of sets $\{B_1\}^K_{l=1}$, we have for any $1 \leq l \leq K$,
\[
\sum_{k} (q_k - p_k - \beta p_k) D_{X|k}(B_1) = (q_l - p_l - \beta_p l) D_{X|l}(B_1) \leq 0.
\]
Dividing by $D_{X|l}(B_1)$ implies that $\beta p_l \geq q_l - p_l$. Due to $\beta$’s nonnegativity, this means that $\beta \geq (\frac{q_l}{p_l} - 1)_+$.

For the per-class case, the same reasoning holds via considering $(q_k - p_k - \beta_k) D_{X|k}$ instead of $(q_k - p_k - \beta p_k) D_{X|k}$.

Proposition 19. Assume $l(\mathbb{H}, \mathbb{E})$ is the space of all measurable functions bounded by 1 over $\mathbb{X}$. Denoting $t$ and $s$ the densities of $T_X$ and $S_X$ with respect to some dominating measure $\mu$, we have for any scoring function $g$
\[
\mathcal{L}_T(g) \leq \mathcal{L}_T(g, h_g) + \int \min(s, t) l(h_g, f_s) + d_1(T_X, S_X) + \int \min(s, t) l(f_S, f_T) \tag{13}
\]
\[
\mathcal{L}_T(g) \leq \mathcal{L}_T(g, f_s) + 1 - T_X(\text{supp} S_X) + \mathcal{L}_T(f_S) \tag{14}
\]
where $d_1$ denotes the total variation distance.
**Proof.** The result is an application of Proposition 10 for the two extreme cases \( r_1 = r_2 = 1 \) (in which case, the localization does not result in any restriction since the loss function \( l \) is assumed to be bounded by 1 by assumption) and \( r_1 = r_2 = 0 \). We will then bound \( \mathcal{C}_H (g) \) and IPM \( \mathcal{F}_{r_1 + r_2} (\mathcal{T}_x, \mathcal{S}_x) \) for the two extreme cases. We will denote by \( \mu \) a measure dominating both \( \mathcal{S}_x \) and \( \mathcal{T}_x \) (e.g., the Lebesgue measure).

**Bounding \( \mathcal{C}_H (h) \) and the ideal joint risk:** First, we have \( \mathcal{C}_H (h) = \inf_{h \in H} \int t(x) l(g(x), h(x)) + l(h(x), f_S(x)) d\mu(x) \). Given that \( \mathcal{H} \) has infinite capacity, we have

\[
\mathcal{C}_H (h) = \int \inf_{h \in \mathcal{H}} t(x) l(g(x), h(x)) + l(h(x), f_S(x)) d\mu(x)
\]

so that we can reason on the integrand \( \inf_{h \in \mathcal{H}} t(x) l(g(x), h(x)) + s(x) l(h(x), f_S(x)) \). For the sake of readability, we omit the dependence on \( x \) the point of interest. At point \( x \), we first bound the integrand using the triangle inequality as

\[
\inf_{h \in \mathcal{H}} t(l(g, h) + s(l(h, f_S)) \leq t(l(g, h) + s(l(h, f_S)) \text{ (33)}
\]

If \( h = f_S \), then setting \( h = f_S = h_g \) achieves a minimum equal to 0. Else, depending on whether \( t \geq s \), we can set \( h = f_S \) or \( h = h_g \), leading to the equality

\[
\inf_{h \in \mathcal{H}} t(l(g, h) + s(l(h, f_S)) = \min(s, t) l(h_g, f_S) \text{ (34)}
\]

Combining (33) and (34), we have

\[
\mathcal{C}_H (h) \leq \mathcal{L}_T (g, h_g) + \int \min(s, t) l(h_g, f_S) d\mu. \text{ (35)}
\]

For the other extreme case corresponding to \( \mathcal{H}^0 \), by definition we have \( \mathcal{L}_S (h) = 0 \) for \( h \in \mathcal{H}^0 \), so that

\[
\mathcal{C}_{H^0} (h) = \inf_{h \in \mathcal{H}^0} \mathcal{L}_T (g, h) \leq \mathcal{L}_T (g, f_S). \text{ (36)}
\]

Since \( \mathcal{C}_{H^0} (f_T) \) is the ideal joint risk, by a similar argument, we have

\[
\inf_{h \in \mathcal{H}^0} \mathcal{L}_T (h) + \mathcal{L}_S (h) = \int \min(s, t) l(f_T, f_S) d\mu \text{ (37)}
\]

and

\[
\inf_{h \in \mathcal{H}^0} \mathcal{L}_T (h) + \mathcal{L}_S (h) \leq \mathcal{L}_T (f_S). \text{ (38)}
\]

**Bounding IPM(F_T, S_x):** We have

\[
\text{IMD}_F (\mathcal{T}_x, \mathcal{S}_x) = \sup_{f \in F} \int f(t-s) d\mu
\]

\[
= \int (t-s)^+ d\mu \quad \text{(choosing the indicator function \([t(\cdot) > s(\cdot)]\text{to achieve the supremum})}
\]

\[
= \frac{1}{2} \int |t-s| + (t-s) d\mu \quad \text{(since \( u_+ = \frac{1}{2}(u + |u|) \text{for } u \in \mathbb{R}})
\]

\[
= \frac{1}{2} \int |t-s| d\mu = \frac{1}{2} d_1 (\mathcal{T}_x, \mathcal{S}_x) \quad \text{(since \( \int s d\mu = \int t d\mu = 1 \). (39)}
\]

For the case of \( \mathcal{F}_0 \), we have

\[
\text{IMD}_{\mathcal{F}_0} (\mathcal{T}_x, \mathcal{S}_x) = \sup_{f \in \mathcal{F}_0} \int f d\mathcal{T}_x \quad \text{(by definition of \( \mathcal{F}_0 \) and the IMD)}
\]

\[
= \sup_{f \in \mathcal{F}_0} \int_{\supp S_x} f d\mathcal{T}_x + \int_{\supp S_x} f d\mathcal{T}_x
\]

\[
= \sup_{f \in \mathcal{F}_0} \int_{\supp S_x} f d\mathcal{T}_x + \int_{\supp S_x} f \frac{t}{s} d\mathcal{S}_x \quad \text{(since \( s(x) > 0 \forall x \in \supp S_x \)}
\]

\[
= \sup_{f \in \mathcal{F}_0} \int_{\supp S_x} f d\mathcal{T}_x \quad \text{(since for any \( f \in \mathcal{F}_0 \), \( f \) is null \( \mathcal{S}_x \) – almost everywhere)},
\]

\[
= \mathcal{T}_x (\supp S_x^c) \text{(choosing the indicator function \([. \in \supp S_x^c]\text{to achieve the supremum). (40)}
\]
Finally, combining (35), (37) and (39) gives the first result. Likewise, combining (36), (38) and (40) gives the second result.

**Corollary 20.** For any \( \beta \geq 0, \beta \geq 0 \), we have

\[
1 - \text{IMD}_{H^\Delta \mathbb{H}}(T_X, (1 + \beta)S_X) = \inf_{f \in H^\Delta \mathbb{H}} \mathbb{P}_T [f = 0] + (1 + \beta)\mathbb{P}_S [f = 1] \quad (15)
\]

\[
1 - \min_{\beta \leq 1, 1 \leq \beta} \text{IMD}_{H^\Delta \mathbb{H}} (T_X, S_X + \sum_{k=1}^K \beta_k S_{Xk}) = \max_{\beta \geq 0} \inf_{g \in H^\Delta \mathbb{H}} \mathbb{P}_T [f = 0] + \sum_{k=1}^{K} (p_k + \beta_k)\mathbb{P}_{S_{Xk}} [f = 1] \quad (16)
\]

**Proof.** In the first equality, for \( \beta \geq 0 \) we have

\[
1 - \text{IMD}_{H^\Delta \mathbb{H}}(T_X, (1 + \beta)S_X) = 1 - \sup_{f \in H^\Delta \mathbb{H}} \mathbb{P}_T [f = 1] - (1 + \beta)\mathbb{P}_S [f = 1]
= \inf_{f \in H^\Delta \mathbb{H}} \mathbb{P}_T [f = 0] + (1 + \beta)\mathbb{P}_S [f = 1]. \quad (41)
\]

Similarly, in the second one, for any \( \beta \in \mathbb{R}_+^K \) we have

\[
1 - \text{IMD}_{H^\Delta \mathbb{H}} (T_X, S_X + \sum_{k=1}^K \beta_k S_{Xk}) = 1 - \sup_{f \in H^\Delta \mathbb{H}} \mathbb{P}_T [f = 1] - \mathbb{P}_S [f = 1] + \sum_{k=1}^{K} \beta_k \mathbb{P}_{S_{Xk}} [f = 1]
= \inf_{f \in H^\Delta \mathbb{H}} \mathbb{P}_T [f = 0] + \sum_{k=1}^{K} \mathbb{P}_{S_{Xk}} [f = 1]. \quad (42)
\]

The result follows by taking the maximum over \( \beta \) such that \( \sum_k \beta_k \leq \beta \).

**Proposition 21.** Given a hypothesis space \( \mathbb{H} \), let \( \mathbb{H} \cdot \mathbb{H} := \{ x \mapsto [h_1(x) = h_2(x)]; h_1, h_2 \in \mathbb{H} \} \), and define the \( \mathbb{H} \cdot \mathbb{H} \)-support of \( S_X \) as

\[
\text{supp}_{\mathbb{H} \cdot \mathbb{H}} S_X := \bigcap_{h_1, h_2 \in \mathbb{H}} \{h_1 = h_2\} \quad (17)
\]

Then

\[
\text{IMD}_{H^\Delta \mathbb{H}_0}(T_X, S_X) \leq 1 - T_X(\text{supp}_{\mathbb{H} \cdot \mathbb{H}} S_X). \quad (18)
\]

**Proof.** We have

\[
\text{IMD}_{H^\Delta \mathbb{H}_0}(T_X, S_X) = \sup_{f \in H^\Delta \mathbb{H}_0} \mathbb{P}_T [f = 1] \quad \text{(since } f \in H^\Delta \mathbb{H}_0 \Rightarrow \mathbb{P}_S [f = 1] = 0)\]

\[
= \sup_{h_1, h_2 \in \mathbb{H}} \mathbb{P}_T [h_1 \neq h_2] \quad \text{(by definition of } H^\Delta \mathbb{H})
= 1 - \inf_{h_1, h_2 \in \mathbb{H}} \mathbb{P}_T [h_1 = h_2]
= 1 - \mathbb{P}_T \left[ \bigcap_{h_1, h_2 \in \mathbb{H}} \{h_1 = h_2\} \right] \quad \text{(the intersection of closed sets is closed hence measurable)}
\]

\[
\leq 1 - \mathbb{P}_T \left[ \bigcap_{h_1, h_2 \in \mathbb{H}} \{h_1 = h_2\} \right] \quad (43)
\]

**Proposition 22** (Optimal transport with per-class localization). Assume \( (\mathcal{X}, d) \) and \( (\gamma, l) \) are metric spaces, and that the hypotheses in \( \mathbb{H} \) are \( \frac{1}{2} \)-Lipschitz. Then \( l(H, \mathbb{H}) \subseteq F \) where \( F \) is the space of nonnegative \( 1 \)-Lipschitz functions.
over $\mathbb{X}$. And for any $\beta \geq 0$, the value of $\text{IMD}_F\left(\mathcal{T}_\mathbb{X}, \mathcal{S}_{\mathbb{X}} + \sum_{k=1}^{K} \beta_k \mathcal{S}_{\mathbb{X}|k}\right)$ can be computed by solving the following transport problem

$$\inf_{\{\mathcal{P}_k\}_{k=1}^{K} \subset \mathcal{M}_+(\mathbb{X}, \mathbb{X})} \sum_{k=1}^{K} \mathbb{E}_{(\mathbf{x}_t, \mathbf{x}_s) \sim \mathcal{P}_k} [d(\mathbf{x}_t, \mathbf{x}_s)]$$

s. t. $\pi_1 \# \sum_{k=1}^{K} \mathcal{P}_k \geq \mathcal{T}_\mathbb{X}$

$$\pi_2 \# \mathcal{P}_k \leq (p_k + \beta_k) \mathcal{S}_{\mathbb{X}|k}$$

where $\pi_1 : (u, v) \mapsto u$, $\pi_2 : (u, v) \mapsto v$, and the first inequality constraint on $\mathcal{T}_\mathbb{X}$ can be replaced by an equality.

Proof. Given that $l$ verifies the triangle inequality, for any $\{y_i\}_{i=1}^{d} \subseteq \mathbb{Y}$ we have

$$l(y_1, y_2) - l(y_3, y_4) \leq l(y_1, y_3) + l(y_3, y_4) + l(y_4, y_2) - l(y_1, y_4) = l(y_1, y_3) + l(y_4, y_2).$$

Hence, given $u, v \in \mathbb{X}$ and $h_1, h_2 \in \mathbb{H}$, by property (44), we have

$$l(h_1(u), h_2(u)) - l(h_1(v), h_2(v)) \leq l(h_1(u), h_1(v)) + l(h_2(u), h_2(v))$$

$$l(h_1(v), h_2(v)) - l(h_1(u), h_2(u)) \leq l(h_1(v), h_1(u)) + l(h_2(v), h_2(u))$$

$$\Rightarrow [l(h_1(u), h_2(u)) - l(h_1(v), h_2(v))] \leq l(h_1(u), h_1(v)) + l(h_2(u), h_2(v)) \quad \text{(by symmetry of $l$)}$$

$$\leq \frac{1}{2}d(u, v) + \frac{1}{2}d(u, v).$$

Thus the $l(\mathbb{H}, \mathbb{H}) \subseteq F$, where $F$ is the space of nonnegative 1–Lipschitz functions.

Given a fixed $\beta \in \mathbb{R}_+^K$, computing $\text{IMD}_F\left(\mathcal{T}_\mathbb{X}, \sum_{k=1}^{K} (p_k + \beta_k) \mathcal{S}_{\mathbb{X}|k}\right)$ is equivalent to solving the following optimization problem.

$$\sup_{f \in \mathcal{P}_F} \int f(u) d\mathcal{T}_\mathbb{X}(u) - (p_k + \beta_k) \int f(v_k) d\mathcal{S}_{\mathbb{X}|k}(v)$$

s. t. $f(u) - f(v_k) \leq d(u, v) \forall u, v_k \in \mathbb{X}; 1 \leq l \leq K$

The problem can then be re-written:

$$\sup_{f \geq 0} \int f(u) d\mathcal{T}_\mathbb{X}(u) - (p_k + \beta_k) \int f(v_k) d\mathcal{S}_{\mathbb{X}|k}(v)$$

s. t. $f(u) - f(v_k) \leq d(u, v)$

$$\inf_{u \in \mathbb{X}} f(u) \geq 0, \inf_{v_k \in \mathbb{X}} f(v_k) \geq 0 \quad \forall 1 \leq k \leq K$$

Now we apply Luenberger (1997, Section 8.6, Theorem 1):

- The space of Lipschitz functions is a convex subset of the space of continuous valued functions of $\mathbb{X}$.
- Any function that outputs a positive constant strictly verifies the inequality constraints.
- By compactness of $\mathbb{X}$, the value of the supremum is finite.
Hence, strong Lagrangian duality holds: denoting $\mathcal{M} + (A)$ the space of nonnegative finite measures on a set $A$, the value of the objective at the optimum is

$$
\inf_{\mathcal{P}_k \in \mathcal{M} + (X)} \sup_{u, V_k \in \mathcal{M} + (X)} \int f(u) d\mathcal{T}_k(u) - \int (p_k + \beta_k) f(v_k) d\mathcal{S}_{X|k}(v_k) + \int d(u, v_k) - f(u) + f(v_k) d\mathcal{P}_k(u, v_k) + \int f(v_k) d\mathcal{V}_k + \int f(u) d\mathcal{U}
$$

Following the same argument in Santambrogio (2015), the supremum in the latter formulation is finite if and only if we have

$$
\pi_1 = \sum_k \mathcal{P}_k = \mathcal{T}_k + \mathcal{U}
$$

$$
\pi_2 = \sum_k (p_k + \beta_k) \mathcal{S}_{X|k} - \mathcal{V}_k.
$$

The nonnegativity of $\mathcal{V}_k$ and $\mathcal{U}$ implies the formulation in the statement of the proposition.

To transform the inequality constraint to an equality, notice that for any $1-$Lipschitz function $f$ that is non-negative on $\text{supp} \mathcal{S}_X$, setting $f$ to $f +$ on $\text{supp} \mathcal{T}_X \setminus \text{supp} \mathcal{S}_X$ cannot decrease the value of the objective, while keeping it in the feasible set of solutions (i.e., it stays nonnegative and $1-$Lipschitz). Hence, it suffices to impose the non-negativity constraint only on $\text{supp} \mathcal{S}_X$. This eliminates the variable $\mathcal{U}$ and the inequality constraint on $\mathcal{T}_X$ becomes an equality.

**Proof for support inclusion for optimal transport** Let $\mathcal{F}$ be the space of nonnegative $1-$Lipschitz functions over $X$. For any $f \in \mathcal{F}_0$, $f$ is nonnegative and continuous with $\int f d\mathcal{S}_X = 0$, so $f$ is null on $\text{supp} \mathcal{S}_X$. Hence, for any $u \in X, v \in \text{supp} \mathcal{S}_X$, we have $f(u) \leq f(v) + d(u, v) = d(u, v)$, implying that $f(u) \leq d(u, \text{supp} \mathcal{S}_X) := \inf_{v \in \text{supp} \mathcal{S}_X} d(u, v)$.

As a result, we have

$$
\text{IMD}_{\mathcal{F}_0}(u, v) = \sup_{f \in \mathcal{F}_0} \int f(u) d\mathcal{T}_X(u) \leq \sup_{f \in \mathcal{F}_0} \int d(u, \mathcal{S}_X) d\mathcal{T}_X(u).
$$

Moreover, the function $d(\cdot, \mathcal{S}_X)$ is $1$-Lipschitz, nonnegative and is null on $\mathcal{S}_X$, meaning that $d(\cdot, \mathcal{S}_X) \in \mathcal{F}_0$. As a result, it achieves the supremum defining $\text{IMD}_{\mathcal{F}_0}$, hence the statement.