A Unified Framework for Comparing Distribution Matching Methods Across Trustworthy Machine Learning Tasks

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Abstract

Distribution matching (DM) is a fundamental tool in trustworthy machine learning (TML), with applications in fairness, calibration, and domain adaptation. While prior work advances individual DM methods based on information-theoretic and geometric divergences, a unified comparative framework remains lacking. We propose a framework integrating DM methods, metrics, and TML tasks to enable systematic comparisons. To our knowledge, this is the first work to compare latent spaces in TML while addressing scaling inconsistencies via PCA whitening. We empirically evaluate MMD, Sinkhorn and adversarial DM calibration methods across fairness, calibration, and domain adaptation. Our findings reveal: (1) simple NLL training objective with post-hoc calibration can outperforms other DM methods; (2) logit-based fairness methods outperform latent-based approaches; and (3) error and DM metrics show a U-shaped trend, and we connect this insight to theory Zhao et al. [2019b]. These insights inform the selection and refinement of DM algorithms for TML applications.

1 Introduction

Domain-invariant representation learning (DIRL) [Zhao et al., 2019a, 2022] aims to learn a representation function $g_\theta : \mathbb{X} \to \mathbb{Z}$, which map data from different domains into a shared latent space where their distributions align, enabling models to focus on task-relevant features while ignoring domain-specific variation as shown in Figure 3. Unlike representation learning for classification which seeeks to maximize the divergence between class distributions, DIRL seeks to minimize the divergence between the domain distribution. This approach is foundational to many trustworthy machine learning (TML) tasks—such as fair classification, domain adaptation, and uncertainty calibration—because it addresses the pervasive challenge of distribution shift that undermines model reliability in real-world applications.

Prior work on distribution matching has primarily been developed within specific TML tasks, often focusing on individual approaches rather than a comparative or unified framework [Han et al., 2023b, Reddy, 2022b, Tao et al., 2023, Gulrajani and Lopez-Paz, 2020, Marx et al., 2024b]. For instance, in uncertainty calibration [Marx et al., 2024b], DM has been explored using kernel-based approaches such as Maximum Mean Discrepancy (MMD) to align predicted and true confidence distributions. In contrast, domain adaptation methods typically rely on adversarial learning, where generative adversarial networks (GANs) or domain classifiers enforce domain-invariant representations [Ganin et al., 2016b]. In fairness, logit-based methods enforce fairness by directly constraining output distributions [Chung et al., 2024a], while latent space-based methods align intermediate feature distributions [Madras et al., 2018]. Consequently, there is limited understanding of which DM methods generalize best across tasks or how different alignment techniques trade off between computational efficiency, stability, and effectiveness.

To bridge this gap, we propose a unified framework for systematically comparing DM methods across multiple TML tasks. Our framework integrates representative DM methods including Maximum Mean Discrepancy (MMD) [Gretton et al., 2012], Sinkhorn divergence [Feydy et al., 2019a], and adversarial domain alignment. We evaluates their performance on three major TML tasks: fairness, calibration, and domain adaptation. While previous studies consider distribution matching (DM) in isolation for individual tasks, our framework enables cross-task comparison. In particu-

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Table 1: Unified distribution-matching (DM) formalization across calibration (Calib), fairness (DP), and domain adaptation (DA).

Task	$L_{\mathbf{task}}$	Domains d	Matched object / matcher	DM constraint (type)
Calib	$\mathbb{E}[\ell(f_\psi(g_\theta(x)), y)]$	$\{\text{FORECAST}, \text{TARGET}\}$	(y', q) with $q = \text{softmax}(f_\psi(g_\theta(x)))$	$D\big(p(y\,\vert\,q),\, p(\hat{y}\,\vert\,q)\big) \le \delta$ (conditional)
Fair (DP)	$\mathbb{E}[\ell(f_\psi(g_\theta(x, \varepsilon)), y)]$ / or $-I(x, z\,\vert\,d)$	sensitive groups ($d \in \{\text{A}, \text{B}\}$)	$z = g_\theta(x, \varepsilon)$ / or q	$D\big(p(z\,\vert\,d{=}1),\, p(z\,\vert\,d{=}2)\big) \le \delta$ (unconditional DP) *EO variant*: $D\big(p(z\,\vert\,d, y),\, p(z\,\vert\,y)\big) \le \delta$
DA	$\mathbb{E}[\ell(f_\psi(g_\theta(x, \varepsilon)), y)]$ (ERM on SRC)	$\{\text{Source}, \text{Target}\}$	domain-invariant $z = g_\theta(x, \varepsilon)$	$D\big(p(z\,\vert\,\text{SRC}),\, p(z\,\vert\,\text{TGT})\big) \le \delta$ (unconditional)

Symbols: x input, y target, $z = g_\theta(\cdot)$ representation, $q = \text{softmax}(f_\psi(z))$; D can be MMD/Sinkhorn/adversarial.

lar, it reveals how intrinsic measures (MMD, Sinkhorn) align with task-specific objectives, including fairness and calibration metrics such as ECE [Guo et al., 2017b] and DP [Han et al., 2023b]. Additionally, we introduce a normalized divergence metric to control for latent space scaling, ensuring fair evaluation DM methods using non-parametric geometric divergences that can be computed directly from samples.

Our empirical results reveal key trends in DM effectiveness across tasks and highlight limitations in current methods that future research must address. First, we find that simple NLL training with post-hoc calibration can outperform other DM-based calibration methods. Second, although most fairness research has focused on representation learning (i.e., latent-based methods), we show that logit-based methods consistently outperform latent-based ones. Lastly, we demonstrate that strictly minimizing distributional discrepancy is not beneficial for domain adaptation by showing that both error and DM metrics exhibit a U-shaped trend. This suggest the existence of a optimal region that minimizes errors by controling DM metrics. Through this study, we aim to guide the selection of DM techniques for TML applications and inspire the development of more robust, generalizable DM algorithms. Our contributions can be summarized as follows:

1. We formalize a common theoretical framework that integrates DIRL and DM methods under a single umbrella, enabling systematic comparisons.
2. We propose a PCA whitened version of a distribution matching metric to be more fair when comparing methods in latent representations spaces.
3. Using the unified DM framework, we evaluate different DM methods across fairness, domain adaptation, and calibration tasks, highlighting their connection between intrinsic metric (e.g., MMD, Sinkhorn) and task specific metric (e.g., DP, ECE), and provide insightful guideline for practical usage.

2 Unified Framework for Distribution Matching and Trustworthy ML Tasks.

Notation. Let $\mathbf{x} \in \mathbb{X}$, $\mathrm{y} \in \mathbb{Y}$, and $\mathrm{d} \in \{1, 2, \ldots, k\}$ denote random variables corresponding to the input, target (optional), and domain label, respectively. Let $\mathbf{z} := g_\theta(\mathbf{x}, \mathrm{y}, \mathrm{d}, \epsilon) \sim p_\theta(\mathbf{z}|\mathrm{y}, \mathbf{x}, \mathrm{d})$ denote the latent representation of $\mathbf{x}$, and for logit based method, we denote $\hat{\mathbf{q}} := g_\theta(\mathbf{x}, \mathrm{y}, \mathrm{d}, \epsilon) \sim p_\theta(\hat{\mathbf{q}}|\mathrm{y}, \mathbf{x}, \mathrm{d})$ where g_θ is called the *matcher* with parameters θ that may optionally depend on the target variable y, the domain d, and exogenous noise ϵ to encompass stochastic aligners. If g does not depend on d and/or ϵ we will suppress notation w.r.t. these random variables for notational simplicity. Let $p_{\text{data}}(\mathbf{x}, \mathrm{y}, \mathrm{d})$ denote the true data distribution. Let ϕ denote parameters of variational models or distributions, e.g., $q_\phi(\mathbf{x}, \mathrm{y}, \mathrm{d})$ will denote a variational distribution and $h_\phi(\mathbf{z})$ will denote a variational discriminator for adversarial learning. Let ψ denote application-specific parameters, e.g., $\hat{\mathrm{y}} := f_\psi(\mathbf{z})$ will denote the predicted class based on the given classifier head in fair classification. Entropy, cross entropy, and mutual information will be denoted by $\mathrm{H}(\mathbf{x})$ and $\mathrm{H_c}(\mathbf{x}, \mathbf{z})$, and $\mathrm{I}(\mathbf{x}, \mathbf{z})$, respectively. Let $\mathrm{D}(p, q)$ denote a distribution divergence between p and q, e.g., $\mathrm{D_{KL}}$, $\mathrm{D_{JSD}}$, and $\mathrm{D_{W_\rho}}$ will denote KL, JSD, and Wasserstein-ρ divergences, respectively. Similarly, let $\widehat{\mathrm{D}}$, $\overline{\mathrm{D}}$, and $\underline{\mathrm{D}}$ denote an approximation, an upper bound, or a lower bound of a divergence respectively. Because DM involves mininizing a divergence w.r.t. the matcher parameters θ, we will let $\mathrm{D}(\theta) := \mathrm{D}(p_\theta(\mathbf{z}|\mathrm{d}{=}1), p_\theta(\mathbf{z}|\mathrm{d}{=}2))$ with slight abuse of notation.

Distribution Matching Problem. The distribution matching problems we consider can be formulated as a task-specific objective plus a distribution matching constraint on the matched representation.

Definition 1. *(Distribution Matching Problem). A distribution matching problem minimizes a task objective* $\mathrm{L}_{\text{task}}(\tilde{f}_\psi, \tilde{g}_\theta)$*, where* $\tilde{f}_\psi$ *is a task-specific model and* $\tilde{g}_\theta$ *is the* matcher *model, subject to a DM constraint on the matched representation* $\tilde{\mathbf{z}} := \tilde{g}_\theta(\mathbf{x}, \mathrm{y}, \mathrm{d}, \epsilon)$*:*

$$\min_{\psi,\theta}\ \mathrm{L}_{\text{task}}(\tilde{f}_\psi, \tilde{g}_\theta) \quad s.t. \quad \mathrm{D}(p_\theta(\tilde{\mathbf{z}}|\mathrm{d}{=}1), p_\theta(\tilde{\mathbf{z}}|\mathrm{d}{=}2)) \leq \delta \tag{1}$$

where $\mathrm{D}(\cdot,\cdot)$ *is a distribution divergence and* δ *is the DM slackness hyperparameter.*

In practice, minimizing a distribution divergence is challenging given only samples. Most approaches use tractable and differentiable approximations to well-known divergences. We will first explain common loss functions that aim to solve trustworthy ML tasks and then review the main approaches to minimizing a distribution divergence.

2.1 Unified Formalization of Trustworthy ML Tasks as Distribution Matching

Many trustworthy ML tasks can be formulated as DM problems. In some cases, DM is fundamental to the trustworthy ML task (e.g., fairness or calibration), while in others, DM is one approach to the task (e.g., domain adaptation). For the tasks where DM is fundamental, the key question is: *What is the empirically achievable Pareto frontier between the task objective and the DM constraint (e.g., fairness-accuracy trade-off)?* For the tasks where DM is an approach, the key question is: *Is DM performance correlated with the relevant task performance (e.g., does better DM yield better domain adaptation performance)?* In particular, we would like to disentangle the effect of the DM algorithm—which may be far from optimal—from the task performance. We conjecture that in some cases, the DM algorithm fails to achieve the DM objective even though the task objective may be reasonable.

Group Fair ML as Distribution Matching The goal of fair learning is to be as accurate as possible while satisfying a fairness constraint. Demographic parity (DP) (also known as statistical parity) is one common notion of group fairness that is satisfied if and only if $p(\hat{\mathrm{y}} = 1|\mathrm{d}{=}1) = p_\theta(\hat{\mathrm{y}} = 1|\mathrm{d}{=}2)$, i.e., these two distributions match. Fair classification seeks to directly learn predictions that are fair. Fair representation learning seeks to learn a representation such that all downstream tasks will be fair. We unify fair learning under our DM framework and notation below.

Proposition 1. *Fair learning [Madras et al., 2018, Song et al., 2019b] w.r.t. DP is a DM problem (1) with* $\tilde{g}_\theta(\mathbf{x}, \mathrm{y}, \mathrm{d}, \epsilon) = g_\theta(\mathbf{x}, \epsilon)$ *and* $\mathrm{L}_{\text{task}} = \mathbb{E}[\ell(f_\psi(g_\theta(\mathbf{x}, \epsilon)), \mathrm{y})]$ *for fair classification and* $\mathrm{L}_{\text{task}} = -\mathrm{I}(\mathbf{x}, \mathbf{z} = g_\theta(\mathbf{x}, \epsilon)|\mathrm{d})$ *for fair representation learning.*

In practice, both the classification and mutual information task objectives are often combined (e.g., [Madras et al., 2018, Gong et al., 2024] approximate mutual information via a VAE objective).

Calibration as DM Problem Vaicenavicius et al. [2019b] formalized canonical calibration for multiclass classification, where calibration means that the predicted probability vector for all classes coincides with the true underlying class probabilities:

$$p(\mathrm{y} = y|\hat{\mathbf{q}}) = p(\hat{\mathrm{y}} = y|\hat{\mathbf{q}}) := \mathrm{q}_y, \quad \forall y \in \mathbb{Y}, \hat{\mathbf{q}} \in \Delta^{|\mathbb{Y}|} \tag{2}$$

where $\hat{\mathbf{q}} := g_\theta(\mathbf{x})$ is the predicted class probabilities for k classes and $\Delta^{|\mathbb{Y}|}$ denotes the probability simplex. This calibration condition is a type of *conditional* distribution matching problem, i.e., match the marginal distribution of predictions to the true distribution *conditioned* on the model's output $\mathbf{q}$. In this case, the domain label is whether it is the real target variable or the predicted target variable. Marx et al. [2023] demonstrated that indeed many types of calibration including regression, classification, and decision calibration can be framed as conditional distribution matching problems. In fact, because the marginal distribution of the conditioning variables is the same regardless of the domain, the problem can be equivalently written as an unconditional DM problem. We now unify the results from Marx et al. [2023] using our framework below.

Proposition 2. *Calibration during training can be interpreted as a distribution matching problem. Let* $\hat{\mathrm{y}}'$*,* y'*, and* c *denote the forecast, target, and conditioning variables, respectively, as defined in Marx et al. [2023, Tables 1 and 2]. Here,* $\hat{\mathrm{y}}'$ *and* y' *are derived transformations of the raw forecast* $\hat{\mathrm{y}}$ *and the true outcome* y*,*[1] *calibration during training is a DM problem (1) with* $\tilde{g}_\theta(\mathbf{x}, \mathrm{y}, \mathrm{d}, \epsilon) = (\tilde{\mathrm{y}}', g_\theta(\mathbf{x}, \epsilon))$*, where* $\tilde{\mathrm{y}}' = \mathbb{1}(\mathrm{d}{=}1)\hat{\mathrm{y}}' + \mathbb{1}(\mathrm{d}{=}2)\mathrm{y}'$ *selects between the forecasted*

[1] Note that in many cases, $\hat{\mathrm{y}}' = \hat{\mathrm{y}}$ and similarly $\mathrm{y}' = \mathrm{y}$, but there are some cases from Marx et al. [2023] such as quantile calibration for regression or top-label calibration for classification that require using either the predicted CDF or indicator functions of $\hat{\mathrm{y}}$ and y.

and target variables, $c = g_\theta(\mathbf{x}, \epsilon)$ represents the conditioning variable, and $\mathrm{L}_{\text{task}} = \mathbb{E}[\ell(g_\theta(\mathbf{x}, \epsilon), \mathrm{y})]$ is the standard negative log-likelihood empiricial risk minimization (ERM) objective.

Domain Adaptation via Domain-Invariant Features Inspired by the bounds on domain adaptation generalization by Ben-David et al. [2006a], many domain adaptation papers aim to learn domain-invariant features (i.e., latent features whose distribution is independent of the domain labels). Specifically, Ben-David et al. [2006a] showed that the risk on the target domain could be bounded by the risk on the source domain plus the divergence between the feature distributions and a constant. A natural approach is to reduce the divergence between the feature distributions (i.e., distribution matching). Thus, domain-invariant domain adaptation can be unified under our framework.

Proposition 3 (Domain-invariant domain adaptation is DM)**.** *Domain-invariant domain adaptation is a DM problem (1) with $\tilde{g}_\theta(\mathbf{x}, \mathrm{y}, \mathrm{d}, \epsilon) = g_\theta(\mathbf{x}, \epsilon)$ and $\mathrm{L}_{\text{task}} = \mathbb{E}[\ell(f_\psi(g_\theta(\mathbf{x}, \epsilon)), \mathrm{y})]$ is the standard ERM objective where f_ψ is the classification head on top of the domain-invariant representation $\mathbf{z} = g_\theta(\mathbf{x}, \epsilon)$.*

2.2 Normalized Geometric Divergences for Evaluating DM Methods

One of the challenges with comparing DM methods is properly evaluating how well the DM constraint was satisfied. Ideally, we would measure the divergence of the latent domain distributions. However, even estimating distribution divergences is known to be a challenging problem in its own right. While the adversarial and VAE-based methods could provide bounds on information theoretic divergences, they would require training an auxiliary model at test time to evaluate each method. Thus, we focus on the non- parametric divergences MMD and Sinkhorn that can be estimated with only samples. However, there is one key challenge with these geometric divergences when comparing across diverse methods. The scale of the latent distribution can significantly affect the absolute MMD or Sinkhorn divergence estimate because geometric divergences are highly sensitive to scale. This is a problem if the latent space is learned since the latent space scale is arbitrary and generally distorted [Jing et al., 2021, Ermolov et al., 2021]. Thus, comparing methods using MMD or Sinkhorn directly would be unfair. To overcome this, we propose a simple approach based on applying principal component analysis (PCA) whitening [Kessy et al., 2018] of the latent space before measuring the divergence. This normalization eliminates the effect of scale in the latent distributions. We do not consider zero phase component analysis (ZCA) whitening, which applies rotation after PCA whitening since L2 based metrics are invariant under rotation. Simple proof can be found on section B. In contrast to latent space, logit space do not suffer from distortion problem since its axes are semantically tied to classes and trained under cross entropy, thus result into well-structured simplex equiangular tight frame (ETF) geometry at convergence also known as neural collapse [Papyan et al., 2020]. Therefore, we do not have to apply PCA whitening.

3 Experimental Setup

Given our unified DM framework for TML tasks, we aim to systematically compare both DM methods and DM evaluation metrics, where we evaluate DM methods both intrinsically (i.e., how well the distributions match) and extrinsically (i.e., how much the DM approach helps the TML task). In particular, we are interested in whether better DM corresponds to better task-specific metrics and vice versa or if the performance tradeoff is more complex—while most methods have theoretic grounding, it is unclear how it translates to empirical results. We are also interested in comparing methods for particular tasks and asking which method is the best method depending on the context. Finally, we explore a few other task-specific ideas along the way such as whether we should match latent representations or logits. To systematically and effectively do this, we fix the model architecture and the form of the objective function and only modify the implementation of the DM regularization to the problem. Specifically, we apply three representative DM methods (kernelized MMD, Sinkhorn, and adversarial) to three representative TML tasks (calibration, group fairness, and domain adaptation) across a variety of datasets. Ultimately we aim to elucidate some of the nuances involved in using DM methods for TML tasks and give practical guidelines for practitioners.

3.1 Experimental Setup

Datasets and Hyperparameter Tuning We consider ADULT dataset [Becker and Kohavi, 1996], COMPAS, and ACS-T datasets for calibration and fairness task. For the domain adaptation task, we use the MNIST and USPS dataset [Deng, 2012, Hull, 1994]. We tune the hyperparameters of each method using a TPE sampler [Bergstra et al., 2011] to find the best model and apply early stopping by tracking the validation loss. More detail can be found on section A.

Calibration Training We follow an individual calibration approach, as described in Marx et al. [2024a]. While prior work primarily used the Maximum Mean

Discrepancy (MMD) method, we extend the study by incorporating both the Sinkhorn divergence and an adversarial method. Since no prior work has applied adversarial techniques in this context, we implemented a GAN-based method designed to match the predicted distribution to the target ground-truth distribution. For post hoc calibration, we apply temperature scaling Hinton [2015].

Fair Classification Training Most fairness benchmark papers [Han et al., 2023a, Reddy, 2022a] focus on fair representation learning, which we refer to as latent-based methods. However, there is a lack of prior work studying logit-based approaches [Chung et al., 2024b]. In this paper, we compare distribution matching using both logit-based and latent-based methods using Sinkhorn, MMD, adversarial.

Domain Adaptation Training In this paper, we focus on unsupervised domain adaptation setting where we do not have access to the target label. [Wilson and Cook, 2020]. We use Sinkhorn based method [Courty et al., 2014], MMD based method [Tzeng et al., 2014], and adversarial based method [Ganin et al., 2016a].

Task Specific Metrics For all tasks, we use accuracy (or equivalently error) as a measure for the raw model performance (for domain adaptation, this is source accuracy). For each task, there is an additional task-specific metric. For the calibration task, we use the *Expected Calibration Error (ECE)* [Naeini et al., 2015a] based on measuring the discrepancy between the model confidence and accuracy: ECE =

$$\sum_{m=1}^{M} \frac{|B_m|}{n} \left| \mathbb{E}\left[\mathbb{I}\left(\hat{y} = y\right) \mid \hat{\mathbf{q}} \in B_m\right] - \mathbb{E}\left[\hat{\mathbf{q}} \mid \hat{\mathbf{q}} \in B_m\right] \right|, \tag{3}$$

where B_m denotes the set of samples in the m-th confidence bin, $|B_m|$ is the number of samples in bin m, n is the total number of samples, $\hat{\mathbf{q}}$ is predicted probability (confidence), and $\hat{y}$ is predicted label For group fairness, we use *Demographic Parity (DP)* difference that measures the discrepancy of the true positive rate between different domains:

$$\mathrm{DP} = |p_\theta(\hat{y} = 1|d = 1) - p_\theta(\hat{y} = 1|d = 2)| \tag{4}$$

For domain adaptation, we simply use the target accuracy (ACC).

4 Experimental Results Across Tasks

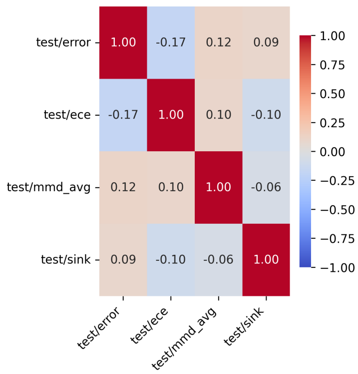
In each of the following sections, we highlight the most interesting results for each task but provide additional discussion in the appendix. For each task, we consider how well DM metrics correlate with accuracy and their corresponding task-specific metrics. In some cases, we find that, despite the theoretic grounding, lower DM metric does not imply a better task-specific metric—particularly for domain adaptation. The other key question is which method is most practical or useful for each task given the results. We also make several other observations that are specific to each task.

4.1 Calibration Task Results

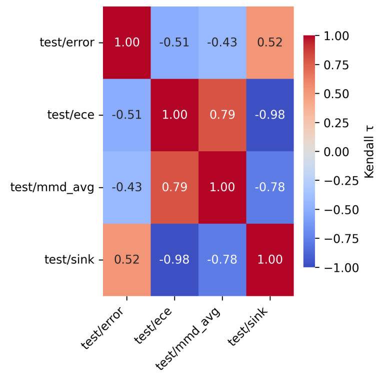
The Sinkhorn divergence best captures distributional differences, whereas MMD fails to do so. As shown in Figure 1, the correlation between Sinkhorn divergence and ECE is mostly negative before temperature scaling (TS), consistent with the definition of calibration Equation (2). In contrast, the correlation between MMD and ECE is sometimes positive Figure 1b. This discrepancy arises from the stronger entropic regularization in MMD, which makes it a noisier estimator compared to the Sinkhorn divergence [Feydy et al., 2019a]. Moreover, the MMD regularizer fails to capture any correlation across metrics on large-scale datasets Figure 1a, even though it can still capture correlations on small-scale datasets. This failure can be explained by the fact that MMD is incomplete when the feature space X is not compact, which often occurs in large-scale datasets due to outliers [Simon-Gabriel et al., 2023, McCarty, 2025]. Lastly, as shown in Table 2, the MMD values across all methods and datasets are so small that they become indistinguishable.

There is a trade-off between Error and ECE (if post-hoc calibration is not used). Extensive research in fairness has investigated the trade-off between Demographic Parity (DP) and accuracy (ACC) [Han et al., 2023a, Plecko and Bareinboim, 2024, Gong et al., 2024]. However, the trade-off between ACC and ECE has not been thoroughly explored in the calibration domain. Recent work reveals a negative correlation between ECE and Error when varying weight decay strength [Wang and Zhang, 2024]. We also observe this trend: before applying Temperature Scaling (TS), Figure 1 shows a negative correlation between ECE and ACC, which indicates such a trade-off. We analyze the the case when post-hoc calibration is used in section C.1.

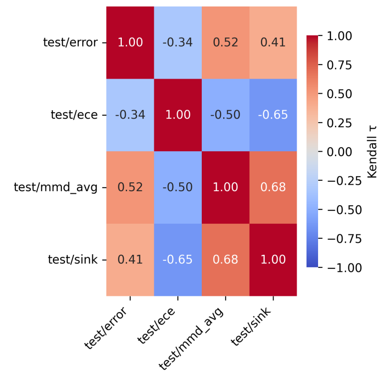
Which DM method should we use for Calibration task? Wang et al. [2021] show that applying TS to an unregularized cross-entropy model can outperform regularized alternatives in terms of ECE. Motivated by this, we include this baseline for comparison with other DM methods. Interestingly, training



(a) Calibration MMD



(b) Calibration Sinkhorn Divergence



(c) Calibration Adversarial

Figure 1: Kendall ranking correlation matrix of task specific metrics (Error and ECE), and DM metrics (MMD and Sinkhorn) across different calibration methods.

Table 2: Experimental results for tabular classification tasks. We display test metrics for each training procedure, with and without post-hoc calibration [Guo et al., 2017b]. n is the number of examples; d is the number of features. We repeat all the experiments across 10 random seeds and report the mean and standard deviation for each metric. We bold top 2 methods if average values are tie.

Dataset	Training Objective	ACC ↑	ECE ↓	SINK ↓	MMD ↓
ADULT	NLL	0.8435 ± 0.002	0.0163 ± 0.003	0.1894 ± 0.002	0.0000 ± 0.000
$n = 30162$	NLL + MMD	0.8438 ± 0.002	0.0175 ± 0.002	0.1887 ± 0.002	0.0000 ± 0.000
$d = 102$	NLL + Sink (Ours)	0.8429 ± 0.003	0.0166 ± 0.003	0.1889 ± 0.003	0.0000 ± 0.000
	NLL + Adv (Ours)	$\mathbf{0.8446 \pm 0.002}$	0.0155 ± 0.003	$\mathbf{0.1884 \pm 0.001}$	0.0000 ± 0.000
COMPAS	NLL	0.6481 ± 0.033	0.0402 ± 0.011	0.2936 ± 0.009	0.0001 ± 0.000
$n = 6172$	NLL + MMD	0.6372 ± 0.033	0.0407 ± 0.014	0.2956 ± 0.010	0.0000 ± 0.000
$d = 401$	NLL + Sink (Ours)	0.6361 ± 0.034	$\mathbf{0.0400 \pm 0.010}$	0.2984 ± 0.008	0.0000 ± 0.000
	NLL + Adv (Ours)	$\mathbf{0.6579 \pm 0.012}$	$\mathbf{0.0402 \pm 0.009}$	$\mathbf{0.2903 \pm 0.007}$	0.0001 ± 0.000
ACS-T	NLL	0.6502 ± 0.003	0.0397 ± 0.004	0.4087 ± 0.002	0.0000 ± 0.000
$n = 172508$	NLL + MMD	0.6496 ± 0.003	0.0430 ± 0.004	0.4081 ± 0.002	0.0000 ± 0.000
$d = 1567$	NLL + Sink (Ours)	$\mathbf{0.6585 \pm 0.001}$	0.1411 ± 0.002	$\mathbf{0.3722 \pm 0.001}$	0.0000 ± 0.000
	NLL + Adv (Ours)	0.6497 ± 0.003	0.0414 ± 0.004	0.4089 ± 0.002	0.0000 ± 0.000

with the *NLL* objective followed by TS often achieves ECE comparable to that of other DM methods, consistent with our explanation in section C.1. Even without TS, *NLL* alone yields competitive ECE on small-scale datasets table 2. While *NLL + Adv* sometimes achieves the lowest ECE (e.g., on Compas), it also introduces instability when the feature dimension is small, as in the German dataset section C.1, leading to high variance in both ACC and ECE.

Takeaway for Calibration

We recommend that practitioners use **NLL + post-hoc calibration** for large-scale datasets, while opting for **NLL** without post-hoc calibration on small-scale datasets, since post-hoc calibration can lead to miscalibration when the validation set is too small.

4.2 Fair Classification Results

Latent-based methods fail to capture consistent correlations due to noise. By definition of demographic parity (DP) in eq. (4), we expect distribution-matching (DM) metrics to exhibit a positive correlation with DP and a negative correlation with error, reflecting the well-known trade-off between error and fairness [Plecko and Bareinboim, 2024]. However, as shown in fig. 8b, both Sink and MMD display the opposite pattern: they are positively correlated with error and negatively correlated with DP. Moreover, 8c indicates that latent-based adversarial methods yield weak or inconsistent correlations between DM and task metrics.

In contrast, the logit-based results (Figure 10) reveal a clearer trend: DM metrics are negatively correlated with error and positively correlated with DP, with the exception of NLL + Sink. Interestingly, NLL + Sink

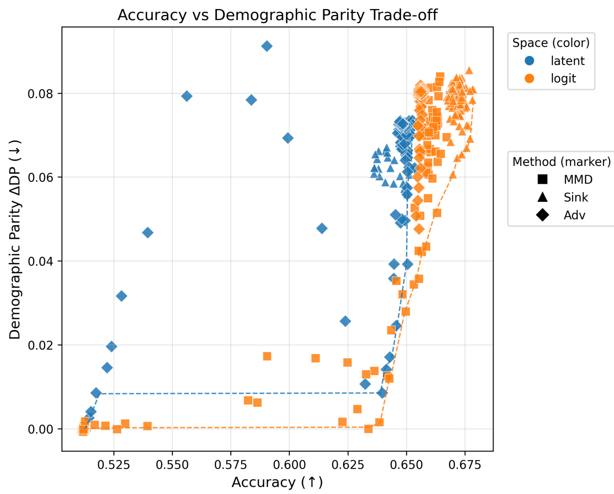


Figure 2: Fairness–accuracy trade-off comparison across methods, with each method distinguished by a unique **shape** and each representation type (latent vs. logit) by a distinct **color**. We can clearly observe that logit (orange) shows better trade off by attaining comparable or higher accuracy at substantially lower Δ DP near the Pareto optimal frontier

appears to break the trade-off entirely, showing almost no relationship between error and DP—as visualized in Figure 7, where its curve forms an almost vertical line in the upper-right corner.

Sinkhorn Divergence can excessively shrink latent representations and validates the need for PCA whitening for a proper DM metric. We observe that *NLL + Sink* often causes extensive distortion of the representation distribution, leading to extremely low DP values (e.g., 0.0025 on ACS-T, see table 6). However, this benefit comes at a substantial cost: accuracy is reduced by nearly 10% compared to other methods. Furthermore, the Sinkhorn distance between distributions is relatively small before applying PCA, which may lead to an unfair comparison across metrics (Table 6). This effect is well known that the learned latent space can have arbitrary scaling and geometric distortion [Jing et al., 2021, Ermolov et al., 2021]. This issue is evident in the SINK values reported in Table 6: before applying PCA, the *NLL + Sink* method often shrinks the distribution excessively, leading to artificially low SINK values. In contrast, logit-based methods do not exhibit this problem. Applying PCA whitening that we introduce mitigates this issue by normalizing the latent space, and we clearly observe that the resulting scales become comparable across methods.

Which DM method should we use for Fairness task We observe that logit-based methods capture a more consistent correlation between DM metrics and task-specific performance (section 4.2).

This consistency enables better control of the DP–ACC trade-off, as shown in fig. 2. Logit-based methods concentrate along the Pareto-optimal frontier of the fairness–utility trade-off (i.e., the lower-right region), and encounter the fairness–utility cliff only in the highest-accuracy regime.

In addition, we note that MMD-based methods can effectively manage the trade-off by producing a wide spread of points across different DP values (fig. 7). Sinkhorn-based methods are primarily concentrated in the high-accuracy region, but they are also associated with elevated DP values. In contrast, adversarial methods exhibit high variance: for latent-based regularization, points scatter widely across the plot, while for logit-based regularization, DP remains within a narrow range but accuracy is consistently the lowest among the three methods.

Takeaway for Fairness

We recommend practitioners to adopt logit-based methods over latent-based ones, as they provide a more favorable DP–ACC trade-off. Sinkhorn-based methods are preferable when achieving high accuracy is the primary goal, even at the cost of moderate DP gaps. In contrast, MMD-based methods are recommended when minimizing DP disparity is the priority, as they offer greater flexibility with respect to the accuracy–fairness trade-off.

4.3 Domain Adaptation Results

U-shaped Trend in Error In domain adaptation, Ben-David et al. [2006b] provide a useful bound on the target error in terms of the source error via the $\mathcal{H}$-divergence, suggesting that a good representation should achieve both low source error and low $\mathcal{H}$-divergence between source and target distributions. However, computing the $\mathcal{H}$-divergence is often impractical in practice, so we instead employ geometric divergences to approximate the distance between distributions. Interestingly, our experimental results deviate from the direct implication of this theoretical bound, a phenomenon also noted by Zhao et al. [2019b]. As shown in section C.3, low geometric divergence does not necessarily correspond to low target error. In fact, as geometric divergence increases up to a certain point, target error decreases, but beyond that point, the target error begins to rise again, forming a U-shaped trend.

Table 3: Experimental results for image classification tasks. n: target examples; d: target features. We repeat all the experiments across 10 random seeds and report the mean and standard deviation for each metric. We bold top 2 methods if average values are tie.

Dataset	Training Objective	Source ACC ↑	Target ACC ↑	SINK ↓	SINK PCA ↓	MMD ↓	MMD PCA ↓
MNIST→USPS	NLL + MMD	$\mathbf{0.9583 \pm 0.006}$	0.6162 ± 0.047	135.9770 ± 17.334	746.6720 ± 0.802	0.1312 ± 0.016	0.0033 ± 0.000
n= 9298	NLL + Sink	0.9461 ± 0.007	$\mathbf{0.6895 \pm 0.029}$	$\mathbf{2.0890 \pm 0.126}$	$\mathbf{741.1450 \pm 0.253}$	$\mathbf{0.0112 \pm 0.002}$	$\mathbf{0.0021 \pm 0.000}$
d= 256	NLL + Adv	0.9412 ± 0.017	0.6053 ± 0.052	192.9870 ± 19.096	746.7900 ± 0.594	0.1315 ± 0.010	0.0033 ± 0.000
USPS→MNIST	NLL + MMD	0.9015 ± 0.025	$\mathbf{0.5647 \pm 0.060}$	78.6320 ± 11.157	742.5810 ± 0.557	0.0269 ± 0.004	0.0023 ± 0.000
n= 70000	NLL + Sink	$\mathbf{0.9106 \pm 0.018}$	0.5451 ± 0.031	$\mathbf{4.6300 \pm 0.260}$	$\mathbf{741.6220 \pm 0.380}$	$\mathbf{0.0040 \pm 0.001}$	$\mathbf{0.0022 \pm 0.000}$
d= 784	NLL + Adv	0.8859 ± 0.015	0.5010 ± 0.012	139.5100 ± 27.899	741.8970 ± 0.599	0.0343 ± 0.008	0.0022 ± 0.000

By leveraging motivating empirical result above, we can explain the information theoretic lower bound on Zhao et al. [2019b] where source error is $\varepsilon_S(h \circ g) = \mathbb{E}_{x\sim D_S}[|h(g(x)) - f_S(x)|]$, $d_{\mathrm{JS}}(\mathcal{D}_S^Y, \mathcal{D}_T^Y)$ represent Jensen Shannon divergence (JSD) between marginal label distribution, and $d_{\mathrm{JS}}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)$ represent JSD between latent distribution.

Theorem 1 (Restatement of Theorem 4.3 in Zhao et al. [2019b])**.** *Suppose the condition in Lemma 4.8 holds and* $d_{JS}(\mathcal{D}_S^Y, \mathcal{D}_T^Y) \geq d_{JS}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)$*, then:*

$$\varepsilon_S(h\circ g)+\varepsilon_T(h\circ g) \geq \frac{1}{2}\left(d_{JS}(\mathcal{D}_S^Y, \mathcal{D}_T^Y) - d_{JS}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)\right)^2.$$

We can treat $d_{\mathrm{JS}}(\mathcal{D}_S^Y, \mathcal{D}_T^Y)$ as constants because they remain fixed while $d_{\mathrm{JS}}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)$ varies. Since $d_{\mathrm{JS}}(\mathcal{D}_S^Y, \mathcal{D}_T^Y)$ is non-negative, we can minimize the target error and source erorr by making $d_{\mathrm{JS}}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)$ close to $d_{\mathrm{JS}}(\mathcal{D}_S^Y, \mathcal{D}_T^Y)$. This trend can also be observed in section C.3. Both errors decrease down to a certain minimum point as increase of DM metrics, which implies that at minimum point i.e. $d_{\mathrm{JS}}(\mathcal{D}_S^Z, \mathcal{D}_T^Z) = d_{\mathrm{JS}}(\mathcal{D}_S^Y, \mathcal{D}_T^Y)$.

One downside of this theorem is that it does not explain the error increase once $d_{\mathrm{JS}}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)$ exceeds $d_{\mathrm{JS}}(\mathcal{D}_S^Y, \mathcal{D}_T^Y)$, because theorem 1 requires $d_{\mathrm{JS}}(\mathcal{D}_S^Y, \mathcal{D}_T^Y) \geq d_{\mathrm{JS}}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)$. Nevertheless, it still provides meaningful insight that we can achieve optimal target accuracy by controlling $d_{\mathrm{JS}}(\mathcal{D}_S^Z, \mathcal{D}_T^Z)$ via varying the regularization weight on distribution divergence.

Which DM method should we use for domain adaptation tasks?

As shown in section C.3, Sinkhorn exhibits a clear correlation with both error and DM metrics, whereas other measures appear noisy. This indicates that optimizing with Sinkhorn can effectively control the error. Furthermore, as presented in section 4.2, Sinkhorn achieves the highest target ACC on *MNIST→USPS* and the second-highest target ACC, which is very close to the best result.

Takeaway for Domain Adaptation

We recommend practitioners use Sinkhorn-based methods, as they can effectively control error by regulating DM metrics. Moreover, the U-shaped trend between error and DM metrics can guide practitioners to tune hyperparameters toward the optimal region.

5 Conclusion

We introduced a unified framework that casts calibration, group fairness, and domain adaptation as distribution matching (DM) problems, enabling fair comparisons of MMD, Sinkhorn, and adversarial approaches across tasks. Normalizing latent spaces via PCA whitening makes geometric DM metrics comparable and reveals consistent trends. Empirically, (i) plain NLL with post-hoc temperature scaling is a strong alibration baseline; (ii) logit-based fairness methods better navigate the DP–ACC trade-off than latent-based ones; and (iii) in domain adaptation, error follows a U-shaped curve versus DM strength, with Sinkhorn providing the most controllable knob. Our findings offer practical guidance and suggest future research directions. (1) Better DM-based calibration methods are needed, since a simple NLL baseline often outperforms most DM approaches. (2) Future work should develop logit-based fairness methods, as most existing algorithms remain latent-based.

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Checklist

1. For all models and algorithms presented, check if you include:
   (a) A clear description of the mathematical setting, assumptions, algorithm, and/or model. [Yes]
   (b) An analysis of the properties and complexity (time, space, sample size) of any algorithm. [No]
   (c) (Optional) Anonymized source code, with specification of all dependencies, including external libraries. [Yes/No/Not Applicable]

2. For any theoretical claim, check if you include:
   (a) Statements of the full set of assumptions of all theoretical results. [Yes]
   (b) Complete proofs of all theoretical results. [Yes]
   (c) Clear explanations of any assumptions. [Yes]

3. For all figures and tables that present empirical results, check if you include:
   (a) The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL). [Yes]
   (b) All the training details (e.g., data splits, hyperparameters, how they were chosen). [Yes]
   (c) A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times). [Yes]
   (d) A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider). [Yes]

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
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5. If you used crowdsourcing or conducted research with human subjects, check if you include:
   (a) The full text of instructions given to participants and screenshots. [Not Applicable]
   (b) Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable. [Not Applicable]
   (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation. [Not Applicable]