Abstract

We consider the multiple-source adaptation (MSA) problem and improve a previously proposed MSA solution, where accurate density estimation per domain is required to obtain favorable learning guarantees. In this work, we replace the difficult task of density estimation per domain with a much easier task of domain classification, and show that the two solutions are equivalent given the true densities and domain classifier, yet the newer approach benefits from more favorable guarantees when densities and domain classifier are estimated from finite samples. Our experiments with real-world applications demonstrate that the new discriminative MSA solution outperforms the previous solution with density estimation, as well as other domain adaptation baselines.

1 Introduction

Learning algorithms are applied to an increasingly broad array of problems. For some tasks, large amounts of labeled data are available to train very accurate predictors. But, for most new problems or domains, no such supervised information is at the learner’s disposal. Furthermore, labeling data is costly since it typically requires human inspection and agreements between multiple expert labelers. Can we leverage past predictors learned for various domains and combine them to devise an accurate one for a new task? Can we provide guarantees for such combined predictors? How should we define that combined predictor? These are some of the challenges of multiple-source domain adaptation.

The problem of domain adaptation from multiple sources admits distinct instances defined by the type of source information available to the learner, the number of source domains, and the amount of labeled and unlabeled data available from the target domain [Mansour et al., 2008, 2009a, Hoffman et al., 2018, Pan and Yang, 2010, Muandet et al., 2013, Xu et al., 2014, Hoffman et al., 2012, Gong et al., 2013a,b, Zhang et al., 2015, Ganin et al., 2016, Tzeng et al., 2015, Motiian et al., 2017b,a, Wang et al., 2019, Konstantinov and Lampert, 2019, Liu et al., 2015]. The specific instance we are considering is one where the learner has access to multiple source domains or distributions and where, for each domain, they only have at their disposal a predictor trained for that domain and some amount of unlabeled data. No other information about the source domains, in particular no labeled data is available. The target domain or distribution is unknown but it is assumed to be in the convex hull of the source distributions, or relatively close to that. The multiple-source adaptation (MSA) problem consists of combining relatively accurate predictors available for each source domain to derive an accurate predictor for any new mixture target domain. This problem was first theoretically studied by Mansour et al. [2008, 2009a] and subsequently by Hoffman et al. [2018],
who further provided an efficient algorithm for this problem and reported a series of experiments with that algorithm.

As pointed out by these authors, this problem arises in a variety of different contexts. In speech recognition, each domain may correspond to a different group of speakers and an acoustic model learned for each domain may be available, and the problem consists of devising a general recognizer for a broader population, a mixture of the source domains [Liao, 2013]. Similarly, in object recognition, there may be accurate models trained on different image databases and the goal is to come up with an accurate predictor for a general domain, which is likely to be close to a mixture of these sources [Torralba and Efros, 2011]. A similar situation often appears in sentiment analysis and various other natural language processing problems where accurate predictors are available for some source domains such as TVs, laptops and CD players, each previously trained on labeled data, but no labeled data or predictor is at hand for the broader category of electronics, which can be viewed as a mixture of the sub-domains [Blitzer et al., 2007, Dredze et al., 2008].

An additional motivation for this instance of multiple-source adaptation is that often the learner does not have access to labeled data from various domains for legitimate reasons such as privacy or storage limitation. This may be for example data from various hospitals, each obeying strict regulations and privacy rules. But, a predictor trained on the labeled data from each hospital may be available. Similarly, a speech recognition system trained on data from some group may be available but the many hours of source labeled data used to train that model may not be accessible anymore, due to the very large amount of disk space it requires. Thus, in many cases, the learner cannot simply merge all source labeled data to learn a predictor.

Here, we build on previous work already mentioned [Mansour et al., 2008, 2009a, Hoffman et al., 2018] where an elegant theoretical solution via a distribution-weighted combination of source predictors was shown to benefit from favorable theoretical guarantees. Our results are based on the observation that, a similar solution to the distribution-weighted combination can be derived by using the estimated conditional probabilities returned by a multi-class classification algorithm such as multinomial logistic regression, instead of density estimates for each domain.

This may at first appear to be a minor change. However, this discriminative solution admits several significant advantages and, with ideal conditional probabilities, this proposed algorithm also has the same optimal guarantees as the ideal density estimation solution of [Hoffman et al., 2018]. First, in general, density estimation is a difficult problem and the guarantees provided by these authors directly depend on the quality of density estimation. Instead, our solution only relies on training an algorithm such as multinomial logistic regression on a full unlabeled sample formed by the union of all domains. The labels used for training the logistic regression are the domain identities. This is a much larger sample and our algorithm thereby benefits from very favorable learning guarantees. Moreover, a more accurate solution can be achieved via discriminative training of a classifier on a large sample than density estimation for each domain based on samples from that domain only.

**Related work.** There is a broad literature on adaptation. Here, we briefly discuss some related work and reserve a more extensive discussion to Appendix B. Using a domain classifier to combine domain-specific predictors has existed in literature. Jacobs et al. [1991], Nowlan and Hinton [1991] considered an adaptive mixture of experts model, where there are multiple expert networks, as well as a gating network to determine which expert to use for each input. The learning consists of jointly training the individual expert networks and the gating network. Instead, we separate the training of expert networks with that of gating network, and our gating network has a special structure. Hoffman et al. [2012] learned a domain classifier via SVM on all source data combined, and predicted on new test points with the weighted sum of domain classifier’s scores and domain-specific predictors. More recently, Xu et al. [2018] deployed multi-way adversarial training to multiple source domains to obtain a domain discriminator, and took a weighted sum of discriminator’s scores and domain-specific predictors to make predictions.

The rest of the paper is organized as follows. In Section 2, we describe our learning problem and give an overview of the generative MSA solution, GMSA, and its theoretical guarantees [Hoffman et al., 2018]. We formally introduce our discriminative MSA solution, DMSA, in Section 3.1, and prove that the ideal DMSA solution benefits from the same guarantees as GMSA solution. Even though DMSA looks syntactically similar to GMSA, the algorithm for GMSA is no more applicable here. Instead, we cast the optimization problem as DC-programming problem and prove a new DC-decomposition for DMSA in Section 3.2. This provides an efficient and practical algorithm for determining our solution.
Next, in Section 4, we present a theoretical comparison of the guarantees for the two MSA solutions. To do so, we extend the previous analysis and derive sample complexity bounds for the exponential of the Rényi divergence between true distribution and kernel density estimation. Finally, we report the results of a series of experiments on several datasets in Section 5 demonstrating the benefits of our new algorithm.

2 Problem setup

In this work we consider a multiple-source domain adaptation (MSA) problem in the general stochastic scenario. We adopt the notation and problem setup of [Hoffman et al., 2018].

Let $X$ denote the input space and $Y$ the output space and assume a distribution over the joint input-output space $X \times Y$. We will identify a domain with a distribution $D_k$ over $X$, and assume that the learner has access to the true, or, more likely, to an estimated distribution for each domain. As in previous work, we adopt the assumption that for all input $x$ and label $y$, the domains share a common conditional probability function $f(y|x): X \times Y \rightarrow [0, 1]$. We then denote by $D_k(x, y)$ the joint distribution over $X \times Y$ for domain $k$: $D_k(x, y) = D_k(x)f(y|x)$. This is a natural assumption in many settings since for example the label of a picture as a dog may not depend much on whether the picture is from a personal collection or a more general dataset. Nevertheless, as in previous work, this condition can be somewhat relaxed. We will also adopt the assumption that $D_k(x) > 0$ for all $x \in X$ and all domains $k \in \{1, \ldots, p\}$ to simplify the presentation. This is not a necessary condition and can be relaxed at the price of adding a small positive quantity to the denominators of our solution, as in previous work. We further assume that the learner has access to a predictor $h_k$ for each domain $D_k$, $k \in \{1, \ldots, p\}$. We consider two types of predictor functions $h_k$, and their associated loss functions $\ell$ under the regression model $(R)$ and the probability model $(P)$ respectively,

$$h_k: X \rightarrow \mathbb{R}, \quad \ell: \mathbb{R} \times \mathbb{Y} \rightarrow \mathbb{R}_+ \quad (R), \quad h_k: \mathcal{X} \times \mathcal{Y} \rightarrow [0, 1], \quad \ell: [0, 1] \rightarrow \mathbb{R}_+ \quad (P).$$

We will denote by $\mathcal{L}(\mathcal{D}, h)$ the expected loss of a predictor $h$ with respect to the distribution $\mathcal{D}$:

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

Our theory assumes that $\ell$ is convex, continuous, and bounded. For the regression model, we will in particularly study the squared loss $\ell(h(x), y) = (h(x) - y)^2$, and for the probability model the cross-entropy loss, $(\log$-loss) $\ell(h(x), y) = -\log h(x, y)$. We will assume that each $h_k$ is a relatively accurate predictor for domain $D_k$: there exists $\epsilon > 0$ such that

$$\mathcal{L}(\mathcal{D}_k, h_k) \leq \epsilon, \forall k \in \{1, \ldots, p\}.$$

We will also assume that the loss of the source predictor $h_k$ is bounded, that is $\ell(h_k(x), y) \leq M$ or $\ell(h_k(x), y) \leq M$, for all $(x, y) \in X \times Y$ and all $k \in \{1, \ldots, p\}$.

The learner’s objective in the MSA problem is to combine these predictors to design a predictor with small expected loss on a target domain $D_T$ that is an arbitrary and unknown mixture of the source domains: $D_T \in \mathcal{D} = \{D_\lambda: D_\lambda = \sum_{k=1}^{p} \lambda_k D_k, \lambda \in \Delta\}$, where $D_\lambda$ is a mixture of source domains with mixture parameter $\lambda \in \Delta$, and where $\Delta$ is the simplex of dimension $p$, $\Delta = \{\lambda_1, \ldots, \lambda_p\}: \sum_{k=1}^{p} \lambda_k = 1, \lambda_k \geq 0, \forall k \in \{1, \ldots, p\}$. To simplify the discussion, in this paper we focus on the case where $D_T \in \mathcal{D}$, but it is straightforward to extend our theoretical results to the case where $D_T$ is some arbitrary distribution outside the mixture of source domains, using the proof techniques of [Mansour et al., 2008, 2009a, Hoffman et al., 2018].

The distribution weighted solution proposed in the previous work has the form

$$h^*_z(x) = \frac{\sum_{k=1}^{p} z_k D_k(x)}{\sum_{k=1}^{p} z_k D_k(x)} h_k(x), \quad (2) \quad h^*_z(x, y) = \frac{\sum_{k=1}^{p} z_k D_k(x)}{\sum_{j=1}^{p} z_j D_j(x)} h_k(x, y), \quad (3)$$

where $z \in \Delta$ is the parameter to learn$^1$. We name this solution GM$\text{MSA}$ with $G$ standing for “generative”, since density estimation explicitly models the distribution of the data. Note that the formula

$^1$ Compare to equation (1) and (2) in Hoffman et al. [2018], we omit the parameter $\eta$, since $D_k$ is assumed to be non-zero for all inputs, and thus $h_k$ is always a continuous function of $z$. Therefore $\eta$ is no longer needed to ensure continuity in the proofs. Furthermore, since all domains share the same conditional probability $f(y|x)$, the formula for the probability (P) models reduces to the stated equation.
slightly varies between the regression (2) and the probability (3) model. It has been shown that there exists a favorable parameter $z$ satisfying the following property (see Footnote 1 for the omitted $\eta$s).

**Lemma 1.** There exists $z \in \Delta$ with $z_k \neq 0$ for all $k \in [p]$, such that the following holds for the distribution-weighted combination $h_z$: $\forall k \in [p], \mathcal{L}(\mathcal{D}_k, h_z) = \sum_{j=1}^{p} z_j \mathcal{L}(\mathcal{D}_j, h_z)$.

In other words, the desired parameter $z$ and its corresponding solution $h_z$ balances the losses $\mathcal{L}(\mathcal{D}_k, h_z)$ across $p$ domains to the same amount. It follows that the loss-balancing $h_z$ is the desired solution: for any target mixture $\mathcal{D}_\lambda \in \mathcal{D}$, $\mathcal{L}(\mathcal{D}_\lambda, h_z) \leq \epsilon$. Lemma 1 therefore motivates MSA algorithms to find a solution $h_z$ that balances the losses across domains.

To use the solution $h_z$ in practice, we need to estimate the densities $\mathcal{D}_k$. The following Theorem shows that the learning guarantees of $h_z$ directly depend on the Rényi divergence (which is given in Appendix C) between the estimated densities $\hat{\mathcal{D}}_k$ and the true ones $\mathcal{D}_k$. Theorem 1 is adapted from Corollary 4 of Hoffman et al. [2018], and its proof is given in Appendix E.

**Theorem 1.** There exist $z \in \Delta$ such that the following inequality holds for any $\alpha > 1$ and arbitrary target mixture $\mathcal{D}_T \in \mathcal{D}$:

$$
\mathcal{L}(\mathcal{D}_T, \hat{h}_z) \leq e^{\frac{(\alpha-1)^2}{\alpha^2}} M^2 \frac{2^{\alpha-1}}{\alpha^2} \left[ \max_{k \in [p]} d_{\alpha}(\hat{\mathcal{D}}_k \parallel \mathcal{D}_k) \right] \left[ \max_{k \in [p]} d_{2\alpha-1}(\mathcal{D}_k \parallel \hat{\mathcal{D}}_k) \right].
$$

However, density estimation is a difficult problem in general. A natural question is if we can obtain an equally favorable solution without density estimation? In the following section, we will show that this is indeed possible.

### 3 Multiple-source adaptation with a domain classifier

#### 3.1 A theoretical solution

Assume that the learner is given access to a domain classifier $d: \mathcal{X} \rightarrow \Delta$, which outputs the likelihood of sample $x$ belonging to each of the $p$ domains. Our proposed MSA solution, $\text{DMSA}$ ($\text{D}$ stands for “discriminative”, as opposed to the “generative” $\text{GMSA}$), with the domain classifier $d$ has the form

$$
g_z(x) = \sum_{k=1}^{p} \frac{z_k d_k(x)}{\sum_{k=1}^{p} z_k d_k(x)} h_k(x), \quad (4) \quad g_z(x, y) = \sum_{k=1}^{p} \frac{z_k d_k(x)}{\sum_{k=1}^{p} z_k d_k(x)} h_k(x, y), \quad (5)
$$

where we denote by $d_k(x) = [d(x)]_k$, the probability of $x$ belonging to domain $k$ according to the classifier. The $\text{DMSA}$ solutions are syntactically the same as the original $\text{GMSA}$ solutions (2) and (3), with the density $\mathcal{D}_k(x)$ replaced by the domain classifier’s probability $d_k(x)$. In fact, we can show that there exists an one-to-one mapping between $\{h_z, z \in \Delta\}$ and $\{g_z, z \in \Delta\}$.

In the rest of this paper, we assume that the domain classifier’s score $d_k(x)$ is the posterior distribution of domain $k$ after observing $x$ and the prior distribution is $(\mathcal{D}(1), \ldots, \mathcal{D}(p)) \in \Delta$ over $p$ domains. Thus, we assume that there exists a joint distribution $\mathcal{D}(\cdot, \cdot)$ over $\mathcal{X} \times [p]$, with $\sum_{x \in X} \mathcal{D}(x, k) = \mathcal{D}(k), \forall k$. The previously defined density $\mathcal{D}_k(x)$ can be viewed as the conditional distribution of $x$ given domain $k$: $\mathcal{D}_k(x) = \mathcal{D}(x|k)$ and the domain classifier’s score is the corresponding posterior distribution of domain $k$ given input $x$: $d_k(x) = \mathcal{D}(k|\mathcal{D}(x))$.

**Proposition 1.** For any parameter $z \in \Delta$ and its corresponding $h_z$, there exists $z' \in \Delta$ such that $g_{z'} = h_z$, with $z'_k = \frac{z_k^{1/2(\alpha)} h_k(x)}{\sum_{j=1}^{p} z_j^{1/2(\alpha)} h_j(y)}$.

The proof is provided in Appendix E. Proposition 1 implies that the $\text{DMSA}$ solution $g_z$ automatically inherits the learning guarantees from the $\text{GMSA}$ solution.

**Theorem 2 (Known target mixture).** If assumption (1) holds, then for any known target mixture parameter $\lambda \in \Delta$, $\mathcal{L}(\mathcal{D}_\lambda, g_\lambda) \leq \epsilon$, where $\lambda'_k = \frac{\lambda_k^{1/2(\alpha)} h_k(x)}{\sum_{j=1}^{p} \lambda_j^{1/2(\alpha)} h_j(y)}$.

**Proof.** Hoffman et al. [2018] showed that, $\mathcal{L}(\mathcal{D}_\lambda, h_\lambda) \leq \epsilon$ for any $\lambda \in \Delta$. Combining this with Proposition 1 concludes the proof. \qed
Theorem 3 (Unknown target mixture). If assumption (1) holds, then there exist \( z \in \Delta \) such that \( \mathcal{L}(\mathcal{D}_\lambda, g_z) \leq \epsilon \) for any mixture parameter \( \lambda \in \Delta \).

**Proof.** By the proof of Hoffman et al. [2018], there exists a \( z \in \Delta \) such that \( \mathcal{L}(\mathcal{D}_\lambda, h_z) \leq \epsilon \) for any mixture parameter \( \lambda \in \Delta \). By Proposition 1, there is a one-to-one mapping from \( h_z \) to \( g_z' \), which ensures the existence of such a \( g_z' \).

3.2 Algorithms for finding \( z \)

When the target mixture is unknown, Theorem 3 proves the existence of a favorable \( z \in \Delta \), and Hoffman et al. [2018] provided a practical algorithm for finding that favorable \( z \) for GMSA based on estimated densities. Here, we adapt that algorithm to DMSA with an estimated domain classifier \( \hat{d} \).

In practice, it is reasonable to assume that the domain prior is uniform: \( \mathcal{D}(k) = 1/p \) for all \( k \in [p] \), and we will train both the domain classifier and the mixture parameter \( z \) under this assumption. Given an estimated domain classifier \( \hat{d} \), denote by \( \hat{g}_z \) the corresponding DMSA solution: 

\[
\hat{g}_z(x) = \sum_{k=1}^{p} \frac{z_k \hat{d}_k(x)}{\sum_{j=1}^{p} z_j \hat{d}_j(x)} h_k(x).
\]

We assume the same amount of labeled data from each of the \( p \) domains:

Let \( Z_k = \{(x^{(k)}_1, y^{(k)}_1), \ldots, (x^{(k)}_{n_k}, y^{(k)}_{n_k}) \} \) be a set of \( n \) i.i.d. labeled samples drawn from domain \( \mathcal{D}_k \), and let \( Z = \bigcup_{k=1}^{p} Z_k \) be the union of all samples. Let \( Z_X = \{x : (x, y) \in Z \} \) denote the input part of \( Z \). When the labeled source samples are unavailable, one could instead use the predicted labels of the supposedly accurate source predictor as the true labels. Note that the combined set of labeled samples will only be used to learn the mixture parameter \( z \), which could be substantially smaller than the combined set of unlabeled samples used to learn the domain classifier. We define an estimate of the marginal distribution \( \mathcal{D}_k(x) \) based on \( \hat{d} \):

\[
\hat{\mathcal{D}}_k(x) = \hat{d}_k(x) \mathcal{D}(x)/\mathcal{D}(k) = p \hat{d}_k(x) \hat{\mathcal{D}}(x), \forall x \in Z_X.
\]

The choice of \( \hat{\mathcal{D}}(x) \) is given by the following optimization problem:

\[
\arg\min_{\hat{\mathcal{D}}} \| \hat{\mathcal{D}} - u \|^2_2, \quad \text{s.t.} \sum_{x \in Z_X} \hat{\mathcal{D}}(x) \hat{d}_k(x) = \frac{1}{p}, \forall k \in [p], \sum_{x \in Z_X} \hat{\mathcal{D}}(x) = 1. \tag{6}
\]

The linear constraints on \( \hat{\mathcal{D}}(x) \) ensure that \( \hat{\mathcal{D}}_k \) and \( \hat{d}_k \) obey the Bayes’ rule. Since there are infinitely many solutions \( \hat{\mathcal{D}}(x) \) satisfying the linear equations, we use the one that is closest to the empirical distribution induced by \( Z_X \), a uniform distribution \( u \). Problem (6) admits a closed-form solution:

\[
\hat{\mathcal{D}} = u - A(A^T A)^{-1}(A^T u - 1), \quad \text{where } A = np \times (p + 1) \text{ matrix with entries } A_i,k = p \hat{d}_k(x_i) \text{ and } A_{i,p+1} = 1, \text{ for all } x_i \in Z_X, 1 \leq i \leq np.
\]

Motivated by Lemma 1, finding the key parameter \( z \) of the DMSA solution \( \hat{g}_z \) consists of solving a min-max optimization problem:

\[
\min_{z \in \Delta} \max_{k \in [p]} \mathcal{L}(\hat{\mathcal{D}}_k, \hat{g}_z) - \mathcal{L}(\hat{\mathcal{D}}_z, \hat{g}_z), \tag{7}
\]

Furthermore, by Lemma 1, the minimal objective value of (7) is zero, thus it is straightforward to check the optimality of any solution \( z \). Problem (7) can be solved by the DC (difference-of-convex) algorithm [Tao and An, 1997, 1998, Sriperumbudur and Lanckriet, 2012]. We present a DC-decomposition of the learning objective for both regression and probability models, which leads to an efficient DC algorithm that guarantees to converge to a stationary point (see Appendix E).

When the context is clear, we write \( \hat{\mathcal{D}}_k \) and \( \hat{d}_k \) instead of \( \hat{\mathcal{D}}_k \) and \( \hat{d}_k \) to avoid clutter of notations.

**Proposition 2 (Regression model).** Let \( \ell \) be the squared loss. Then, for any \( k \in [p], \mathcal{L}(\hat{\mathcal{D}}_k, g_z) - \mathcal{L}(\hat{\mathcal{D}}_z, g_z) = u_k(z) - v_k(z), \) where \( u_k \) and \( v_k \) are convex functions defined for all \( z \) by

\[
u_k(z) = \sum_{(x,y) \in Z} \mathcal{D}_k(x,y) [y - g_z(x)]^2 - 2M \left( \sum_{x \in Z_X} \mathcal{D}_k(x) \log d_z(x) \right),
\]

\[
u_k(z) = \sum_{(x,y) \in Z} \mathcal{D}_z(x,y) [y - g_z(x)]^2 - 2M \left( \sum_{x \in Z_X} \mathcal{D}_k(x) \log d_z(x) \right).
\]

All proofs are given in Appendix E.
Proposition 3 (Probability model). Let $\ell$ be the cross-entropy loss. Then, for $k \in [p]$, $\mathcal{L}(\mathcal{D}_k, g_z) = \mathcal{L}(\mathcal{D}_k, g_z) = u_k(z) - v_k(z)$, where $u_k$ and $v_k$ are convex functions defined for all $z$ by

$$u_k(z) = \sum_{(x,y) \in Z} -D_k(x,y) \log g_z(x,y) - D_k(x,y) \log d_z(x),$$

$$v_k(z) = \sum_{(x,y) \in Z} -D_z(x,y) \log g_z(x,y) - D_k(x,y) \log d_z(x).$$

4 Learning guarantees

In this section, we prove favorable learning guarantees for $\hat{g}_z$ with domain classifier $\hat{d}_k(x)$ learned by multinomial logistic regression. We first provide learning guarantees for multinomial logistic regression in Section 4.1, and then use them to prove favorable learning guarantees for DMSA with a domain classifier, and finally discuss its advantage over GMSA with density estimation (Section 4.2). All the proofs are given in Appendix E.

4.1 Multinomial logistic regression

Let $\mathcal{D}(x, k) : \mathcal{X} \times [p] \rightarrow \mathbb{R}$ denote the joint distribution over the input space $\mathcal{X}$ and $p$ domains. Let $S = \{(x_1, k_1), \ldots, (x_M, k_M)\}$ be a set of $M$ i.i.d. samples drawn from $\mathcal{D}(\cdot, \cdot)$. The multinomial logistic regression has the learning objective:

$$\arg\min_{w \in \mathbb{R}^N} \xi \|w\|^2 - \frac{1}{M} \sum_{i=1}^{M} \log p_w[k_i|x_i],$$

where $\xi \geq 0$ is the regularizer. The model for the conditional distribution $\mathcal{D}(k|x)$ is $p_w[k|x] = \frac{1}{Z(x)} \exp(w \cdot \Phi(x,k))$, with $Z(x) = \sum_{k \in [p]} \exp(w \cdot \Phi(x,k))$, and $\Phi(x,k)$ is a feature mapping $\mathcal{X} \times [p] \rightarrow \mathbb{R}^N$ with bounded values, $|\Phi(x,k)| \leq R$. Multinomial logistic regression problem (8) benefits from favorable guarantees.

Theorem 4. Let $\hat{w}$ be the solution to problem (8) and $w^*$ be the solution under the true distribution:

$$w^* = \arg\min_{w \in \mathbb{R}^N} \xi \|w\|^2 - \mathbb{E}_{(x,k) \sim \mathcal{D}} \log p_w[k|x].$$

Then, for any $\delta > 0$, with probability at least $1 - \delta$,

$$\left| \mathbb{E}_{(x,k) \sim \mathcal{D}} \log p_{w^*}[k|x] - \mathbb{E}_{(x,k) \sim \mathcal{D}} \log p_{w^*}[k|x] \right| \leq \frac{2\sqrt{2\xi R^2}}{\sqrt{M}} (1 + \sqrt{\log 1/\delta}).$$

Theorem 4 shows that the expected log-loss of the logistic regression solution $p_{\hat{w}}$ converges to that of the best-in-class classifier $p_{w*}$ at the rate of $O(1/\sqrt{M})$, and it does not depend on the dimension of the feature mapping $\Phi$.

4.2 Comparison of the guarantees of DMSA and GMSA

As in Section 3.2, we assume a uniform domain prior $\mathcal{D}(k) = \frac{1}{p}, \forall k \in [p]$, and thus $\mathcal{D}(x) = \frac{1}{p} \sum_{k=1}^{p} D_k(x)$. Let $p_{\hat{g}_z}$ be the logistic regression solution learned on the combined set of $m$ samples per domain: $\cup_{k=1}^{m} \{(x_i^{(k)}, k) : i \in [m], x_i \sim \mathcal{D}_k\}$, and denote by $\hat{g}_z$ the DMSA solution based on $p_{\hat{g}_z}$.

Theorem 5. There exist $z \in \Delta$ such that the following inequality holds for any $\alpha > 1$ and arbitrary target mixture $\mathcal{D}_T$:

$$\mathcal{L}(\mathcal{D}_T, \hat{g}_z) \leq \mathcal{E}^{-2\alpha - 1} \left[ d_m(\alpha) d_2(\alpha) \right] \left[ \mathcal{E}^{2\alpha - 2} \left( d_m^*(\alpha) \right) \right]^{1/\alpha},$$

where

$$d_1(\alpha) = \left[ \mathbb{E}_{x \sim \mathcal{D}_T(x)} \left[ d_m(\alpha) \left( d(x) \right) \left( \mathcal{E}^{2\alpha - 2} \left( d_m^*(\alpha) \right) \right) \right] \right]^{1/\alpha},$$

$$d_2(\alpha) = \left[ \mathbb{E}_{x \sim \mathcal{D}_T(x)} \left[ d_m^*(\alpha) \left( d(x) \right) \right] \right]^{1/\alpha}.$$
Next, we prove learning guarantees for GMSA with densities estimated by KDE. Assume the estimated density \( \hat{D}_k \) is learned on the same \( p \) unlabeled samples from domain \( D_k \), \( \{x_i^{(k)}; i \in [m]\} \), via kernel density estimation with a normalized kernel function \( K_\sigma (\cdot, \cdot) \) that satisfies \( \int_{x \in X} K_\sigma (x, x') dx = 1 \) for all \( x' \in X \).

**Theorem 6.** There exist \( z \in \Delta \) such that, for any \( \delta > 0 \), with probability at least \( 1 - \delta \) the following inequality holds for any \( 1 < \alpha < 2 \) and arbitrary target mixture \( D_T \):

\[
\mathcal{L}(D_T, \hat{h}_z) \leq \epsilon^2 \frac{(\alpha - 1)^2}{\alpha} M_2(\frac{1}{\alpha}) \sqrt{m \log \frac{4}{\epsilon}} \frac{d_3(\alpha)}{d_4(\alpha)},
\]

with \( M_m = 1 + \frac{2}{m} \left[ \max_{x_i, x_j, x \in X} \frac{K_\sigma (x, x_j) - K_\sigma (x, x_i)}{K_\sigma (x, x_i)} \right] \), and

\[
d_3(\alpha) = \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_\alpha (K_\sigma (\cdot, x) \| D_k) \right], \quad d_4(\alpha) = \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_2(\alpha - 1) (D_k \| K_\sigma (\cdot, x)) \right].
\]

**Remark:** Both Theorem 5 and Theorem 6 have two sets of terms in the generalization bound, sample complexity, and Rényi divergence. We compare two MSA guarantees in terms of both.

**Sample complexity:** The dependence on the number of samples for DMSA (Theorem 5) is determined by the term \( e^{(2 + \frac{1}{\alpha - 2})/2} \| \hat{w} - w^* \| \). From the proof of Theorem 4, for any \( \delta > 0 \), with probability at least \( 1 - \delta \), \( \| \hat{w} - w^* \| \leq \frac{R}{\zeta \sqrt{mp/2}} (1 + \sqrt{\log 1/\delta}) \), where \( mp \) is the total number of samples used to learn the domain classifier. Thus, \( \hat{D}_z \) has error on the order of \( O(e^{1/\sqrt{m}}) \). On the other hand, the sample complexity of GMSA (Theorem 6) with KDE trained on the same set of unlabeled samples has error \( O(e^{1/\sqrt{m}}) \). Thus, DMSA benefits from combining all unlabeled samples to learn an accurate domain classifier.

**Rényi divergence:** The generalization guarantees for DMSA (Theorem 5) depends on two critical terms that measure the divergence between logistic regression’s best-in-class solution and the true domain classifier:

\[
\mathbb{E}_{x \sim D(x)} \left[ d_{2\alpha - 1} (d^*(x) \| d(x)) \right], \quad \mathbb{E}_{x \sim D(x)} \left[ d_{4\alpha - 2} (d(x) \| d^*(x)) \right].
\]

When the feature mapping for logistic regression is rich enough, such as reproducing kernel Hilbert space (RKHS) with a Gaussian kernel, one can expect the two divergences to be close to one. On the other hand, the generalization guarantees for GMSA (Theorem 6) also depend on two divergence terms:

\[
\max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_\alpha (K_\sigma (\cdot, x) \| D_k) \right], \quad \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_2(\alpha - 1) (D_k \| K_\sigma (\cdot, x)) \right].
\]

Comparing to learning a domain classifier for posterior distribution \( d(x) \), it is more difficult to chose a good density kernel \( K_\sigma (\cdot, \cdot) \) to make the divergence between marginal distributions to be small. This demonstrates another benefit of DMSA.

## 5 Experiments

We evaluated the DMSA solution with domain classifier on the same datasets used in Hoffman et al. [2018], and compared its performances with various baselines, including GMSA.

**Sentiment analysis.** To evaluate the DMSA solution under the regression model, we used the sentiment analysis dataset [Blitzer et al., 2007], which consists of product review text and rating labels taken from four domains: books (B), dvd (D), electronics (E), and kitchen (K), with 2,000 samples for each domain. We adopted the same training procedure and hyper-parameters from Hoffman et al. [2018] to obtain base predictors: first define a vocabulary of 2,500 words that occur at least twice in each of the four domains, then use this vocabulary to define word-count feature vectors for every review text, and finally train base predictors for each domain using support vector regression. We use the same word-count features to train the domain classifier via logistic regression. We randomly split 2,000 samples into 1,600 train and 400 test samples for each domain, and learn the base predictors, domain classifier, density estimations, and parameter \( z \) for both MSA solutions.
We compared our method (DMSA) against each source predictor, $h_k$, the uniform combination of all predictors ($\text{unif}$), $\sum_k h_k/p$, and GMSA with kernel density estimation. Each column in Table 1 corresponds to a different target test mixtures as indicated by the column name: four single domains, and uniform mixtures of two, three, and four domains, respectively. Our distribution-weighted method DMSA outperforms all baseline predictors across almost all test domains. In particular, DMSA improves upon the GMSA by a big margin on all test mixtures, verifying the advantage of using a domain classifier over estimated densities in the distribution-weighted combination.

**Recognition tasks with the cross-entropy loss.** To evaluate the DMSA solution under the probability model, we considered a digit recognition task consists of three datasets: Google Street View House Numbers (SVHN), MNIST, and USPS. Dataset statistics can be found in Table 2. For each individual domain, we trained a convolutional neural network (CNN) with the same setup as in Hoffman et al. [2018], and used the output from the softmax score layer as our base predictors $h_k$. Furthermore, for every input image, we extract the last layer before softmax from each of the base networks and concatenate them to obtain the feature vector for training the domain classifier. We used the full training sets per domain to train the source model, and used 6,000 samples per domain to learn the domain classifier. Finally, for our DC-programming algorithm we used a 1000 image-label pairs from each domain to learn the parameter $z$.

We compared our method (DMSA) against each source predictor ($h_k$), the uniform combination of all predictors ($h_{\text{unif}}$), a network jointly trained on all source data combined ($h_{\text{joint}}$), and GMSA with KDE. We evaluated these baselines on each of the three test datasets, on combinations of two test datasets, and on all test datasets combined. Results are given in Table 3. Once again, DMSA outperforms all baselines on all test mixtures, and when the target is a single test domain, DMSA admits comparable performance to the predictor which is trained and tested on the same domain. And, as in the sentiment analysis experiments, DMSA wins over GMSA by a big margin on all test domains.

### 6 Conclusion

We presented a new algorithm for the important problem of multiple-source adaptation, which commonly arises in applications. Our algorithm was shown to benefit from favorable theoretical guarantees and a superior empirical performance, compared to previous work. Moreover, our algorithm is practical: it is straightforward to train a multi-class classifier in the setting we described and our

---

**Table 1:** MSE on the sentiment analysis dataset of source-only baselines for each domain, $K$, D, B, E, the uniform weighted predictor $\text{unif}$, the distribution-weighted predictor $\text{DW-dens}$ based on density estimation, and $\text{DW-class}$ based on learned posterior distribution.

| $K$ | D | B | E | unif | GMSA | DMSA (ours) |
|-----|---|---|---|------|------|-------------|
| 0.12 | 0.10 | 0.13 | 0.20 | 0.20 | 0.21 | 0.10 |
| 1.42 | 2.09 | 2.16 | 1.50 | 1.42 | 1.42 | 1.42 |
| 0.12 | 0.13 | 0.12 | 0.06 | 0.06 | 0.06 | 0.06 |
| 1.81 | 2.01 | 2.07 | 1.96 | 1.59 | 1.59 | 1.59 |
| 0.06 | 0.06 | 0.06 | 0.06 | 0.06 | 0.06 | 0.06 |
| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 1.91 | 2.02 | 2.02 | 1.95 | 1.55 | 1.55 | 1.55 |

**Table 2:** Digit dataset statistics.

| SVHN | MNIST | USPS |
|------|-------|------|
| # train images | 73,257 | 26,032 | 92,300 |
| # test images | 60,000 | 10,000 | 99,200 |
| image size | 32x32 | 28x28 | 16x16 |
| color | rgb | gray | gray |

**Table 3:** Digit dataset accuracy.

| SVHN | MNIST | USPS | CNN | GMSA | DMSA (ours) |
|------|-------|------|-----|------|-------------|
| mean | mean | mean | mean | mean | mean |
| 92.3 | 99.2 | 96.6 | 92.3 | 92.3 | 92.3 |
| 66.9 | 65.6 | 66.7 | 66.9 | 66.9 | 66.9 |
| 57.9 | 79.7 | 96.0 | 97.9 | 97.9 | 97.9 |
| 16.7 | 62.3 | 68.1 | 68.1 | 68.1 | 68.1 |
| 75.7 | 91.3 | 92.2 | 91.4 | 91.4 | 91.4 |
| 90.9 | 99.1 | 96.0 | 98.6 | 98.6 | 98.6 |
| 91.4 | 98.8 | 95.6 | 98.3 | 98.3 | 98.3 |
| 92.3 | 99.2 | 96.6 | 98.8 | 98.8 | 98.8 |

---

Note that one can slightly improve the two Rényi divergences to $\max_k \max_{p \in [p]} d_\alpha \left( \mathbb{E}_{x \sim \mathcal{D}_k} \left[ K(x, \cdot) \right] \right) \parallel \mathcal{D}_k$, and $\max_k \max_{p \in [p]} d_{2\alpha-1} \left( \mathcal{D}_k \parallel \mathbb{E}_{x \sim \mathcal{D}_k} \left[ K(x, \cdot) \right] \right)$, using Theorem 9 in Appendix D.
DC-programming solution is very efficient. A key research problem to design a solution for active adaptation from multiple sources to a single target domain, that is by actively requesting labels from the target, while preserving strong theoretical and algorithmic guarantees as well as practical and empirical benefits.

**Broader impact.** This paper presents a significant improvement over previous solutions for the difficult task of multiple-source domain adaptation. Providing a robust solution for the problem is particularly important for under-represented groups, whose data is not necessarily well-represented in the classifiers to be combined and trained on source data. Our solution demonstrates improved performance even in the cases where the target distribution is not included in the source distributions, see the appendix for more experimental results (Appendix A). We hope that continued efforts in this area will result in more equitable treatment of under-represented groups.

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Table 4: Train on two domains and test on all domains combined. Column name dom means that the learner is given features and base predictors from all domains except from domain dom.

| Train data | svhn | mnist | usps |
|------------|------|-------|------|
| CNN-svhn   | -    | 84.2  | 84.2 |
| CNN-mnist  | 41.0 | -     | 41.0 |
| CNN-usps   | 32.9 | 32.9  | -    |
| CNN-unif   | 43.8 | 85.1  | 90.9 |
| DMSA        | 43.4 | 85.4  | 93.3 |

Table 5: Train on four domains and test on all domains combined. Column name dom means that the learner is given features and base predictors from all domains except from domain dom.

| Train data | svhn | mnist | usps | mnistm | synth |
|------------|------|-------|------|--------|-------|
| CNN-svhn   | -    | 78.0  | 78.0 | 78.0   | 78.0  |
| CNN-mnist  | 43.5 | -     | 43.5 | 43.5   | 43.5  |
| CNN-usps   | 28.4 | 28.4  | -    | 28.4   | 28.4  |
| CNN-mnistm | 59.4 | 59.4  | 59.4 | -      | 59.4  |
| CNN-synth  | 83.8 | 83.8  | 83.8 | -      | 83.8  |
| CNN-unif   | 77.0 | 91.7  | 90.3 | 87.7   | 77.2  |
| DMSA        | **91.1** | **93.5** | **94.0** | **89.8** | **92.4** |

A More experiments

In this section, we report experimental results for the scenario where the target domain is close to being a mixture of the source domains but where it may not necessarily be such a mixture.

We begin with the three datasets used in Section 5: Google Street View House Numbers (SVHN), MNIST, and USPS. We adopt the learning scenario where the learner is only given access to feature vectors and base predictors for two of the three domains, and is asked to predict on all three domains combined. Thus, the target domain is not a mixture of the source domains, but is not too far away from that.

Table 4 presents the accuracy on all test data combined, for various baselines: the base predictors, the uniform combination of two base predictors, and DMSA trained on two domains. DMSA outperforms the unif combination in two of the three cases, and is very close to unif in the other case.

Next, we increase the number of source domains by introducing two additional digit datasets: MNIST-M (MNIST digits superimposed on patches randomly extracted from color photos), and a synthetic dataset. Again, we left out one domain and trained on the other four, and then tested on all domains combined. The results are given in Table 5.

With more source domains, DMSA significantly outperforms other baselines in all cases. This robust performance of the algorithm on domains that poorly represented or even unrepresented during training makes it a strong candidate to tackle fairness concerns.

B Related and previous work on multiple-source adaptation (MSA)

The general theoretical problem of adaptation from a single domain to a target domain has been studied in a series of publications in the last two decades or so [Kifer et al., 2004, Ben-David et al., 2007, Blitzer et al., 2008, Mansour et al., 2009b, Cortes and Mohri, 2014, Cortes et al., 2019b]. There are many distinct instances of adaptation problems.

Using a domain classifier to combine domain-specific predictors has existed in literature. Jacobs et al. [1991], Nowlan and Hinton [1991] considered an adaptive mixture of experts model, where there are multiple expert networks, as well as a gating network to determine which expert to use for each input. The learning consists of jointly training the individual expert networks as well as the gating network. Instead, we separate the training of expert networks with that of gating network, and our gating network has a special structure. Hoffman et al. [2012] learned a domain classifier via SVM on all source data combined, and predicted on new test points.

For details of the two additional datasets, see http://yaroslav.ganin.net/.
with the weighted sum of domain classifier’s scores and domain-specific predictors. More recently, Xu et al. [2018] deployed multi-way adversarial training to obtain a multi-way discriminator, and took a weighted sum of discriminator’s scores and domain-specific predictors to make predictions.

Multiple-source adaptation has been extensively studied from various aspects. Yang et al. [2007] proposed to learn a linear combination of pre-trained auxiliary classifiers using SVMs on labeled target data. Duan et al. [2009, 2012] further assumed plenty of unlabeled target data to form a meaningful regularizer, and a small set of labeled target data for training. Khosla et al. [2012], Blanchard et al. [2011] combined all the source data to jointly train a single predictor. Pei et al. [2018], Zhao et al. [2018] extended single domain adversarial learning techniques to the multiple-source setting to extract domain-invariant features. Ghifary et al. [2015] extended auto-encoders to the multi-task setting and minimized the sum of reconstruction errors across domains. Peng et al. [2019] proposed to align moments of feature distribution across source and target domains. Muandet et al. [2013] proposed Domain-Invariant Component Analysis to transform features onto a low dimensional subspace that minimizes the dissimilarity across domains. Zhang et al. [2015] adopted a causal view of MSA where label Y is the cause for features X, estimated the weights for combining source conditional probabilities (P(X|Y)), and proposed various ways to construct target predictor based on estimated weights. Crammer et al. [2008] considered learning accurate models for each source domain, using “nearby” data of other domains. Gong et al. [2012] ranked multiple source domains by how good can they adapt to a target domain. Gong et al. [2013a] learned domain-invariant features by constructing multiple auxiliary tasks, and learning new feature representations from each auxiliary task. Gong et al. [2013b] proposed to discover multiple latent domains by maximizing distinctiveness and learnability between latent domains. Jhuo et al. [2012] transferred source samples into an intermediate representation such that each transformed source sample can be linearly reconstructed by target samples. Wen et al. [2019] adjusted the weight of each source domain during training based on discrepancy minimization theory. Fernando et al. [2013] considered aligning subspaces for visual domain adaptation. Liu et al. [2016] proposed to preserve the structure information from source domains via clustering. Gan et al. [2016] tackled the multiple-source adaptation problem via attributes possessing. Sun et al. [2011] considered a two-stage adaptation where in the first stage one combines weighted source data based on marginal probability, and in the second stage based conditional probability as well.

C Rényi divergence

The Rényi Divergence is parameterized by $\alpha \in [0, +\infty]$ and denoted by $D_\alpha$. The $\alpha$-Rényi Divergence of two distributions $\mathcal{D}$ and $\mathcal{D}'$ is defined by

$$D_\alpha(\mathcal{D} \parallel \mathcal{D}') = \frac{1}{\alpha - 1} \log \sum_{(x,y) \in X \times Y} \mathcal{D}(x, y) \left(\frac{\mathcal{D}(x, y)}{\mathcal{D}'(x, y)}\right)^{\alpha - 1},$$

where, for $\alpha \in \{0, 1, +\infty\}$, the expression is defined by taking the limit. For $\alpha = 1$, the Rényi divergence coincides with the relative entropy. For $\alpha = +\infty$, it coincides with $\log \sup_{x \in \mathcal{X}} \frac{\mathcal{D}(x)}{\mathcal{D}'(x)}$. It can be shown that the Rényi Divergence is always non-negative and that for any $\alpha > 0$, $D_\alpha(\mathcal{D} \parallel \mathcal{D}') = 0$ iff $\mathcal{D} = \mathcal{D}'$ [Arndt, 2004]. We will denote by $d_\alpha(\mathcal{D} \parallel \mathcal{D}')$ the exponential:

$$d_\alpha(\mathcal{D} \parallel \mathcal{D}') = e^{D_\alpha(\mathcal{D} \parallel \mathcal{D}')} = \sum_{(x,y) \in X \times Y} \frac{\mathcal{D}(x, y)}{d_\alpha^{1/(\alpha - 1)}(x, y)}.$$

The following lemma from Van Erven and Harremos [2014] summarizes some useful properties of the Rényi divergence.

**Lemma 2.** The Rényi divergence admits the following properties:

1. $D_\alpha(\mathcal{D} \parallel \mathcal{D}')$ is a non-decreasing function of $\alpha$.
2. $D_\alpha(\mathcal{D} \parallel \mathcal{D}')$ is jointly convex in $(\mathcal{D}, \mathcal{D}')$ for $\alpha \in [0, 1]$.
3. $D_\alpha(\mathcal{D} \parallel \mathcal{D}')$ is convex in $\mathcal{D}'$ for $\alpha \in [0, \infty]$.
4. $D_\alpha(\mathcal{D} \parallel \mathcal{D}')$ is jointly quasi-convex in $(\mathcal{D}, \mathcal{D}')$ for $\alpha \in [0, \infty]$.

We prove another useful lemma that presents a family of “triangle inequality” of the Rényi divergence.

**Lemma 3.** Let $\mathcal{P}, \mathcal{Q}, \mathcal{R}$ be three distributions on $\mathcal{X}$. Then, for any $\gamma \in (0, 1)$ and any $\alpha > \gamma$,

$$\left[ d_\alpha(\mathcal{P} \parallel \mathcal{Q}) \right]^{\alpha - 1} \leq \left[ d_\alpha(\mathcal{P} \parallel \mathcal{R}) \right]^{\alpha - \gamma} \left[ d_{\frac{\alpha - \gamma}{\alpha - 1}}(\mathcal{R} \parallel \mathcal{Q}) \right]^{\alpha - 1}. $$
Proof. Let $\gamma \in (0, 1)$ be a constant. When the context is clear, we write $P$ instead of $P(x)$ for simplicity. By Hölder’s inequality and the definition of Rényi divergence,

$$
\left[ d_{\alpha}(P \parallel Q) \right]^{\alpha - 1} = \sum_{x} P^{\alpha}(x) = \sum_{x} P^{\alpha} \frac{Q^{\alpha - \gamma}}{Q^{\alpha - 1}} = \left[ \sum_{x} \left( \frac{P^{\alpha}}{Q^{\alpha - \gamma}} \right) \right]^{1/\alpha - 1} \left[ \sum_{x} \frac{Q^{\alpha - \gamma}}{Q^{\alpha - 1}} \right]^{\gamma/\alpha - 1} \leq \left[ \sum_{x} \left( \frac{P^{\alpha}}{Q^{\alpha - \gamma}} \right) \right]^{1/\alpha - 1} \left[ \sum_{x} \frac{Q^{\alpha - \gamma}}{Q^{\alpha - 1}} \right]^{\gamma/\alpha - 1} = \left[ d_{\alpha}(P \parallel Q) \right]^{\alpha - 1} \left[ d_{\alpha}(P \parallel Q) \right]^{\alpha - 1}.
$$

(\text{Hölder’s inequality})

Lemma 3 gives a family of multiplicative triangle inequalities for the exponentiated Rényi divergence, where the parameter $\gamma$ trades off the two Rényi divergences on the right-hand side, and one can choose $\gamma$ to obtain desired inequalities.

Given above results, we can rewrite Corollary 4 of Hoffman et al. [2018] in terms of domain-specific Rényi divergences. For readability, we present a simplified version first, and give the full result (Corollary 2) at the end of this section.

Corollary 1. For any $\delta > 0$, there exist $\eta > 0$ and $z \in \Delta$, such that the following inequality holds for any $\alpha > 1$ and arbitrary target distribution $D_T$:

$$
\mathcal{L}(D_T, \hat{D}) \leq (\hat{\epsilon} + \delta)^{\alpha - 1} M^\frac{\alpha}{\alpha - 1} \left[ d_{2\alpha}(D_T \parallel \hat{D}) \right]^{\frac{2\alpha - 1}{2\alpha}} \left[ \max_{k \in [p]} d_{2\alpha - 1}(D_{k} \parallel \hat{D}_{k}) \right]^{\frac{\alpha - 1}{\alpha - 1}},
$$

where $\hat{\epsilon} = \max_{k \in [p]} \left[ \epsilon d_{\alpha}(\hat{D}_{k} \parallel D_{k}) \right]^{\frac{\alpha - 1}{\alpha}} M^{\frac{\alpha}{\alpha - 1}}$.

Corollary 1 replaces the less straightforward term $d_{\alpha}(D_T \parallel \hat{D})$ in Corollary 4 of Hoffman et al. [2018] with $d_{2\alpha}(D_T \parallel \hat{D})$ and domain-specific density estimation accuracies $d_{\alpha}(D_{k} \parallel \hat{D}_{k})$. In the special case where the target domain $D_T$ is an unknown mixture of source domains, $D_T \in D$, and thus $d_{2\alpha}(D_T \parallel D) = 1$, which gives Theorem 1.

Corollary 1 states that, there exists a solution $\hat{D}$ based on estimated distributions that is $\hat{\epsilon}$-accurate on arbitrary target distribution $D_T$, as long as $D_T$ is close to the family of mixtures $D$, and the estimated distributions $\hat{D}_{k}$ are close to the true ones $D_{k}$, where closeness is measured via the Rényi divergence. The quality of density estimation yields a multiplicative effect on the learning guarantee of $\hat{D}$. To better understand the result, we consider a few examples of $\alpha$: when $\alpha = +\infty$,

$$
\mathcal{L}(D_T, \hat{D}) \leq \epsilon \left( \max_{k \in [p]} d_{\infty}(D_{k} \parallel D_{k}) \right) + \delta \left( \max_{k \in [p]} d_{\infty}(D_{k} \parallel D_{k}) \right) \left( \max_{k \in [p]} d_{\infty}(D_{k} \parallel D_{k}) \right);
$$

and when $\alpha = 2$,

$$
\mathcal{L}(D_T, \hat{D}) \leq \left[ \max_{k \in [p]} \left( \epsilon M d_{2}(D_{k} \parallel D_{k}) \right)^{\frac{1}{2}} + \delta \right] M^{\frac{1}{2}} \left[ \max_{k \in [p]} d_{2}(D_{k} \parallel D_{k}) \right]^{\frac{1}{2}} \left( \max_{k \in [p]} d_{2}(D_{k} \parallel D_{k}) \right)^{\frac{1}{2}}.
$$

Finally, since $d_{\alpha} \geq 1$, we can slightly relax the upper bound: for any $\alpha > 1$,

$$
\mathcal{L}(D_T, \hat{D}) \leq (\hat{\epsilon} + \delta)^{\frac{\alpha - 1}{\alpha}} M^{\frac{\alpha}{\alpha - 1}} \left[ d_{2\alpha}(D_T \parallel \hat{D}) \right]^{\frac{\alpha - 1}{\alpha}} \left[ \max_{k \in [p]} d_{2\alpha - 1}(D_{k} \parallel \hat{D}_{k}) \right].
$$

Corollary 2. For any $\delta > 0$, there exist $\eta > 0$ and $z \in \Delta$, such that the following inequality holds for any $\alpha > 1$, $\beta > 0$, $0 < \gamma < 1$, and arbitrary target distribution $D_T$:

$$
\mathcal{L}(D_T, \hat{D}) \leq (\hat{\epsilon} + \delta)^{\frac{\alpha - 1}{\alpha}} M^{\frac{\alpha}{\alpha - 1}} \left[ d_{2\alpha}(D_T \parallel \hat{D}) \right]^{\frac{\alpha - 1}{\alpha}} \left[ \max_{k \in [p]} d_{2\alpha - 1}(D_{k} \parallel \hat{D}_{k}) \right],
$$

where $\hat{\epsilon} = \max_{k \in [p]} \left[ \epsilon d_{\alpha}(\hat{D}_{k} \parallel D_{k}) \right]^{\frac{\alpha - 1}{\alpha}} M^{\frac{\alpha}{\alpha - 1}}$.

Proof. By Lemma 2, $d_{\alpha}(D \parallel \hat{D})$ is quasi-convex in $(D, \hat{D})$, thus for any $\lambda \in \Delta$,

$$
d_{\alpha}(\hat{D}_{\lambda} \parallel D_{\lambda}) = \exp\{D_{\alpha}(\hat{D}_{\lambda} \parallel D_{\lambda})\} \leq \exp\left\{ \max_{k \in [p]} D_{\alpha}(\hat{D}_{k} \parallel D_{k}) \right\} = \max_{k \in [p]} d_{\alpha}(\hat{D}_{k} \parallel D_{k}).
$$
By Lemma 3, for any $\lambda \in \Delta$,
\[
\left[ d_\alpha(D_T \mid \hat{D}_\lambda) \right]^{\alpha-1} \leq \left[ d_\beta(D_T \mid \hat{D}_\lambda) \right]^{\alpha-\gamma} \left[ d_\gamma(D_T \mid \hat{D}_\lambda) \right]^{\alpha-1} \\
\leq \left[ d_\beta(D_T \mid \hat{D}_\lambda) \right]^{\alpha-\gamma} \left[ \max_{k \in [p]} d_\gamma(D_k \mid \hat{D}_\lambda) \right]^{\alpha-1}.
\]

From the proof of Theorem 1, for any $\lambda \in \Delta$,
\[
\mathcal{L}(D_T, \hat{h}_\lambda) \leq \left[ (\tilde{\alpha} + \delta) d_\beta(D_T \mid \hat{D}_\lambda) \right] \frac{\beta-1}{\beta} M^\frac{\beta}{\beta-1} \\
= (\tilde{\alpha} + \delta) \frac{\beta-1}{\beta} M^\frac{\beta}{\beta-1} \left[ d_\beta(D_T \mid \hat{D}_\lambda) \right]^{\beta-1} \\
\leq (\tilde{\alpha} + \delta) \frac{\beta-1}{\beta} M^\frac{\beta}{\beta-1} \left[ \max_{k \in [p]} d_\gamma(D_k \mid \hat{D}_\lambda) \right]^{\frac{\beta-1}{\beta}}.
\]

where $\tilde{\alpha} = \max_{k \in [p]} \left[ \epsilon d_\alpha(D_k \mid \hat{D}_k) \right]^{\frac{\beta-1}{\beta}} M^\frac{\beta}{\beta-1}$. Taking the infimum of $d_\beta(D_T \mid \hat{D}_\lambda)$ over all $D_\lambda \in \mathcal{D}$ completes the proof.

Corollary 2 uses Rényi divergences with various parameters ($\alpha, \beta, \gamma$). To better understand the result, we look at some explicit examples:

1. When $\gamma = \frac{1}{2}$,
\[
\mathcal{L}(D_T, \hat{h}_\lambda) \leq (\tilde{\alpha} + \delta) \frac{\beta-1}{\beta} M^\frac{\beta}{\beta-1} \left[ d_\beta(D_T \mid \hat{D}_\lambda) \right]^{\beta-1} \left[ \max_{k \in [p]} d_\gamma(D_k \mid \hat{D}_\lambda) \right]^{\frac{\beta-1}{\beta}}.
\]

Let $\alpha = \beta$ and we retrieve the result of Corollary 1.

2. Let $\gamma \to 0$. Since the exponentiated Rényi divergence $d_\alpha(\mathcal{P} \mid \mathcal{Q})$ is continuous in $\alpha$, we have
\[
\mathcal{L}(D_T, \hat{h}_\lambda) \leq (\tilde{\alpha} + \delta) \frac{\beta-1}{\beta} M^\frac{\beta}{\beta-1} \left[ d_\alpha(D_T \mid \hat{D}_\lambda) \right]^{\beta-1} \left[ \max_{k \in [p]} d_\gamma(D_k \mid \hat{D}_\lambda) \right]^{\frac{\beta-1}{\beta}}.
\]

Furthermore, when $\beta = 2$,
\[
\mathcal{L}(D_T, \hat{h}_\lambda) \leq \left[ d_\alpha(D_T \mid \hat{D}_\lambda) \right]^{\frac{\beta}{2}} \left[ (\tilde{\alpha} + \delta) M \max_{k \in [p]} d_\gamma(D_k \mid \hat{D}_\lambda) \right]^{\frac{\beta-1}{\beta}}.
\]

3. Similarly, let $\gamma \to 1$, we have
\[
\mathcal{L}(D_T, \hat{h}_\lambda) \leq (\tilde{\alpha} + \delta) \frac{\beta-1}{\beta} M^\frac{\beta}{\beta-1} \left[ d_\beta(D_T \mid \hat{D}_\lambda) \right]^{\beta-1} \left[ \max_{k \in [p]} d_\gamma(D_k \mid \hat{D}_\lambda) \right]^{\frac{\beta-1}{\beta}}.
\]

Furthermore, when $\beta = 2$,
\[
\mathcal{L}(D_T, \hat{h}_\lambda) \leq \left[ (\tilde{\alpha} + \delta) M d_2(D_T \mid \hat{D}_\lambda) \max_{k \in [p]} d_\gamma(D_k \mid \hat{D}_\lambda) \right]^{\frac{\beta}{2}}.
\]

From the examples above, we see that $\gamma$ trades off between $d_\alpha(D_T \mid \hat{D}_\lambda)$, the divergence between the target distribution $D_T$ and the family of mixtures $\mathcal{D}$, and $\max_{k \in [p]} d_\alpha(D_k \mid \hat{D}_k)$, the maximum divergence between the true and the estimated domain-specific densities, by tuning the parameters $\alpha$ and $\alpha'$ that define these divergences.

D Convergence results for kernel density estimation

In this section, we show that the true distribution $\mathcal{D}$ can be closely approximated via kernel density estimation (KDE), where the quality of approximation depends on the choice of the kernel function $K_\sigma(\cdot, \cdot)$. More precisely, we present two convergence results for the $\alpha$-Rényi divergence between the true and the estimated distribution: the first result (Theorem 8) is in terms of the expected pointwise divergence, $\mathbb{E}_{x \sim D} [d_\alpha(K_\sigma(\cdot, x) \mid \mathcal{D})]$, and the second result (Theorem 9) is in terms of a single divergence term, $d_\alpha([\mathbb{E}_{x \sim D} K_\sigma(\cdot, x)] \mid \mathcal{D})$. For certain values of Rényi parameter $\alpha$, $d_\alpha(\mathcal{P} \mid \mathcal{Q})$ is convex in $\mathcal{P}$, and thus by Jensen’s inequality the second result can be more favorable than the first one.

Kernel density estimation (KDE) is a widely-used nonparametric method for estimating densities. Let $K_\sigma(\cdot, \cdot) \geq 0$ be a normalized kernel function that satisfies $\int_{x \in \mathcal{X}} K_\sigma(x, x') dx = 1$ for all $x' \in \mathcal{X}$,
and $\sigma$ is the bandwidth parameter. A well-known kernel function is the Gaussian kernel: $K_\sigma(x, x') = \left(\frac{1}{\sqrt{2\pi} \sigma}\right)^d \exp\left\{-\frac{||x-x'||^2}{2\sigma^2}\right\}$, where $d$ is the dimension of the input space $\mathcal{X} \subseteq \mathbb{R}^d$. Let $S_n = \{x_1, \ldots, x_n\}$ be a sample of size $n$ drawn from the true distribution $\mathcal{D}$. Then, the kernel density estimation based on the sample $S_n$ is defined as $\hat{D}_{S_n}() = \frac{1}{n} \sum_{i=1}^{n} K_\sigma(., x_i)$. With a slight abuse of notation, we denote $\mathcal{D}_{S_{\infty}}(\cdot) = \mathbb{E}_{\mathcal{X}, \mathcal{D}} K_\sigma(., x)$ the kernel density estimation based on the entire population.

We introduce the notion of “Rényi stability” of kernel density estimation: given two samples $S_n$ and $S'_n$ that only differ by one point: $S_n = S_{n-1} \cup \{x_n\}$, $S'_n = S_{n-1} \cup \{x'_n\}$, where $x_n \neq x'_n$, what is the Rényi divergence between $\mathcal{D}_{S_n}$ and $\mathcal{D}_{S'_n}$?

**Theorem 7.** For any $\alpha \in [1, 2] \cup \{+\infty\}$,

$$d_\alpha(\mathcal{D}_{S_n} \parallel \mathcal{D}_{S'_n}) \leq \left(1 - \frac{1}{n}\right)^2 + \frac{(2n-1)}{n^2} \max_{x, x' \in S_n \cup S'_n} d_\alpha\left(K_\sigma(., x_i) \parallel K_\sigma(., x_j)\right).$$

$$d_\alpha(\mathcal{D}_{S'_n} \parallel \mathcal{D}_{S_n}) \leq \left(1 - \frac{1}{n}\right)^2 + \frac{(2n-1)}{n^2} \max_{x, x' \in S'_n \cup S_n} d_\alpha\left(K_\sigma(., x_i) \parallel K_\sigma(., x_j)\right).$$

**Proof.** First, observe that $\mathcal{D}_{S_{n}}$ (or $\mathcal{D}_{S'_{n}}$) is a convex combination of $\mathcal{D}_{S_{n-1}}$ and $K_\sigma(., x_n)$ (or $K_\sigma(., x'_n)$):

$$\mathcal{D}_{S_n}(x) = \left(1 - \frac{1}{n}\right) \mathcal{D}_{S_{n-1}}(x) + \frac{1}{n} K_\sigma(x, x_n),$$

$$\mathcal{D}_{S'_n}(x) = \left(1 - \frac{1}{n}\right) \mathcal{D}_{S_{n-1}}(x) + \frac{1}{n} K_\sigma(x, x'_n).$$

By Lemma 2, $d_\alpha(\mathcal{P} \parallel \Omega)$ is convex in $\Omega$ for $\alpha \geq 0$. Thus, $d_\alpha(\mathcal{P} \parallel \Omega)$ is also convex in $\Omega$: for some constant $\lambda \in [0, 1]$,

$$d_\alpha(\mathcal{P} \parallel \lambda\Omega + (1 - \lambda)\Omega') \leq \exp\{\lambda d_\alpha(\mathcal{P} \parallel \Omega) + (1 - \lambda)d_\alpha(\mathcal{P} \parallel \Omega')\} \quad (d_\alpha(\mathcal{P} \parallel \Omega) \text{ is convex in } \Omega)$$

$$\lambda \exp\{d_\alpha(\mathcal{P} \parallel \Omega)\} + (1 - \lambda) \exp\{d_\alpha(\mathcal{P} \parallel \Omega')\} \quad (e^x \text{ is convex})$$

$$= \lambda d_\alpha(\mathcal{P} \parallel \Omega) + (1 - \lambda) d_\alpha(\mathcal{P} \parallel \Omega').$$

Furthermore, we can show that $d_\alpha(\mathcal{P} \parallel \Omega)$ is convex in $\mathcal{P}$ for $1 \leq \alpha \leq 2$ as well as for $\alpha = +\infty$. We first prove for $\alpha \in [1, 2]$. Fix a constant $\lambda \in [0, 1]$,

$$\left[d_\alpha(\lambda\mathcal{P} + (1 - \lambda)\mathcal{P}' \parallel \Omega)\right]^{\alpha - 1} = \sum_x \frac{(\lambda \mathcal{P}(x) + (1 - \lambda)\mathcal{P}'(x))^\alpha}{\Omega^{-\alpha}(x)}$$

$$\leq \sum_x \frac{\lambda \mathcal{P}(x) + (1 - \lambda)\mathcal{P}'(x)}{\Omega^{-\alpha}(x)} \quad (x^\alpha \text{ is convex for } \alpha \geq 1)$$

$$= \lambda \sum_x \frac{\mathcal{P}(x)}{\Omega^{-\alpha}(x)} + (1 - \lambda) \sum_x \frac{\mathcal{P}'(x)}{\Omega^{-\alpha}(x)}$$

$$= \lambda \left[d_\alpha(\mathcal{P} \parallel \Omega)\right]^{\alpha - 1} + (1 - \lambda) \left[d_\alpha(\mathcal{P}' \parallel \Omega)\right]^{\alpha - 1}.$$

Since $x^{\alpha - 1}$ is convex for $1 \leq \alpha \leq 2$, we have

$$d_\alpha(\lambda\mathcal{P} + (1 - \lambda)\mathcal{P}' \parallel \Omega) \leq \left(\lambda \left[d_\alpha(\mathcal{P} \parallel \Omega)\right]^{\alpha - 1} + (1 - \lambda) \left[d_\alpha(\mathcal{P}' \parallel \Omega)\right]^{\alpha - 1}\right)^{\frac{1}{\alpha}}$$

$$\leq \lambda d_\alpha(\mathcal{P} \parallel \Omega) + (1 - \lambda) d_\alpha(\mathcal{P}' \parallel \Omega).$$

Next we prove the convexity for $\alpha = +\infty$:

$$d_\infty(\lambda\mathcal{P} + (1 - \lambda)\mathcal{P}' \parallel \Omega) = \max_{x \in \mathcal{X}} \frac{\lambda \mathcal{P}(x) + (1 - \lambda)\mathcal{P}'(x)}{\mathcal{Q}(x)} = \max_{x \in \mathcal{X}} \frac{\lambda \mathcal{P}(x)}{\mathcal{Q}(x)} + (1 - \lambda) \frac{\mathcal{P}'(x)}{\mathcal{Q}(x)}$$

$$\leq \lambda \max_{x \in \mathcal{X}} \frac{\mathcal{P}(x)}{\mathcal{Q}(x)} + (1 - \lambda) \max_{x \in \mathcal{X}} \frac{\mathcal{P}'(x)}{\mathcal{Q}(x)} \quad (\text{max is convex})$$

$$= \lambda d_\infty(\mathcal{P} \parallel \Omega) + (1 - \lambda) d_\infty(\mathcal{P}' \parallel \Omega).$$
Thus, for $\alpha \in [1, 2] \cup \{+\infty\}$, $d_\alpha(\mathcal{P} \parallel \mathcal{Q})$ is convex in $\mathcal{P}$ and $\mathcal{Q}$ separately, which implies,

$$
d_\alpha(\mathcal{D}_{S_n} \parallel \mathcal{D}_{S'_n}) \leq \left(1 - \frac{1}{n}\right)^2 d_\alpha(\mathcal{D}_{S_{n-1}} \parallel \mathcal{D}_{S_{n-1}}) + \left(1 - \frac{1}{n}\right) \frac{1}{n} d_\alpha(\mathcal{D}_{S_{n-1}} \parallel K_\sigma(\cdot, x'_n)) + \left(1 - \frac{1}{n}\right) \frac{1}{n} d_\alpha(K_\sigma(\cdot, x_n) \parallel \mathcal{D}_{S_{n-1}}) + \frac{1}{n} d_\alpha(K_\sigma(\cdot, x_n) \parallel K_\sigma(\cdot, x'_n)) \leq \left(1 - \frac{1}{n}\right)^2 + \frac{1}{n^2} \left[\sum_{i=1}^{n-1} d_\alpha(K_\sigma(\cdot, x_i) \parallel K_\sigma(\cdot, x'_i))\right] + \frac{1}{n^2} \left[\sum_{i=1}^{n-1} d_\alpha(K_\sigma(\cdot, x_i) \parallel K_\sigma(\cdot, x'_i))\right] + \frac{1}{n^2} d_\alpha(K_\sigma(\cdot, x_n) \parallel K_\sigma(\cdot, x'_n)) \leq \left(1 - \frac{1}{n}\right)^2 + \frac{(2n-1)}{n^2} \left[\max_{x_i, x_j \in \mathcal{S}_n} d_\alpha(K_\sigma(\cdot, x_i) \parallel K_\sigma(\cdot, x_j))\right].$$

The upper bound for $d_\alpha(\mathcal{D}_{S'_n} \parallel \mathcal{D}_{S_n})$ holds by a similar proof.

When $\alpha = +\infty$, Theorem 7 implies that

$$
d_\infty(\mathcal{D}_{S_n} \parallel \mathcal{D}_{S'_n}) \leq \left(1 - \frac{1}{n}\right)^2 + \frac{(2n-1)}{n^2} \left[\max_{x_i, x_j \in \mathcal{K}} d_\infty(K_\sigma(\cdot, x_i) \parallel K_\sigma(\cdot, x_j))\right].
$$

Suppose the kernel function is bounded from above and below, that is, there exists $0 < m_K < M_K$ such that $m_K \leq K_\sigma(\cdot, \cdot) \leq M_K$. Then, for any $S_n, S'_n$ that differ by one point, $d_\infty(\mathcal{D}_{S_n} \parallel \mathcal{D}_{S'_n}) \leq 1 + 2M_K/n = 1 + O\left(n^{-1/2}\right)$, and thus the two distributions are close under the Rényi divergence when sample size $n$ is large.

Given the “Rényi stability”, we can now derive convergence results for the divergence between $\mathcal{D}_{S_n}$ and $\mathcal{D}$. Consider two samples $S_n$ and $S'_n$ that only differ by one point: $S_n = S_{n-1} \cup \{x_n\}$, $S'_n = S_{n-1} \cup \{x'_n\}$, where $x_n \neq x'_n$. Assume that, for all such pairs of samples $S_n, S'_n$, $d_\infty(\mathcal{D}_{S_n} \parallel \mathcal{D}_{S'_n}) \leq M_\infty$ for some positive constant $M_\infty$. The following result depends on $M_\infty$ and the choice of the kernel function.

**Theorem 8.** For any $\delta > 0$, with probability at least $1 - \delta$, each of the following two inequalities holds:

$$
d_\alpha(\mathcal{D}_{S_n} \parallel \mathcal{D}) \leq \mathbb{E}_{x \sim \mathcal{D}} \left[d_\alpha(K_\sigma(\cdot, x) \parallel \mathcal{D})\right] M_\infty \sqrt{n \log \frac{1}{\delta}}, \quad \text{for all } 1 \leq \alpha \leq 2,
$$

$$
d_\alpha(\mathcal{D} \parallel \mathcal{D}_{S_n}) \leq \mathbb{E}_{x \sim \mathcal{D}} \left[d_\alpha(\mathcal{D} \parallel K_\sigma(\cdot, x))\right] M_\infty \sqrt{n \log \frac{1}{\delta}}, \quad \text{for all } \alpha \geq 1.
$$

**Proof.** Consider two samples $S_n$ and $S'_n$ that only differ by one point. We prove the first inequality for $1 \leq \alpha \leq 2$. Given a sample $S$, define $\Phi(S) = \log \left[d_\alpha(\mathcal{D}_S \parallel \mathcal{D})\right]$. Let $\gamma \to 0$ in Lemma 3,

$$
\alpha - 1 \leq d_\alpha(\mathcal{P} \parallel \mathcal{Q})\right) \alpha - 1 \Rightarrow d_\alpha(\mathcal{P} \parallel \mathcal{Q}) \leq \left[d_\alpha(\mathcal{P} \parallel \mathcal{Q})\right]^{\alpha - 1}.
$$

Thus,

$$\Phi(S_n) - \Phi(S'_n) = \log \left[d_\alpha(\mathcal{D}_{S_n} \parallel \mathcal{D})\right] \leq \frac{\alpha}{\alpha - 1} \log \left[d_\alpha(\mathcal{D}_{S_n} \parallel \mathcal{D})\right].$$

By assumption, $d_\infty(\mathcal{D}_{S_n} \parallel \mathcal{D}_{S'_n})$ is upper bounded by some positive constant $M_\infty$. Thus, by McDiarmid’s inequality,

$$\mathbb{P}(\Phi(S_n) - \mathbb{E}[\Phi(S_n)] \geq \epsilon) \leq \exp\left(-\frac{2\epsilon^2}{n(\alpha^{-1} \log M_\infty)}\right),$$

which implies that with probability at least $1 - \delta$ over the drawn of $S_n$,

$$\Phi(S_n) \leq \mathbb{E}[\Phi(S_n)] + \left(\frac{\alpha}{\alpha - 1} \log M_\infty\right) \sqrt{\frac{n \log \frac{1}{\delta}}{2}}.$$

Furthermore, since $\log$ is concave, and $d_\alpha(\mathcal{P} \parallel \mathcal{Q})$ is convex in $\mathcal{P}$ for $1 \leq \alpha \leq 2$, we have

$$\mathbb{E}[\Phi(S_n)] = \mathbb{E}_{S_n \sim \mathcal{D}^n} \log \left[d_\alpha(\mathcal{D}_{S_n} \parallel \mathcal{D})\right] \leq \mathbb{E}_{S_n \sim \mathcal{D}^n} \left[d_\alpha(\mathcal{D}_{S_n} \parallel \mathcal{D})\right] \leq \log \left\{ \mathbb{E}_{S_n \sim \mathcal{D}^n} \left[\frac{1}{n} \sum_{i=1}^{n} d_\alpha(K_\sigma(\cdot, x_i) \parallel \mathcal{D})\right]\right\} \leq \log \left\{ \mathbb{E}_{x \sim \mathcal{D}} \left[d_\alpha(K_\sigma(\cdot, x) \parallel \mathcal{D})\right]\right\} = \log \left\{ \mathbb{E}_{x \sim \mathcal{D}} \left[d_\alpha(K_\sigma(\cdot, x) \parallel \mathcal{D})\right]\right\}.$$
Therefore, with probability at least $1 - \delta$ over the draw of $S_n$, for all $1 \leq \alpha \leq 2$,
\[
\Phi(S_n) \leq \log \left\{ \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( K_\alpha(\cdot, x) \right) \mathcal{D} \right] \right\} + \left( \frac{\alpha}{\alpha - 1} \log M_\alpha \right) \sqrt{\frac{n \log \frac{1}{\delta}}{2}}
\]
\[
\Rightarrow d_\alpha \left( \hat{\mathcal{D}}_{S_n} \mathcal{D} \right) \leq \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( K_\alpha(\cdot, x) \right) \mathcal{D} \right] \exp \left\{ \left( \frac{\alpha}{\alpha - 1} \log M_\alpha \right) \sqrt{\frac{n \log \frac{1}{\delta}}{2}} \right\}
\]
\[
= \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( K_\alpha(\cdot, x) \right) \mathcal{D} \right] M_n^{\frac{n \log \frac{1}{\delta}}{2}}.
\]

Similarly, if we define $\Phi(S) = \log \left[ d_\alpha \left( \mathcal{D} \| \hat{\mathcal{D}}_S \right) \right]$, then for $\alpha \geq 1$,
\[
\Phi(S_n) - \Phi(S_n^*) \leq \log \left[ d_\alpha \left( \hat{\mathcal{D}}_{S_n} \| \hat{\mathcal{D}}_{S_n^*} \right) \right] \leq \log \left[ d_\alpha \left( \hat{\mathcal{D}}_{S_n} \| \hat{\mathcal{D}}_{S_n^*} \right) \right],
\]
where the last inequality follows from setting $\gamma \to 1$ in Lemma 3:
\[
\left[ d_\alpha \left( \mathcal{P} \mathcal{D} \right) \right]^{\alpha - 1} \leq \left[ d_\alpha \left( \mathcal{P} \mathcal{D} \right) \right]^{\alpha - 1} \left[ d_\alpha \left( \mathcal{R} \mathcal{O} \right) \right]^{\alpha - 1} \Rightarrow d_\alpha \left( \mathcal{P} \mathcal{D} \right) \leq d_\alpha \left( \mathcal{R} \mathcal{O} \right).
\]
Furthermore, since $\log$ is concave, and $d_\alpha \left( \mathcal{P} \mathcal{Q} \right)$ is convex in $\mathcal{Q}$ for any $\alpha \geq 0$,
\[
\mathbb{E}(\Phi(S_n)) = \mathbb{E}_{S_n \sim \mathcal{D}^n} \log \left[ d_\alpha \left( \mathcal{D} \| \hat{\mathcal{D}}_{S_n} \right) \right] \leq \log \left\{ \mathbb{E}_{S_n \sim \mathcal{D}^n} \left[ d_\alpha \left( \mathcal{D} \| \hat{\mathcal{D}}_{S_n} \right) \right] \right\}
\]
\[
\leq \log \left\{ \mathbb{E}_{S_n \sim \mathcal{D}^n} \left[ \frac{1}{n} \sum_{i=1}^{n} d_\alpha \left( \mathcal{D} \| K_\alpha(\cdot, x_i) \right) \right] \right\} = \log \left\{ \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( \mathcal{D} \| K_\alpha(\cdot, x) \right) \right] \right\}.
\]
Thus, by McDiarmid’s inequality again, with probability at least $1 - \delta$ over the draw of $S_n$,
\[
d_\alpha \left( \mathcal{D} \| \hat{\mathcal{D}}_{S_n} \right) \leq \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( \mathcal{D} \| K_\alpha(\cdot, x) \right) \right] \exp \left\{ \left( \log M_\alpha \right) \sqrt{\frac{n \log \frac{1}{\delta}}{2}} \right\}
\]
\[
= \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( \mathcal{D} \| K_\alpha(\cdot, x) \right) \right] M_n^{\frac{n \log \frac{1}{\delta}}{2}}.
\]

\[\square\]

Theorem 8 shows that the Rényi divergence between $\hat{\mathcal{D}}_{S_n}$ and $\mathcal{D}$ is upper bounded by the product of two terms: the first term is the expected pointwise divergence, or more precisely, the expected Rényi divergence between the kernel function centered at $x$, $K_\alpha(\cdot, x)$, and the true distribution $\mathcal{D}$, with the expectation taken over $x \sim \mathcal{D}$. Thus, the first term is purely determined by the choice of the kernel function $K_\alpha(\cdot, \cdot)$. The second term is a polynomial function of $M_n^\alpha$. As shown in the next Theorem 7, we have $M_n = 1 + O(\frac{1}{n})$ under mild conditions, which implies $M_n^\alpha \to 1$ as $n$ increases, and thus the second term converges to 1. Therefore, as the sample size $n$ goes to infinity, we have
\[
d_\alpha \left( \hat{\mathcal{D}}_{S_n} \| \mathcal{D} \right) \leq \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( K_\alpha(\cdot, x) \| \mathcal{D} \right) \right] \quad \text{for all } 1 \leq \alpha \leq 2, \quad (9)
\]
\[
d_\alpha \left( \mathcal{D} \| \hat{\mathcal{D}}_{S_n} \right) \leq \mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( \mathcal{D} \| K_\alpha(\cdot, x) \right) \right] \quad \text{for all } \alpha \geq 1. \quad (10)
\]
Thus, the kernel density estimations will be accurate provided that the expected pointwise Rényi divergence is small with a properly chosen kernel function $K_\alpha(\cdot, \cdot)$.

Instead of using the expected pointwise Rényi divergence, $\mathbb{E}_{x \sim \mathcal{D}} \left[ d_\alpha \left( K_\alpha(\cdot, x) \| \mathcal{D} \right) \right]$, we can also derive an upper bound in terms of a single divergence term, $d_\alpha \left( S_{n} \mathcal{D} \right)$. To do so, we first decompose $d_\alpha \left( \hat{\mathcal{D}}_{S_n} \| \mathcal{D} \right)$ into $d_\alpha \left( \hat{\mathcal{D}}_{S_n} \| D_{S_n} \right)$ and $d_\alpha \left( S_{n} \| \mathcal{D} \right)$. This decomposition is motivated by the classic statistical learning theory, where one can decompose excess risk into estimation error and approximation error, and analyze the two errors separately. We can proceed in a similar way here: instead of directly studying the divergence between $\hat{\mathcal{D}}_{S_n}$ and $\mathcal{D}$ (equivalent to the “excess risk”), we can decompose the divergence into two terms, the divergence between $\hat{\mathcal{D}}_{S_n}$ and $\mathcal{D}_{S_n}$ (the “estimation error”), and the divergence between $\mathcal{D}_{S_n}$ and $\mathcal{D}$ (the “approximation error”).

**Lemma 4.** For any $\alpha \geq 1$,
\[
d_\alpha \left( \hat{\mathcal{D}}_{S_n} \| \mathcal{D} \right) \leq d_\alpha \left( \hat{\mathcal{D}}_{S_n} \| S_{n} \| \mathcal{D}_{S_n} \right) \leq d_\alpha \left( \mathcal{D} \| D_{S_n} \right) \quad \text{and} \quad d_\alpha \left( \mathcal{D} \| \hat{\mathcal{D}}_{S_n} \right) \leq d_\alpha \left( \mathcal{D} \| S_{n} \| \mathcal{D}_{S_n} \right) d_\alpha \left( \mathcal{D} \| \mathcal{D}_{S_n} \right).
\]

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Lemma 4 is a straightforward result from the generalized “triangle inequality” of Rényi divergence (Lemma 3). Given Lemma 4, we can show that the “estimation error” $d_{\alpha}(\widehat{D}_{S_n} \parallel D)$ converges to 1 as the sample size $n$ increases, and thus the divergence between $\widehat{D}_{S_n}$ and $D$ is essentially upper bounded by the “approximation error” $d_{\alpha}(D \parallel \widehat{D}_{S_n})$, which can be more favorable than the expected pointwise divergence in Theorem 8. We need the following definition of the complexity of the set of functions $Q = \{ x \rightarrow 1_{K_\sigma(x,x') > t}, x' \in X, t \in \mathbb{R} \}$. Given a sample $S = \{ x_1, \ldots, x_n \}$, let $Q(S)$ denote the number of distinct dichotomies generated by $Q$ over $S$: $Q(S) = \text{Card}(\{ q(x_1), \ldots, q(x_n) : q \in Q \})$.

**Theorem 9.** For any $\delta > 0$, with probability at least $1 - \delta$, for any $\alpha \geq 1$, each of the following two inequalities holds,

$$d_{\alpha}(\widehat{D}_{S_n} \parallel D) \leq \left[ \frac{1}{1 - A(n, \delta)} \right]^{\alpha - 1} d_{\alpha}(D_{S_{\infty}} \parallel D),$$

$$d_{\alpha}(D \parallel \widehat{D}_{S_n}) \leq \left[ \frac{1}{1 - A(n, \delta)} \right] d_{\alpha}(D \parallel D_{S_{\infty}}),$$

where $A(n, \delta) = 2\sqrt{B(n, \delta)} \Gamma_0 \left( 2, 2\sqrt{B(n, \delta)} n \right), B(n, \delta) = 2 \log \mathbb{E}_{S \sim D_{\infty}} [Q(S)] + \log \frac{1}{\delta}$, and $\Gamma(2, \epsilon) = \min_{r \in (0, \epsilon)} \left( \frac{1}{2} (1 + \frac{r}{2}) \right)^{\frac{1}{2}} [1 + \log(1/s)]^{\frac{1}{2}}$.

To prove Theorem 9, we need the following relative deviation bound (Corollary 7) from Cortes et al. [2019a], which is adapted to the learning scenario of kernel density estimation.

**Lemma 5.** For any $x' \in X$, assume $\mathbb{E}_x [K_\sigma^2(x, x')] \leq \infty$. Then, for any $\delta > 0$, with probability at least $1 - \delta$, each of the following inequalities holds for all $x' \in X$,

$$D_{S_{\infty}}(x') \leq \widehat{D}_{S_n}(x') + \sqrt{\mathbb{E}_{x \sim D} [K_\sigma^2(x, x')]} A(n, \delta),$$

$$\widehat{D}_{S_n}(x') \leq D_{S_{\infty}}(x') + \sqrt{\mathbb{E}_x [K_\sigma^2(x, x')] A(n, \delta)},$$

where $A(n, \delta) = 2\sqrt{B(n, \delta)} \Gamma_0 \left( 2, 2\sqrt{B(n, \delta)} n \right), B(n, \delta) = 2 \log \mathbb{E}_{S \sim D_{\infty}} [Q(S)] + \log \frac{1}{\delta}$, and $\Gamma(2, \epsilon) = \min_{r \in (0, \epsilon)} \left( \frac{1}{2} (1 + \frac{r}{2}) \right)^{\frac{1}{2}} [1 + \log(1/s)]^{\frac{1}{2}}$.

**Proof.** (of Theorem 9) By inequality (13), with probability at least $1 - \delta$, for any $x' \in X$,

$$D_{S_{\infty}}(x') \leq \widehat{D}_{S_n}(x') + \sqrt{\mathbb{E}_{x \sim D} [K_\sigma^2(x, x')]} A(n, \delta) \leq \widehat{D}_{S_n}(x') + \sqrt{\mathbb{E}_x [K_\sigma^2(x, x')] A(n, \delta)} = \widehat{D}_{S_n}(x') + D_{S_{\infty}}(x') A(n, \delta),$$

where the last inequality follows from the fact that $\mathbb{E}[x^2] \leq (\mathbb{E}[x])^2$. Thus, with probability at least $1 - \delta$, for any $\alpha \geq 1$,

$$d_{\alpha}(D_{S_{\infty}} \parallel \widehat{D}_{S_n}) = \sum_{x' \in X} D_{S_{\infty}}(x') \left( \frac{\widehat{D}_{S_n}(x')}{D_{S_{\infty}}(x')} \right)^{\alpha - 1} \leq \sum_{x' \in X} D_{S_{\infty}}(x') \left( \frac{1}{1 - A(n, \delta)} \right)^{\alpha - 1} = \left( \frac{1}{1 - A(n, \delta)} \right)^{\alpha - 1} \cdot \frac{1}{1 - A(n, \delta)}.$$  

Similarly, by inequality (11), with probability at least $1 - \delta$, for any $x' \in X$,

$$\widehat{D}_{S_n}(x') \leq D_{S_{\infty}}(x') + \sqrt{\mathbb{E}_x [K_\sigma^2(x, x')] A(n, \delta)} \leq D_{S_{\infty}}(x') + \mathbb{E}_x [K_\sigma(x, x')] A(n, \delta) = D_{S_{\infty}}(x') + \widehat{D}_{S_n}(x') A(n, \delta).$$

Thus, with probability at least $1 - \delta$, $d_{\alpha}(D_{S_{\infty}} \parallel \widehat{D}_{S_n}) \leq \frac{1}{1 - A(n, \delta)}$. Finally, combine the above results with Lemma 4 gives the desired upper bounds.  

When $K_\sigma(\cdot, \cdot)$ is bounded, $\mathbb{E}_x [K_\sigma^2(x, x')] \leq \infty$. In addition, when $K_\sigma(\cdot, x)$ is a unimodal and symmetric function, such as the Gaussian kernel, then the pseudo-dimension of the hypothesis set $\{ K_\sigma(\cdot, x) : x \in \mathcal{X} \}$...
is finite, and thus $B(n, δ)$ is of the order $O(\frac{d \log \frac{1}{δ}}{n})$, where $d$ is the pseudo-dimension. This implies that $A(n, δ) = O(\frac{\log \frac{1}{δ}}{n})$. As $n$ increases, the upper bound of $d_\alpha(D_{S_n} || \mathcal{D})$ and $d_\alpha(D || \widehat{D}_{S_n})$ is eventually determined by $d_\alpha(D_{S_m} || \mathcal{D})$ and $d_\alpha(D || \widehat{D}_{S_m})$, respectively. Comparing inequalities (11) and (12) to inequalities (9) and (10) from Theorem 8, the new bounds are tighter for certain values of $\alpha$, since

\[
\begin{align*}
    d_\alpha(D_{S_m} || \mathcal{D}) &= d_\alpha \left( \mathbb{E}_{x \sim \mathcal{D}} [K_\sigma(\cdot, x)] || \mathcal{D} \right), \quad (1) \\
d_\alpha(D || \widehat{D}_{S_m}) &= d_\alpha \left( \mathbb{E}_{x \sim \widehat{D}} [K_\sigma(\cdot, x)] || \mathcal{D} \right), \quad (2)
\end{align*}
\]

where the inequalities follow from Jensen’s inequality and the fact that $d_\alpha(\mathcal{D} || \Omega)$ is convex in $\mathcal{D}$ for $1 \leq \alpha \leq 2$, and convex in $\Omega$ for all $\alpha \geq 0$.

### E Proofs

**Theorem 1.** There exist $\mathbf{z} \in \Delta$ such that the following inequality holds for any $\alpha > 1$ and arbitrary target mixture $D_T \in \mathcal{D}$:

\[
\mathcal{L}(D_T, \hat{h}_z) \leq \epsilon \left[ \frac{(\alpha - 1)}{\alpha} - \epsilon \left( \frac{1}{\alpha - 1} - \frac{1}{\alpha} \right) \right] M \frac{d_0}{\alpha} \left[ \max_{k \in [p]} d_\alpha(D_k || \widehat{D}_k) \right].
\]

**Proof.** By Corollary 1 in Appendix C, there exist $\mathbf{z} \in \Delta$ such that the following inequality holds for any $\alpha > 1$ and arbitrary target mixture $D_T \in \mathcal{D}$:

\[
\mathcal{L}(D_T, \hat{h}_z) \leq \epsilon \left[ \frac{(\alpha - 1)}{\alpha} - \epsilon \left( \frac{1}{\alpha - 1} - \frac{1}{\alpha} \right) \right] M \frac{d_0}{\alpha} \left[ \max_{k \in [p]} d_\alpha(D_k || \widehat{D}_k) \right].
\]

where $\hat{h}_z = \max_{k \in [p]} \left[ d_0(D_k || \widehat{D}_k) \right]$. Since $d_0 \geq 1$ for any $\alpha$, $\left[ d_\alpha(D_k || \widehat{D}_k) \right] \alpha^{-1} \leq d_\alpha(D_k || \widehat{D}_k)$.

The rest of the proof concludes the proof.

**Proposition 1.** For any parameter $\mathbf{z} \in \Delta$ and its corresponding $h_z$, there exists $\mathbf{z}' \in \Delta$ such that $g_{\mathbf{z}'} = h_z$, with $\mathbf{z}' = \mathbf{z} \frac{d_\alpha(D_k || \widehat{D}_k)}{\sum_{j=1}^{p} d_\alpha(D_k || \widehat{D}_k)}$.

**Proof.** By Bayes’ rule,

\[
d_k(x) = D(x | k) = \frac{D(x, k)}{D(x)} = \frac{D(k) D_k(x)}{\sum_{j=1}^{p} D(j) D_k(x)}
\]

First consider the regression model. Observe that,

\[
h_z(x) = \sum_{k=1}^{p} \frac{z_k D_k(x)}{z_n} h_k(x) = \sum_{k=1}^{p} \frac{z_k D_k(x)}{z_n} \frac{D_k(x)}{D(x)} \frac{D(x)}{D(x)} h_k(x)
\]

\[
= \sum_{k=1}^{p} \sum_{j=1}^{p} \frac{z_k D_k(x) D_j(x)}{z_n} \frac{D_k(x)}{D(x)} \frac{D(x)}{D(x)} h_k(x) = \sum_{k=1}^{p} \frac{z_k D_k(x) D_j(x)}{z_n} \frac{D_k(x)}{D(x)} \frac{D(x)}{D(x)} h_k(x) = g_{\mathbf{z}'}(x)
\]

The proof for probability model $h_z(x, y)$ is syntactically the same.

**Proposition 4.** The optimization problem

\[
\arg\min_{\hat{D}} \| \hat{D} - \mathbf{u} \|_2^2, \quad s.t. \quad \sum_{x \in \mathcal{X}} \hat{D}(x) \hat{h}_k(x) = \frac{1}{p}, \forall k \in [p], \quad \sum_{x \in \mathcal{X}} \hat{D}(x) = 1,
\]

admits a closed-form solution: $\hat{D} = \mathbf{u} - A(A^T A)^{-1}(A^T \mathbf{u} - \mathbf{1})$, where $A$ is an $np \times (p + 1)$ matrix with entries $A_{i,k} = p d_k(x_i)$ and $A_{i,p+1} = 1$ for $x_i \in \mathcal{X}, 1 \leq i \leq np$.

**Proof.** Given the notation, we can rewrite the optimization problem as

\[
\min_{x \in \mathbb{R}^{n+1}} (x - \mathbf{u})^T (x - \mathbf{u}), \quad s.t. \ A^T x = 1.
\]

Using the method of Lagrange multipliers, let $\lambda \in \mathbb{R}^{p+1}$ denote the vector of Lagrange multipliers, and the Lagrangian function is

\[
L(x, \lambda) = x^T x - 2u^T x - \lambda^T (A^T x - 1) + u^T u
\]
Taking derivative with respect to \( x \) and setting to 0 yields
\[
2x - 2u - A\lambda = 0 \Rightarrow x = u + \frac{A\lambda}{2}.
\]
Plugging into the constraints, we have
\[
A^T x = 1 \Rightarrow A^T (u + \frac{A\lambda}{2}) = 1 \Rightarrow \lambda = 2(A^T A)^{-1}(1 - A^T u)
\]
\[
\Rightarrow x = u + A(A^T A)^{-1}(1 - A^T u).
\]

**Proposition 2.** Let \( \ell \) be the squared loss. Then, for any \( k \in [p] \), \( \mathcal{L}(D_k, g_z) - \mathcal{L}(D_k, g_z) = u_k(z) - v_k(z) \), where \( u_k \) and \( v_k \) are convex functions defined for all \( z \) by
\[
u_k(z) = \sum_{(x,y) \in \mathcal{Z}} D_k(x,y)[y - g_z(x)]^2 - 2M \left( \sum_{x \in \mathcal{X}} D_k(x) \log d_z(x) \right),
\]
\[
v_k(z) = \sum_{(x,y) \in \mathcal{Z}} D_k(x,y)[y - g_z(x)]^2 - 2M \left( \sum_{x \in \mathcal{X}} D_k(x) \log d_z(x) \right).
\]

**Proof.** Denote by \( j_z(x) = \sum_{k=1}^p z_k d_k(x) h_k(x) \) and \( k_z(x) = d_z(x) \). By definition, \( g_z(x) = j_z(x)/k_z(x) \).

First, observe that \( (g_z(x) - y)^2 = (z - y)^2 - 2M \log d_z(x), \quad G_z(x) = -2M \log d_z(x). \)

The convexity holds since the Hessian matrix of \( F_z(x) \) and \( G_z(x) \) with respect to \( z \) are positive semidefinite:
\[
H_{F_z}(z) = \frac{2}{d_z(x)^2} \left[ h_{d_z}(x)h_{d_z}(x)^T + (M - (y - g_z(x))^2) D(x)D^T(x) \right],
\]
\[
H_{G_z}(z) = \frac{2M}{d_z(x)^2} D(x)D^T(x),
\]

where \( h_{d_z}(x) \) is a \( p \)-dimensional vector defined as \( [h_{d_z}]_k = d_k(h_k + y - 2g_z) \) for \( k \in [p] \), and \( D(x) = (d_1(x), \ldots, d_p(x))^T \). Using the fact that \( M \geq (y - g_z(x))^2 \), \( H_{F_z}(z) \) and \( H_{G_z}(z) \) are positive semidefinite matrices, and thus \( F_z \), \( G_z \) are convex functions of \( z \) for all \( (x,y) \in \mathcal{X} \times \mathcal{Y} \). Therefore, \( u_k(z) \) is a convex function of \( z \), since
\[
u_k(z) = \sum_{(x,y) \in \mathcal{Z}} D_k(x,y)[y - g_z(x)]^2 - 2M \log d_z(x) = \sum_{(x,y) \in \mathcal{Z}} D_k(x,y)F_z(x,y).
\]

Similarly, we can write the second term of \( v_k(z) \) as \( \sum_{x \in \mathcal{X}} D_k(x)G_z(x) \), which is convex. Using the notation previously defined, we can write the first term of \( v_k(z) \) as
\[
\sum_{(x,y) \in \mathcal{Z}} D_z(x,y) \left[ y - \frac{j_z(x)}{k_z(x)} \right]^2
\]
\[
= \sum_{(x,y) \in \mathcal{Z}} \left( pD(x)f(y|x) \right) d_z(x) \left[ y - \frac{j_z(x)}{k_z(x)} \right]^2
\]
\[
= \sum_{(x,y) \in \mathcal{Z}} \left( pD(x)f(y|x) \right) \left( \frac{j_z(x)^2}{k_z(x)} - 2yj_z(x) + y^2k_z(x) \right).
\]

The Hessian matrix of \( j_z(x)^2/k_z(x) \) with respect to \( z \) is
\[
\nabla^2 \left( \frac{j_z(x)^2}{k_z(x)} \right) = \frac{1}{k_z(x)} (h_D(x) - g_z(x)D(x)) (h_D(x) - g_z(x)D(x))^T
\]

where \( h_D(x) = (d_1(x), \ldots, d_p(x), d_1(x))^T \) and \( D(x) = (d_1(x), \ldots, d_p(x))^T \); Thus \( j_z(x)^2/k_z(x) \) is convex. \( -2yj_z(x) + y^2k_z(x) \) is an affine function of \( z \) and is therefore convex. Therefore the first term of \( v_k(z) \) is convex, which completes the proof.

**Proposition 3.** Let \( \ell \) be the cross-entropy loss. Then, for \( k \in [p] \), \( \mathcal{L}(D_k, g_z) - \mathcal{L}(D_k, g_z) = u_k(z) - v_k(z) \), where \( u_k \) and \( v_k \) are convex functions defined for all \( z \) by
\[
u_k(z) = \sum_{(x,y) \in \mathcal{Z}} -D_k(x,y) \log g_z(x,y) - D_k(x,y) \log d_z(x),
\]
\[
v_k(z) = \sum_{(x,y) \in \mathcal{Z}} -D_z(x,y) \log g_z(x,y) - D_k(x,y) \log d_z(x).
\]
Proof. Denote by $j_z(x, y) = \sum_{k=1}^{p} z_k d_k(x) h_k(x, y)$, $k_z(x) = d_z(x)$. By definition, $g_z(x, y) = j_z(x, y) / k_z(x)$. We can write
\[
\mathcal{L}(\mathcal{D}_k, g_z) - \mathcal{L}(\mathcal{D}_z, g_z) = \sum_{(x, y) \in Z} (\mathcal{D}_z(x, y) - \mathcal{D}_k(x, y)) \log \frac{j_z(x, y)}{k_z(x)}
\]
\[
= \sum_{(x, y) \in Z} p\mathcal{D}(f(y|x)(d_z(x) - d_k(x)) \log \frac{k_z(x)}{j_z(x, y)}
\]
\[
= \left[ \sum_{(x, y) \in Z} p\mathcal{D}(f(y|x)d_k(x)) \log \frac{k_z(x)}{j_z(x, y)} - p\mathcal{D}(f(y|x)d_k(x)) \log k_z(x) \right]
\]
\[
= \left[ \sum_{(x, y) \in Z} \mathcal{D}_z(x, y) \log j_z(x, y) \right] - \left[ \sum_{(x, y) \in Z} \mathcal{D}_z(x, y) \log \frac{k_z(x)}{j_z(x, y)} - \mathcal{D}_k(x, y) \log k_z(x) \right]
\]
\[
u_k(z) - \nu_k(z).
\]

$u_k$ is convex since $-\log j_z$ is convex as the composition of the convex function $-\log$ with an affine function. Similarly, $-\log k_z$ is convex, which shows that the second term in the expression of $v_k$ is a convex function. The first term of $v_k$ can be written in terms of the unnormalized relative entropy:
\[
\sum_{(x, y) \in Z} \mathcal{D}_z(x, y) \log \frac{k_z(x)}{j_z(x, y)} = \sum_{(x, y) \in Z} K_z(x, y) \log \frac{K_z(x, y)}{J_z(x, y)}
\]
\[
= B(K_z || J_z) + \sum_{(x, y) \in Z} (K_z - J_z)(x, y),
\]
where we denote by $J_z(x, y) = \sum_{k=1}^{p} z_k \mathcal{D}_k(x, y) h_k(x, y)$, and $K_z(x, y) = \mathcal{D}_z(x, y)$. It is easy to show that $J_z(x, y) / K_z(x, y) = j_z(x, y) / k_z(x) = g_z(x, y)$, since $\mathcal{D}_k(x, y)$’s share the same conditional probability $f(y|x)$. The rest of the proof follows from Hoffman et al. [2018]: The unnormalized relative entropy $B(\cdot || \cdot)$ is jointly convex, thus $B(K_z || J_z)$ is convex; $(K_z - J_z)$ is an affine function of $z$ and is therefore convex too. \hfill \Box

Given the DC decomposition from Proposition 2 and 3, one can cast the min-max optimization problem (7) into the following variational form of a DC-programming problem [Tao and An, 1997, 1998, Sriperumbudur and Lanckriet, 2012]:
\[
\min_{z \in \Delta, \gamma \in \mathbb{R}} \mathbb{E} \left[ (u_k(z) - v_k(z) \leq \gamma) \wedge \left( -z_k \leq 0 \right) \wedge \left( \sum_{k=1}^{p} z_k - 1 = 0 \right) \right], \forall k \in [p]. \tag{15}
\]
The DC-programming algorithm works by repeatedly solving the following convex optimization problem:
\[
z_{t+1} = \arg\min_{z \in \Delta, \gamma \in \mathbb{R}} \gamma
\]
\[
\text{s.t. } u_k(z) - v_k(z) - (z - z_t) \nabla v_k(z_t) \leq \gamma
\]
\[
n - z_k \leq 0 \text{, } \sum_{k=1}^{p} z_k - 1 = 0, \forall k \in [p],
\]
where $z_0 \in \Delta$ is an arbitrary starting value, and $(z_t)_t$ denotes the sequence of solutions. Then, $(z_t)_t$ is guaranteed to converge to a local minimum of Problem (7) [Sriperumbudur and Lanckriet, 2012].

Theorem 4. Let $\tilde{w}$ be the solution to problem (8), and $w^*$ be the solution under the true distribution:
\[
w^* = \arg\min_{w \in \mathbb{R}^N} \mathbb{E} \left[ \log p_w[k|x] \right].
\]

Then, for any $\delta > 0$, with probability at least $1 - \delta$,
\[
\mathbb{E} \left[ \log p_{\tilde{w}}[k|x] - \log p_{w^*}[k|x] \right] \leq \frac{2\sqrt{2}p^2}{\xi \sqrt{m}} (1 + \sqrt{\log 1/\delta}).
\]

Proof. From Theorem 2 of McDonald et al. [2009], for any $\delta > 0$, with probability at least $1 - \delta$,
\[
||\tilde{w} - w^*|| \leq \frac{R}{\xi \sqrt{m/2}} (1 + \sqrt{\log 1/\delta}).
\]

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Next, for a fixed pair of \((x_i, k_i)\), observe that
\[
\nabla_w \left[ \log p_w[k_i|x_i] \right] = \mathbb{E}_{k \sim p_w[|x|]} \Phi(x_i, k_i) - \Phi(x_i, k)
\]
Thus, \(|\nabla_w \log p_w[k_i|x_i]| \leq 2R\) for any \((x_i, k_i) \in \mathcal{X} \times [p]\). It follows that, with probability at least \(1 - \delta\),
\[
\left| \mathbb{E}_{(x, k) \sim D} \log p_w[k|x] - \mathbb{E}_{(x, k) \sim D} \log p_w*[k|x] \right| \leq 2R \|\hat{w} - w^*\| \leq \frac{2\sqrt{T}R^2}{\xi \sqrt{m}} (1 + \sqrt{\log 1/\delta}).
\]

**Theorem 5.** There exist \(z \in \Delta\) such that the following inequality holds for any \(\alpha > 1\) and arbitrary target mixture \(D_T\):
\[
\mathcal{L}(D_T, \hat{g}_z) \leq e^{(\frac{\alpha - 1}{2} \text{Max})} M \frac{2^{\alpha - 1} - 1}{\text{Max}} \left[ e^{(2 + \frac{\alpha - 1}{2})2R \|\hat{w} - w^*\|} \right] d_1(\alpha) d_2(\alpha),
\]
with
\[
d_1(\alpha) = \left[ \sum_{x \sim D(x)} d_2(x \| d(x)) \right]^{2\alpha - 1} \left[ \sum_{x \sim D(x)} d_2(x \| d(x)) \right]^{(2 - \alpha)},
\]
\[
d_2(\alpha) = \left[ \sum_{x \sim D(x)} d_2(x \| d(x)) \right]^{4\alpha - 1} \left[ \sum_{x \sim D(x)} d_2(x \| d(x)) \right]^{(4 - \alpha)}.
\]

**Proof.** Note that in Theorem 1, the learning guarantees are essentially determined by \(\max_{k \in [p]} d_\alpha(D_k \| \hat{D}_k)\) and \(\max_{k \in [p]} d_\alpha(D_k \| D_k)\), for some Rényi parameter \(\alpha > 1\). We extend Theorem 1 to \(g_z\) as follows: Given \(\hat{D}_k(x)\), construct a “fake” density estimator \(\tilde{D}_k(x) := D(x)d_k(x)/D(k)\). Since we will not actually use \(\tilde{D}_k(x)\) in practice, but only use it for proofs, we can assume access to the true \(D(x)\) and \(D(k)\). For any \(\alpha > 1\),
\[
\max_{k \in [p]} \left[ d_\alpha(D_k \| \tilde{D}_k) \right]^{\alpha - 1}
\]
\[
= \max_{k \in [p]} \left[ \sum_x D_k^\alpha(x) \| \tilde{D}_k^{\alpha - 1}(x) \right] = \max_{k \in [p]} \left[ \sum_x \left( \frac{d_k(x)D(x)/D(k)}{d_k(x)D(x)/D(k)} \right)^\alpha \right] = \max_{k \in [p]} \left[ \sum_x \frac{d_k(x)}{D(k)} \frac{d_k^\alpha(x)}{D_k^{\alpha - 1}(x)} \right]
\]
\[
\leq p \sum_{k \in [p]} \left[\sum_x D(x) d_k^\alpha(x) \| d_k^{\alpha - 1}(x) \right]^{\alpha - 1} \quad \text{(Assume } D(k) = 1/p, \text{ upper bound max by sum)}
\]
\[
= p \mathbb{E}_{x \sim D(x)} \left[ d_\alpha(x \| \tilde{D}(x)) \right]^{\alpha - 1}
\]
Let \(d^*(x) = p_{\Phi}[x|x]\), and \(d_k(x) = p_\Phi[x|x]\), the population and empirical solution of logistic regression problem (8), respectively. Then, by Lemma 3,
\[
\mathbb{E}_{x \sim D(x)} \left[ d_\alpha(x \| \tilde{D}(x)) \right]^{\alpha - 1}
\]
\[
\leq \sum_x D(x) \left[ \sum_k \frac{d_k^\alpha(x)}{d_k^{\alpha - 1}(x)} \right]^{\gamma} \left[ \sum_k \frac{d_k^{\alpha - 1}(x)}{d_k^\alpha(x)} \right]^{1 - \gamma}
\]
\[
= \sum_x D(x) \left[ \sum_k \frac{d_k^\alpha(x)}{d_k^{\alpha - 1}(x)} \right]^{\gamma} D(x) \left[ \sum_k \frac{d_k^{\alpha - 1}(x)}{d_k^\alpha(x)} \right]^{1 - \gamma}
\]
\[
\leq \sum_x D(x) \left[ \sum_k \frac{d_k^\alpha(x)}{d_k^{\alpha - 1}(x)} \right]^{\gamma} \left[ \sum_x D(x) \sum_k \frac{d_k^{\alpha - 1}(x)}{d_k^\alpha(x)} \right]^{1 - \gamma}
\]
\[
= \left[ \mathbb{E}_{x \sim D(x)} \left[ d_\alpha(x \| d^*(x)) \right]^{\gamma - 1} \right]^{\frac{1}{\gamma - 1}} \left[ \mathbb{E}_{(x, k) \sim D(x) \times d^*(x)} \left[ d_k(x) \right]^{\frac{1}{\gamma - 1}} \right]^{1 - \gamma},
\]
where the last inequality follows from Hölder’s inequality. When the population best domain classifier \(d^*(x)\) can closely approximate the true posterior distribution \(d(x)\), the first term of (17) is close to 1. The second term
of (17) can be upper bounded by

\[
\left[ (x,k) \sim \mathcal{D}(x) \times \mathcal{D} \right] \sum_{x} \mathbb{P}_{\mathcal{D}(x)} \left[ \mathcal{D}(x) \mid d^*(x) \right]^{\gamma - 1} \leq \mathbb{E}_{\mathcal{D}(x)} \left[ d^*(x) \right]^{\gamma - 1}. 
\]

Thus,

\[
\max_{k \in [p]} \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq p \mathbb{E}_{x \sim \mathcal{D}(x)} \left[ d^*(x) \right]^{\gamma - 1}. 
\]

Similarly, for any \( \alpha > 1 \),

\[
\max_{k \in [p]} \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\alpha - 1} = \max_{k \in [p]} \left[ \sum_{x} \mathcal{D}(x) \left( \mathcal{D}(x) \right)^{\alpha - 1} \right] = \max_{k \in [p]} \left[ \sum_{x} \mathcal{D}(x) \right]^{\alpha - 1} 
\]

\[
\leq p \mathbb{E}_{x \sim \mathcal{D}(x)} \left[ d^*(x) \right]^{\alpha - 1}. 
\]

Pick \( \gamma = \frac{1}{2} \), and the above results simplify to

\[
\max_{k \in [p]} \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq p \mathbb{E}_{x \sim \mathcal{D}(x)} \left[ d^*(x) \right]^{\gamma - 1}. 
\]

\[
\Rightarrow \max_{k \in [p]} \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq p \mathbb{E}_{x \sim \mathcal{D}(x)} \left[ d^*(x) \right]^{\gamma - 1}. 
\]

And,

\[
\max_{k \in [p]} \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq p \mathbb{E}_{x \sim \mathcal{D}(x)} \left[ d^*(x) \right]^{\gamma - 1}. 
\]

Plug into Theorem 1.

\[
\mathcal{L}(\mathcal{D}, \mathcal{G}) \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1}. 
\]

\[
\Rightarrow \max_{k \in [p]} \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq p \mathbb{E}_{x \sim \mathcal{D}(x)} \left[ d^*(x) \right]^{\gamma - 1}. 
\]

\[\Box\]

**Theorem 6.** There exist \( z \in \Delta \) such that, for any \( \delta > 0 \), with probability at least \( 1 - \delta \) the following inequality holds for any \( 1 < \alpha < 2 \) and arbitrary target mixture \( \mathcal{D} \) :

\[
\mathcal{L}(\mathcal{D}, \mathcal{G}) \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1}. 
\]

with \( M_m = 1 + \frac{2}{m} \left[ \max_{\alpha, \beta} \mathbb{E}_{x \sim \mathcal{D}(x)} \left[ \frac{K_\alpha(x, \cdot)}{K_\beta(x, \cdot)} \right] \right] \), and

\[
\mathcal{L}(\mathcal{D}, \mathcal{G}) \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1}. 
\]

and

\[
\mathcal{L}(\mathcal{D}, \mathcal{G}) \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1} \leq \epsilon \left[ \mathcal{D}(x) \mid \mathcal{D}(x) \right]^{\gamma - 1}. 
\]
Proof. By Theorem 8, for any $\delta > 0$, with probability at least $1 - \delta$, each of the following two inequalities holds for all domains:

$$d_\alpha(\hat{D}_k \parallel D_k) \leq \mathbb{E}_{x \sim D_k} \left[ d_\alpha(K_\sigma(\cdot, x) \parallel D_k) \right] M_{mn}^{\frac{\alpha}{2} \sqrt{m \log \frac{2}{2\delta}}}, \quad \text{for all } 1 \leq \alpha \leq 2,$$

$$d_\alpha(D_k \parallel \hat{D}_k) \leq \mathbb{E}_{x \sim D_k} \left[ d_\alpha(D_k \parallel K_\sigma(\cdot, x)) \right] M_{mn}^{\frac{\alpha}{2} \sqrt{m \log \frac{2}{2\delta}}}, \quad \text{for all } \alpha \geq 1.$$

It follows that, for all $1 < \alpha < 2$,

$$\max_{k \in [p]} d_\alpha(\hat{D}_k \parallel D_k) \leq \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_\alpha(K_\sigma(\cdot, x) \parallel D_k) \right] M_{mn}^{\frac{\alpha}{2} \sqrt{m \log \frac{2}{2\delta}}},$$

$$\max_{k \in [p]} d_\alpha(D_k \parallel \hat{D}_k) \leq \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_\alpha(D_k \parallel K_\sigma(\cdot, x)) \right] M_{mn}^{\frac{\alpha}{2} \sqrt{m \log \frac{2}{2\delta}}}.$$

Plug into Theorem 1, for $1 < \alpha < 2$,

$$\mathcal{L}(D_T, \hat{h}_z) \leq \epsilon \frac{(\alpha - 1)^2}{2\alpha^2} M \left[ \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_\alpha(\hat{D}_k \parallel D_k) \right] \left( \max_{k \in [p]} d_{2\alpha - 1}(D_k \parallel \hat{D}_k) \right) \right]$$

$$\leq \epsilon \frac{(\alpha - 1)^2}{2\alpha^2} M \left( \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_\alpha(D_k \parallel \hat{D}_k) \right] \left( \max_{k \in [p]} d_{2\alpha - 1}(D_k \parallel K_\sigma(\cdot, x)) \right) \right),$$

with

$$d_3(\alpha) = \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_\alpha(K_\sigma(\cdot, x) \parallel D_k) \right], \quad d_4(\alpha) = \max_{k \in [p]} \mathbb{E}_{x \sim D_k} \left[ d_{2\alpha - 1}(D_k \parallel K_\sigma(\cdot, x)) \right] .$$