

# Fair and Optimal Classification via Post-Processing Predictors\*

Ruicheng Xian<sup>1</sup>

Lang Yin<sup>1</sup>

Han Zhao<sup>1</sup>

## Abstract

To address the bias exhibited by machine learning models, fairness criteria impose statistical constraints to ensure equal treatment to all demographic groups, but typically at a cost to model performance. Understanding this tradeoff, therefore, underlies the design of fair and effective algorithms. This paper completes the characterization of the inherent tradeoff of demographic parity on classification problems in the most general multigroup, multiclass, and noisy setting. Specifically, we show that the minimum error rate achievable by randomized and attribute-aware classifiers is given by the optimal value of a Wasserstein-barycenter problem. More practically, this reformulation leads to a simple procedure for post-processing any pre-trained predictors to satisfy demographic parity in the general setting, which, in particular, yields the optimal fair classifier when applied to the Bayes optimal predictor. We provide suboptimality and finite sample analyses for our procedure, and demonstrate precise control of the tradeoff of error rate for fairness on real-world datasets provided sufficient data.

## 1 Introduction

Machine learning models trained on biased data are observed to propagate and exacerbate the bias against historically underrepresented and disadvantaged demographic groups at inference time (Barocas and Selbst, 2016; Berk et al., 2021). This has prompted studies on aspects of fairness concerning their usage, especially as they expand to high-stakes domains such as criminal justice, healthcare, and finance (Berk et al., 2021). To mitigate the potential bias, a variety of fairness criteria and algorithms have been proposed (Barocas et al., 2019; Caton and Haas, 2020), which impose mathematical or statistical constraints on the model to ensure equal treatment under the respective notion of fairness. Typically, these algorithms induce a cost to model performance as they improve model fairness (Calders et al., 2009; Corbett-Davies et al., 2017).

It is often unclear, however, whether the degraded performance is attributed to artifacts of the algorithm, or possibly to the *inherent tradeoff*—predictive power that must be given up for satisfying the criteria (Hardt et al., 2016; Zhao and Gordon, 2022). Hence, the design of fair and effective algorithms necessitates the understanding of this tradeoff, which would also provide insight to the implications of fairness in machine learning. Yet, it remains open for most fairness criteria and problem settings.

For the group fairness criterion of *demographic parity* (DP; Definition 2.1), a.k.a. statistical parity, which requires statistical independence between model output and demographic group membership (Calders et al., 2009), Le Gouic et al. (2020) and Chzhen et al. (2020) characterized the tradeoff of mean squared error (MSE) for fairness on regression problems. On classification problems, the inherent tradeoff in terms of error rate has only been studied under special cases: Denis et al. (2022) assumed binary groups, Zeng et al. (2022a) and Gaucher et al. (2022) assumed binary

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<sup>1</sup>University of Illinois Urbana-Champaign. {rxian2,langyin2,hanzhao}@illinois.edu.

class labels, and Zhao and Gordon (2022) assumed that the data distribution is *noiseless*, i.e., the (unconstrained) Bayes error rate is zero. Our work closes this gap and completes the characterization of the tradeoff of DP fairness in the most general classification setting.

**Contributions.** This paper considers learning *randomized* and *attribute-aware* classifiers under DP fairness (allowing relaxations) in the general setting of multigroup, multiclass, and potentially *noisy* data distributions with nonzero (unconstrained) Bayes error rate. We show that:

1. The minimum classification error rate under DP is given by the optimal value of a (relaxed) Wasserstein-barycenter problem (Section 3.1).
2. This reformulation reveals that the *optimal fair classifier*, one that satisfies DP while achieving the minimum error, is composed of the (unconstrained) Bayes optimal predictor (minimum MSE regressor of the one-hot labels) and optimal transports, which arise from solving the barycenter problem (Section 3.2).
3. Based on the decomposition, we propose a post-processing procedure that is applicable to any pre-trained predictors for DP fairness (Section 3.3). Our procedure is instantiated to operate on finite samples of unlabeled data (Section 4).

To our knowledge, this is the first DP post-processing procedure for the general classification setting with suboptimality and finite sample analyses.<sup>2</sup>

4. Experiments on real-world datasets demonstrate the effectiveness of our procedure (Section 5). Provided sufficient training data, it achieves precise control of the tradeoff during inference.

## 1.1 Related Work

**Inherent Tradeoff.** Many analyses of the tradeoff of DP fairness leverage the concept of barycenter (reviewed below), because of the analogy to the independence constraint. Intuitively, by treating the barycenter as the model output distribution that is required to be identical across groups, and setting the quantities over which the barycenter is computed to the optimal unconstrained (output) distributions on each group, the sum of distances to the barycenter naturally emerges as the minimum error under DP.

We review such characterizations established in prior work in Table 1, and compare them to ours. Let the input be denoted by  $X$ , group membership by  $A$ , and target variable by  $Y$  (set to the one-hot label on classification problems). Let  $r_a^*$  denote the distribution of the conditional mean,  $\mathbb{E}[Y \mid X, A = a]$ , i.e., the minimum MSE estimates of  $Y$  given  $X$  on each group (for classification, these are the class probabilities). Then under the strict DP constraint, for group-balanced error, on

- regression problems with MSE (Le Gouic et al., 2020; Chzhen et al., 2020), the minimum *excess* risk is given by the Wasserstein-2-barycenter (under the  $\ell_2$  metric) over the  $r_a^*$ 's: Eq. (1);
- noiseless classification problems (Zhao and Gordon, 2022), the minimum (excess) error rate is given by the TV-barycenter over the class marginals,  $p_a^*(e_i) := \mathbb{P}(Y = e_i \mid A = a)$ : Eq. (2), where  $\frac{1}{2} \|\cdot\|_1$  computes the total variation (TV);
- classification in the general setting (ours), the minimum error rate is given by the Wasserstein-1 barycenter (under the  $\ell_1$  metric): Eq. (3).

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<sup>2</sup>Our code is available at <https://github.com/rxian/fair-classification>.

Table 1: Characterizations of the inherent tradeoff of (strict) DP fairness.

Problem Setting	Minimum Achievable Risk	
Regression with MSE (Le Gouic et al., 2020; Chzhen et al., 2020)	excess risk =	$\min_{q: \text{supp}(q) \subseteq \mathbb{R}} \frac{1}{ \mathcal{A} } \sum_{a \in \mathcal{A}} W_2^2(r_a^*, q) \quad (1)$
Noiseless Classification (Zhao and Gordon, 2022)	excess = min. risk =	$\min_{q: \text{supp}(q) \subseteq \{e_1, \dots, e_k\}} \frac{1}{ \mathcal{A} } \sum_{a \in \mathcal{A}} \frac{1}{2} \ p_a^* - q\ _1 \quad (2)$
Classification (Theorem 3.2)	minimum risk =	$\min_{q: \text{supp}(q) \subseteq \{e_1, \dots, e_k\}} \frac{1}{ \mathcal{A} } \sum_{a \in \mathcal{A}} \frac{1}{2} W_1(r_a^*, q) \quad (3)$

First, the barycenter in Eq. (3) is restricted to the vertices of the simplex, which correspond to the one-hot labels. Combined with the fact that the error rate is the expected  $\frac{1}{2}\ell_1$  distance between the true class probabilities and the output labels, the sum of  $\frac{1}{2}W_1$  distances to the barycenter gives the minimum classification error. Similarly, the  $W_2^2$  distance under the  $\ell_2$  metric in Eq. (1) arises from the choice of the MSE loss. Second, our Eq. (3) recovers Eq. (2) in the noiseless setting, under which  $r_a^* = p_a^*$  and  $\frac{1}{2}W_1 = \frac{1}{2}\|\cdot\|_1$ . Denis et al. (2022) and Gaucher et al. (2022) also derived expressions for the tradeoff that resemble ours, but they assumed binary group or class labels.

**Post-Processing.** Given a biased model (e.g., pre-trained on biased data without constraints), this family of algorithms post-process the model to satisfy fairness, e.g., via remapping the outputs (Hardt et al., 2016; Pleiss et al., 2017). For DP fairness, existing procedures include but not limited to Fish et al. (2016); Menon and Williamson (2018); Chzhen et al. (2019); Jiang et al. (2020); Zeng et al. (2022a); Denis et al. (2022), but a major limitation is that they only handle binary group or class labels. In contrast, our proposed DP post-processing procedure works in the most general classification setting, and is accompanied by suboptimality and finite sample analyses. Moreover, it yields the optimal fair classifier when applied to the Bayes optimal predictor.

## 2 Preliminaries

**Notation.** Denote the  $(k-1)$ -dimensional probability simplex by  $\Delta_k := \{x \in \mathbb{R}^k : x \geq 0, \sum_{i=1}^k x_i = 1\}$ , whose  $k$  vertices are  $\{e_1, \dots, e_k\}$ , with  $e_i \in \mathbb{R}^k$  being the vector of all zeros and a single 1 on the  $i$ -th coordinate. Let  $\mathcal{Q}_k$  denote the collection of distributions supported on the vertices of  $\Delta_k$ . We will work with *randomized functions*, whose outputs are not deterministic but rather follow a distribution conditioned on the input; a formal definition via the *Markov kernel* is provided in Definition B.2. Given a (randomized) function  $f : \mathcal{X} \rightarrow \mathcal{Y}$  and a measure  $p$  on  $\mathcal{X}$ , the *push-forward* of  $p$  is denoted by  $f\#p$  (Definition B.3).

**Problem Setup.** A  $k$ -class classification problem is defined by a joint distribution  $\mu$  of input  $X$ , demographic group membership  $A$  (a.k.a. sensitive attribute), and class label  $Y$ , supported on  $\mathcal{X} \times \mathcal{A} \times \mathcal{Y}$ ; the labels may contain noise originating from e.g. the data collection process. We assume a finite number of groups,  $\mathcal{A} = [m] := \{1, \dots, m\}$ , and use one-hot representation for the

class labels, i.e.,  $\mathcal{Y} = \{e_1, \dots, e_k\}$ . We denote the distribution under  $\mu$  conditioned on group  $A = a$  by  $\mu_a$ , and the marginal distribution of input  $X$  by  $\mu^X$ .

For fair classification, we aim to find a *randomized* and *attribute-aware* classifier  $h : \mathcal{X} \times \mathcal{A} \rightarrow \mathcal{Y}$  on  $\mu$  that achieves the minimum group-balanced classification error rate,<sup>3</sup>

$$\text{err}(h; \mu) := \frac{1}{m} \sum_{a \in [m]} \mathbb{P}(h(X, A) \neq Y \mid A = a) = \frac{1}{m} \sum_{a \in [m]} \int_{\mathcal{X} \times \mathcal{Y}} \mathbb{P}(h(x, a) \neq y) d\mu_a(x, y), \quad (4)$$

(the decomposition in the last expression is due to randomization), under the constraints set by the designated fairness criteria. This work considers the group fairness criterion of demographic parity, with relaxations:

**Definition 2.1** (Demographic Parity with Relaxation). Let  $\alpha \in [0, 1]$ . A classifier  $h : \mathcal{X} \times \mathcal{A} \rightarrow \mathcal{Y}$  satisfies  $\alpha$ -DP if  $\Delta_{\text{DP}}(h; \mu) \leq \alpha$ , defined as

$$\begin{aligned} \Delta_{\text{DP}}(h; \mu) &:= \max_{\substack{a, a' \in [m] \\ y \in \mathcal{Y}}} |\mathbb{P}(h(X, A) = y \mid A = a) - \mathbb{P}(h(X, A) = y \mid A = a')| \\ &= \max_{a, a' \in [m]} \|h_{\#}(\mu_a^X \times \{a\}) - h_{\#}(\mu_{a'}^X \times \{a'\})\|_{\infty}, \end{aligned}$$

where  $\|p - q\|_{\infty} := \max_{z \in \mathcal{Z}} |p(z) - q(z)|$  bounds the differences of the pmfs of  $p, q$  uniformly, and

$$\mathbb{P}(h(X, A) = y \mid A = a) = \int_{\mathcal{X}} \mathbb{P}(h(x, a) = y) d\mu_a^X(x)$$

is the proportion of outputs with label  $y$  on group  $a$ .

A classifier is called  $\alpha$ -fair when it satisfies  $\alpha$ -DP, where the parameter  $\alpha$  controls the tradeoff between DP fairness and the maximal attainable accuracy; setting  $\alpha = 0$  recovers the standard strict definition of DP.<sup>4</sup>

Lastly, we make the distinction between a *classifier* and a *predictor*: given an input, whereas the former assigns a class label, the latter outputs a probability vector that estimates the class probabilities, meaning  $f : \mathcal{X} \times \mathcal{A} \rightarrow \Delta_k$  and  $f(x, a)_i \approx \mathbb{P}_{\mu}(Y = e_i \mid X = x, A = a)$ . We denote the component of  $f$  conditioned on group  $a$  by  $f_a(x)$ . The predictor that exactly computes the true class probabilities is called the *Bayes optimal predictor*, and denoted by  $f_{\mu}^*$ , where for all  $(x, a)$ ,

$$f_{\mu, a}^*(x)_i := \mathbb{P}_{\mu_a}(Y = e_i \mid X = x) = \mathbb{E}_{\mu_a}[Y_i \mid X = x];$$

it coincides with the minimum MSE estimator of the one-hot labels  $Y$  given  $(X, A = a)$ . In addition, we will often work with the quantity  $r_{a, \mu}^* := f_{a, \mu}^* \# \mu_a^X$ , which is the distributions of true class probabilities conditioned on group  $a$ .

In this paper, we seek fair classifiers via post-processing (pre-trained) predictors, i.e., finding  $g_1, \dots, g_m : \Delta_k \rightarrow \mathcal{Y}$  s.t. the derived classifier  $h(x, a) = g_a \circ f_a(x)$  is fair.

**Optimal Transport and Wasserstein Distance.** Our study of fair classification involves the concept of optimal transports and Wasserstein distance, which defines a metric between distributions (Villani, 2003).

<sup>3</sup>We extend our results to weighted errors in Appendix A.1, and consider balanced error in the main sections for clarity.

<sup>4</sup>The dependencies of  $f^*$ ,  $r$ ,  $\text{err}$  and  $\Delta_{\text{DP}}$  on  $\mu$  will be omitted.

**Definition 2.2** (Coupling). Let  $p, q$  be probability measures on  $\mathcal{X}$  and  $\mathcal{Y}$ , respectively. A coupling  $\gamma$  of  $p$  and  $q$  is a joint distribution on  $\mathcal{X} \times \mathcal{Y}$  s.t.  $p(x) = \int_{y \in \mathcal{Y}} d\gamma(x, y)$  for all  $x \in \mathcal{X}$ , and  $q(y) = \int_{x \in \mathcal{X}} d\gamma(x, y)$  for all  $y \in \mathcal{Y}$ . We denote the collection of all couplings of  $p$  and  $q$  by  $\Gamma(p, q)$ .

**Definition 2.3** (Optimal Transport). Let  $p, q$  be probability measures on  $\mathcal{X}$  and  $\mathcal{Y}$ , respectively, and  $c : \mathcal{X} \times \mathcal{Y} \rightarrow [0, \infty)$  a cost function. The optimal transportation cost between  $p$  and  $q$  under  $c$  is  $\inf_{\gamma \in \Gamma(p, q)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\gamma(x, y)$ ; let  $\gamma^*$  be a minimizer, then the optimal transport from  $p$  to  $q$ ,  $\mathcal{T}_{p \rightarrow q, c}^* : \mathcal{X} \rightarrow \mathcal{Y}$ , is a (randomized) function s.t.  $\gamma^* = (\text{Id} \times \mathcal{T}_{p \rightarrow q, c}^*) \# p$ , where  $\text{Id}$  denotes the identity map.

Intuitively, the (randomized) function  $\mathcal{T}_{p \rightarrow q, c}^*$  specifies an optimal plan of transporting masses distributed according to  $p$  to  $q$  with the minimum total cost, by moving the mass located at each  $x \in \mathcal{X}$  (probabilistically) to  $\mathcal{T}_{p \rightarrow q, c}^*(x) \in \mathcal{Y}$ . The optimal transport is equivalently represented by the optimal coupling  $\gamma^* \in \Gamma(p, q)$ , because the randomized function  $\mathcal{T}$  satisfying  $\mathbb{P}(\mathcal{T}(X) = y \mid X = x) = \gamma^*(x, y) / \gamma^*(x, \mathcal{Y})$ ,  $\forall x, y$ , is an optimal transport.<sup>5</sup>

Lastly, when  $\mathcal{X} = \mathcal{Y}$  and is a metric space equipped with distance  $d$ , the optimal transportation cost between  $p$  and  $q$  under  $c = d$  coincides with their Wasserstein-1 distance:

**Definition 2.4** (Wasserstein Distance). Let  $p, q$  be probability measures on a metric space  $(\mathcal{X}, d)$ , and  $r \in [1, \infty]$ . The Wasserstein- $r$  distance between  $p$  and  $q$  is

$$W_r(p, q) = \left( \inf_{\gamma \in \Gamma(p, q)} \int_{\mathcal{X} \times \mathcal{X}} d(x, x')^r d\gamma(x, x') \right)^{1/r}.$$

### 3 Fair and Optimal Classification

The first goal of this section is to give a characterization of the inherent tradeoff of DP fairness (Section 3.1), based on which, we will then build a DP post-processing procedure with suboptimality analyses (Sections 3.2 and 3.3).

#### 3.1 Characterizing the Inherent Tradeoff

Our characterization is due to a reformulation of the classification problem assuming access to the Bayes optimal predictor. For any generic classification problem, we have:

**Lemma 3.1.** *Let  $\mu$  with  $|\mathcal{A}| = 1$  be given along with the Bayes optimal predictor  $f^*$ , define  $r^* := f^* \# \mu^X$ , and fix  $q \in \mathcal{Q}_k$ . Then for any (randomized) classifier  $h : \mathcal{X} \rightarrow \mathcal{Y}$  satisfying  $h \# \mu^X = q$ , there exists a coupling  $\gamma \in \Gamma(r^*, q)$  s.t.*

$$\text{err}(h) = \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 d\gamma(s, y).$$

*Conversely, for any  $\gamma \in \Gamma(r^*, q)$ , there exists a randomized classifier  $h$  satisfying  $h \# \mu^X = q$  s.t. the above equality holds.*

The reformulation converts the problem of minimizing classification error while satisfying the output distribution of  $q \in \mathcal{Q}_k$  into an optimal transport problem from  $r^*$  to  $q$  under the  $\ell_1$  cost, because by Definition 2.4,

$$\min_{h: h \# \mu^X = q} \text{err}(h) = \frac{1}{2} \min_{\gamma \in \Gamma(r^*, q)} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 d\gamma(s, y) = \frac{1}{2} W_1(r^*, q).$$

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<sup>5</sup>We will only consider transportation under the of  $\ell_1$  cost of  $(x, y) \mapsto \|x - y\|_1$ , hence omit the dependency of  $\mathcal{T}_{p \rightarrow q}^*$  on  $c$ .

This is particularly convenient to the analysis of DP fairness, which only puts constraints on the output distributions,  $q_a := h^\#(\mu_a^X \times \{a\})$ ,  $\forall a \in [m]$ : from Definition 2.1,

$$\Delta_{\text{DP}}(h) \leq \alpha \iff \max_{a, a' \in [m]} \|q_a - q_{a'}\|_\infty \leq \alpha.$$

Therefore, for attribute-aware classifiers, where the components on each group,  $h(\cdot, a)$ , can be optimized independently, the discussions above directly lead to the following characterization of the minimum error rate under DP:

**Theorem 3.2** (Minimum Error Rate Under DP). *Let  $\mu$  be given along with Bayes optimal predictor  $f_a^*$ 's, and  $\alpha \in [0, 1]$ . Let  $r_a^* := f_a^\# \mu_a^X$ ,  $\forall a \in [m]$ , then with  $W_1$  under the  $\ell_1$  metric,  $\min_{h: \Delta_{\text{DP}}(h) \leq \alpha} \text{err}(h) = \text{err}_\alpha^*$ , where*

$$\text{err}_\alpha^* := \min_{\substack{q_1, \dots, q_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q_a - q_{a'}\|_\infty \leq \alpha}} \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a^*, q_a). \quad (5)$$

It is described as a *relaxed Wasserstein-barycenter problem* of the  $r_a^*$ 's restricted to the vertices, because when  $\alpha = 0$ ,  $q_1 = \dots = q_m \in \mathcal{Q}_k$  and represent the barycenter under  $W_1$  distance. It is a convex problem (in the primal form presented above), and can be simplified given assumptions: in the noiseless setting with  $\alpha = 0$ , it reduces to the TV-barycenter problem in Eq. (2). Zhao and Gordon (2022) established this equality for  $m = k = 2$ , whereas our reduction in Theorem A.2 holds generally.

Under strict DP ( $\alpha = 0$ ), the inherent tradeoff, namely the excess risk induced by the DP constraint, is

$$\frac{1}{2m} \left( \min_{q \in \mathcal{Q}_k} \sum_{a \in [m]} W_1(r_a^*, q) - \sum_{a \in [m]} \min_{q_a \in \mathcal{Q}_k} W_1(r_a^*, q_a) \right) \geq 0,$$

where the second term is the Bayes error rate and is achieved by the classifier  $(x, a) \mapsto e_{\arg \max_i f_a^*(x)_i}$ . So we may expect the tradeoff to be larger on problem instances where the  $r_a^*$ 's differ, and equal to zero when they are identical ( $\mathbb{E}_\mu[Y | X, A] \perp\!\!\!\perp A$ ), since all groups would have the same optimal decision rule.

However, we point out that the tradeoff could be zero even if  $\mathbb{E}_\mu[Y | X, A] \not\perp\!\!\!\perp A$ , meaning that on such instances, enforcing DP would not degrade model performance. These scenarios arise from the nonuniqueness of the optimal classifier, which we illustrate in Example A.5.

Lastly, Zhao and Gordon (2022) concluded that in the noiseless setting, the tradeoff is zero iff the class marginals are the same,  $\mathbb{E}_\mu[Y | A] \perp\!\!\!\perp A$ . But this is no longer sufficient in the general noisy setting, by a counterexample (Example A.6).

### 3.2 Optimal Fair Classifier via Post-Processing

Theorem 3.2 only reformulates the fair classification problem, but the construction used in the proof of Lemma 3.1 for the equivalence (deferred to Appendix B) provides that the optimal fair classifier can be obtained by composing the Bayes optimal predictors  $f_a^*$  with post-processing functions.

More precisely, the post-processing functions are the optimal transport from  $r_a^*$ 's to the minimizing  $q_a^*$ 's of Eq. (5) (see Fig. 1 for a picture of these distributions):

**Theorem 3.3** (Optimal Classifier Under DP). *Let  $\alpha \in [0, 1]$ ,  $q_1^*, \dots, q_m^*$  be a minimizer of Eq. (5), and  $\mathcal{T}_{r_a^* \rightarrow q_a^*}^*$  the optimal transport from  $r_a^*$  to  $q_a^*$  under the  $\ell_1$  cost. Then*

$$(x, a) \mapsto \mathcal{T}_{r_a^* \rightarrow q_a^*}^* \circ f_a^*(x) \in \arg \min_{h: \Delta_{\text{DP}}(h) \leq \alpha} \text{err}(h).$$

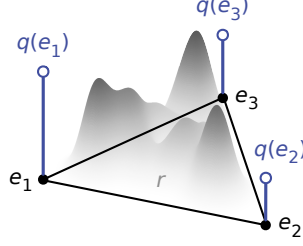


Figure 1: A distribution  $r$  on the 2d simplex  $\Delta_3$  (grey surface), and a distribution  $q \in \mathcal{Q}_3$  on the vertices  $\{e_1, e_2, e_3\}$  (blue spikes).

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**Algorithm 1** Post-Process Predictor for  $\alpha$ -DP

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- 1: **Input:** marginal input distributions  $\mu_1^X, \dots, \mu_m^X$ , predictors  $f_1, \dots, f_m : \mathcal{X} \rightarrow \Delta_k$ , relaxation  $\alpha \in [0, 1]$
  - 2:  $r_a := f_a \# \mu_a^X, \forall a \in [m]$
  - 3:  $q_1, \dots, q_m \leftarrow$  minimizer of Eq. (5) on  $r_1, \dots, r_m, \alpha$   $\triangleright$  relaxed barycenter problem
  - 4: **for**  $a = 1$  **to**  $m$  **do**
  - 5:    $\mathcal{T}_{r_a \rightarrow q_a}^* \leftarrow$   $r_a$  to  $q_a$  optimal transport under  $\ell_1$  cost
  - 6: **end for**
  - 7: **Return:**  $(x, a) \mapsto \mathcal{T}_{r_a \rightarrow q_a}^* \circ f_a(x)$
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To summarize, optimal fair classifiers can be computed in 3 steps: (1) learn  $f_a^*$  by minimizing MSE w.r.t. the one-hot  $Y$ ,

$$f_a^* = \arg \min_{f: \mathcal{X} \rightarrow \Delta_k} \mathbb{E}_\mu [\|f(X) - Y\|_2^2 \mid A = a], \quad (6)$$

(2) find the minimizing  $q_a^*$ 's of Eq. (5), the barycenter problem, and (3) compute the optimal transports  $\mathcal{T}_{r_a^* \rightarrow q_a^*}^*$ , then return  $(x, a) \mapsto \mathcal{T}_{r_a^* \rightarrow q_a^*}^* \circ f_a^*(x)$ . The last two are post-processing steps, reproduced in Algorithm 1.

In practice, however, the Bayes optimal  $f_a^*$ 's may not be exactly obtained due to computational cost, or difficulties in representation, optimization, and generalization (Woodworth et al., 2017). Instead, we will often work with suboptimal predictors  $f_a \approx f_a^*$  (pre-trained by a vendor). The following section analyzes the applicability of Algorithm 1 to post-processing  $f_a$ 's that are not Bayes optimal.

### 3.3 Post-Processing Pre-Trained Predictors

Let  $f_1, \dots, f_m : \mathcal{X} \rightarrow \Delta_k$  be arbitrary (randomized) predictors on each group. We want to find post-processing functions  $g_a : \Delta_k \rightarrow \mathcal{Y}$  such that when applied to  $f_a$ , the derived classifier  $(x, a) \mapsto g_a \circ f_a(x)$  satisfies fairness, and ideally achieves the minimum error rate among all fair classifiers derived from the  $f_a$ 's.

The classifier returned from calling Algorithm 1 on the  $f_a$ 's,  $\bar{h}(x, a) := \mathcal{T}_{r_a \rightarrow q_a}^* \circ f_a(x)$  (where  $r_a := f_a \# \mu_a^X$ ), is  $\alpha$ -fair, because  $\bar{h} \# (\mu_a^X \times \{a\}) = q_a$  for all  $a$  by construction, and  $\Delta_{\text{DP}}(\bar{h}) = \max_{a, a'} \|q_a - q_{a'}\|_\infty \leq \alpha$  from Eq. (5) constraints. Its suboptimality can be upper bounded by the  $L^1$  error of the  $f_a$ 's w.r.t. the Bayes optimal predictors  $f_a^*$ :

**Theorem 3.4** (Error Propagation). *Let predictor  $f_a$ 's be given,  $\alpha \in [0, 1]$ , and  $\text{err}_\alpha^*$  as in Eq. (5). For the  $\alpha$ -fair classifier  $\bar{h}$  returned from Algorithm 1,*

$$0 \leq \text{err}(\bar{h}) - \text{err}_\alpha^* \leq \frac{1}{m} \sum_{a \in [m]} \mathbb{E}_{\mu_a^X}[\|f_a(X) - f_a^*(X)\|_1].$$

Hence, while the decrease in performance of the post-processed  $\bar{h}$  when  $f_a = f_a^*$  the Bayes optimal predictor is attributed entirely to the inherent tradeoff (Theorem 3.3), this may not be the case if  $f_a \neq f_a^*$ , due to information loss. But, to guarantee that the returned  $\bar{h}$  is (at least) optimal among all fair classifiers derived from  $f_a$ , we require them to be *calibrated* prior to calling Algorithm 1:

**Definition 3.5** (Calibration). Let  $\mu$  with  $|\mathcal{A}| = 1$  be given. The predictor  $f : \mathcal{X} \rightarrow \Delta_k$  is said to be calibrated if  $\mathbb{P}_\mu(Y = e_i \mid f(X) = s) = s_i$  for all  $s \in \Delta_k$  and  $i \in [k]$ .

The predictors  $f_a$ 's can be calibrated by composing with calibration maps  $u_a : \Delta_k \rightarrow \Delta_k$  as extra post-processing. The optimal calibration maps  $u_a^*$ 's (in the sense that no further information loss is incurred) are by definition the minimum MSE estimators of  $Y$  given  $(f_a(X), A = a)$ , which can be learned from labeled data. When the  $f_a$ 's are already calibrated (e.g., Bayes optimal predictors),  $u_a^* = \text{Id}$  identity map. Alternatively, calibration could be achieved with more efficient methods, e.g., Guo et al. (2017) calibrates neural networks via histogram binning.

Note that finding the optimal fair post-processing functions on the  $f_a$ 's is equivalent to finding the optimal fair classifier on a new problem  $\mu'$  derived from the original  $\mu$  under an input transformation—the joint distribution of  $(f_A(X), A, Y)$ . Also, the Bayes optimal predictors on  $\mu'$  coincide with the optimal calibration maps,  $\mathbb{E}_{\mu'}[Y \mid X' = s, A = a] = u_a^*(s)$ . Hence, by Theorem 3.3, the optimal fair classifier on  $\mu'$  equal the post-processing maps found by Algorithm 1 on the optimally calibrated predictors,  $u_a^* \circ f_a$ , which implies that the returned  $\bar{h}$  is optimal among all derived fair classifiers. Lastly, we remark that the suboptimality due to miscalibration can also be bounded using Theorem 3.4 after replacing  $f_a^*$  in the statement with  $u_a^* \circ f_a$ .

## 4 Algorithms for Finite Samples

In this section, we instantiate our proposed DP post-processing procedure, Algorithm 1, to scenarios where only finite (unlabeled) samples are available:

**Assumption 4.1.** We have  $n$  i.i.d. samples of  $X$  conditioned on each group  $a \in [m]$ ,  $S_a := (x_{a,i})_{i=1}^n$ ,  $x_{a,i} \sim \mu_a^X$ , which are independent of the predictor  $f_a$ 's being post-processed.

We provide finite sample guarantees for both the fairness and the error rate of the returned classifier; the latter is stated in terms of the suboptimality relative to the optimal fair classifier derived from calibrated versions of the predictors:

**Assumption 4.2.** The predictor  $f_a$ 's being post-processed are *calibrated*. Let  $r_a := f_a \# \mu_a^X$ , by discussions in Section 3.3, the optimal derived  $\alpha$ -fair classifier has error rate

$$\text{err}_{\alpha,f}^* := \min_{\substack{q_1, \dots, q_m \in \mathcal{Q}_k \\ \max_{a,a'} \|q_a - q_{a'}\|_\infty \leq \alpha}} \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a, q_a).$$



## 4.1 The Finite Case

We begin with the case where the  $\text{supp}(r_a) =: \mathcal{R}_a$ 's are finite (but the input distribution  $\mu^X$  need not be finite). Note that this covers the scenario of post-processing pre-trained *classifiers*,  $f_a : \mathcal{X} \rightarrow \mathcal{Y}$ , which have a finite output space.

If the true probability mass of the  $r_a$ 's are known, then Algorithm 1 is instantiated by a linear program:

$$\begin{aligned} \text{LP}(r_1, \dots, r_m, \alpha) : \quad & \min_{\substack{q_1, \dots, q_m \\ \gamma_1, \dots, \gamma_m}} \sum_{a \in [m]} \sum_{s \in \mathcal{R}_a, y \in \mathcal{Y}} \|s - y\|_1 \cdot \gamma_a(s, y) \\ \text{s.t.} \quad & \sum_{s' \in \mathcal{R}_a} \gamma_a(s', y) = q_a(y), \quad \forall a \in [m], y \in \mathcal{Y}, \\ & \sum_{y' \in \mathcal{Y}} \gamma_a(s, y') = r_a(s), \quad \forall a \in [m], s \in \mathcal{R}_a, \\ & |q_a(y) - q_{a'}(y)| \leq \alpha, \quad \forall a, a' \in [m], y \in \mathcal{Y}, \\ & q_a \geq 0, \quad \gamma_a \geq 0, \quad \forall a \in [m], \end{aligned}$$

where  $q_1, \dots, q_m \in \mathbb{R}^k$ , and  $\gamma_a \in \mathbb{R}^{|\mathcal{R}_a| \times k}$ . This program simultaneously finds the minimizers  $q_1^*, \dots, q_m^*$  of the relaxed barycenter problem in Eq. (5) and the optimal transports in Theorem 3.3, which are stored in the solution  $\gamma_1^*, \dots, \gamma_m^*$  of LP: each  $\mathcal{T}_{r_a \rightarrow q^*}^*$  is a randomized function satisfying  $\mathbb{P}(\mathcal{T}_{r_a \rightarrow q^*}^*(R) = y \mid R = s) = \gamma_a^*(s, y) / \sum_{y' \in \mathcal{Y}} \gamma_a^*(s, y')$ , for all  $s \in \mathcal{R}_a$ .

If the pmfs of the  $r_a$ 's are unknown but finite samples  $S_a$  are given, we proceed with the empirical pmfs,  $\hat{r}_a := \frac{1}{n} \sum_{i=1}^n \delta_{f_a(x_{a,i})}$ , where  $\delta$  denotes the Dirac delta function, and estimate  $\hat{q}_a$  and compute the  $\hat{\mathcal{T}}_{\hat{r}_a \rightarrow \hat{q}_a}^*$ 's by solving  $\text{LP}(\hat{r}_1, \dots, \hat{r}_m, \alpha)$ . Then, we post-process the predictors via  $\hat{h}(x, a) = \mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^* \circ f_a(x)$  (assign arbitrary label to unseen inputs during inference,  $f_a(x) \notin f_a(S_a)$ ). It has the following guarantees:

**Theorem 4.3** (Generalization, Finite Case). *Let predictor  $f_a$ 's be given, and  $\alpha \in [0, 1]$ . Under Assumption 4.1, let  $|\mathcal{R}| := \max_a |\text{supp}(r_a)|$ , w.p. at least  $1 - \delta$  over the random draw of the samples, for the classifier  $\hat{h}$  derived from above,*

$$\Delta_{\text{DP}}(\hat{h}) \leq \alpha + \sqrt{\frac{128|\mathcal{R}|}{n} \left( \frac{1}{4} + \ln \left( \frac{2mk}{\delta} \right) \right)},$$

and additionally with Assumption 4.2,

$$\text{err}(\hat{h}) - \text{err}_{\alpha, f}^* \leq \sqrt{\frac{72|\mathcal{R}|}{n} \left( \frac{1}{4} + \ln \left( \frac{2m}{\delta} \right) \right)}.$$

## 4.2 The Continuous Case

When the  $r_a$ 's are continuous,<sup>6</sup> we may still use the program  $\text{LP}(\hat{r}_1, \dots, \hat{r}_m, \alpha)$  to estimate the optimal target output distributions,  $\hat{q}_1, \dots, \hat{q}_m$ , but the empirical transports  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$  are no longer usable for post-processing here, since the inputs at inference time will be unseen almost surely ( $f_a(x) \notin f_a(S_a)$ ). Instead, after obtaining the  $\hat{q}_a$ 's, we need to approximate the optimal transports  $\mathcal{T}_{r_a \rightarrow \hat{q}_a}^*$  from  $r_a$ 's (population) to the  $\hat{q}_a$ 's from finite samples for all  $a \in [m]$ .

<sup>6</sup>I.e., the probability measure does not give mass to sets whose intersection with  $\Delta_k$  has Hausdorff dimension less than  $k - 1$ .

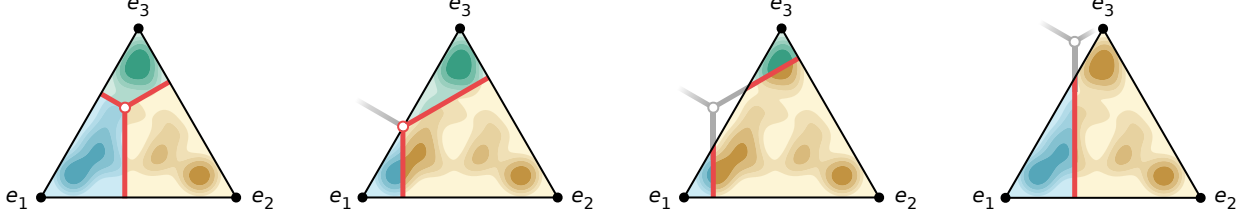


Figure 2: Examples of simplex-vertex optimal transports for  $k = 3$  (vertex distributions are different). All points in the lower-left blue partition are transported to  $e_1$ , lower-right yellow to  $e_2$ , and upper green to  $e_3$ . The transports are described by a Y-shaped boundary.

Note that this is a semi-discrete optimal transport problem, studied in a long line of work (Genevay et al., 2016; Staib et al., 2017; Chen et al., 2019), where a common procedure is to reformulate optimal transport as a convex optimization problem over a vector  $\psi_a \in \mathbb{R}^k$  using the Kantorovich-Rubinstein dual and the  $c$ -transform of the Kantorovich potential  $\phi_a$ . Namely, for each  $a \in [m]$ ,

$$\begin{aligned} \inf_{\gamma_a \in \Gamma(r_a, \hat{q}_a)} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 d\gamma_a(s, y) &= \sup_{\substack{\phi_a: \Delta_k \rightarrow \mathbb{R}, \psi_a \in \mathbb{R}^k \\ \phi_a(s) + \psi_{a,i} \leq \|s - e_i\|_1}} \left( \int_{\Delta_k} \phi_a(s) dr_a(s) + \sum_{i=1}^k \psi_{a,i} \hat{q}_a(e_i) \right) \\ &= \sup_{\psi_a \in \mathbb{R}^k} \left( \int_{\Delta_k} \min_i (\|s - e_i\|_1 - \psi_{a,i}) dr_a(s) + \sum_{i=1}^k \psi_{a,i} \hat{q}_a(e_i) \right), \end{aligned}$$

whereby the optimal  $\psi_a^*$  can be found by e.g. (stochastic) gradient ascent w.r.t. the last expression. Moreover, Gangbo and McCann (1996) showed that in the semi-discrete case, the optimal transport  $\mathcal{T}_{r_a \rightarrow \hat{q}_a}^*$  belongs to the class of deterministic functions of

$$\mathcal{G}_k := \left\{ s \mapsto e_{\arg \min_{i \in [k]} (\|s - e_i\|_1 - \psi_i)} : \psi \in \mathbb{R}^k \right\}$$

(break ties to the tied  $e_i$  with the largest index  $i$ ); specifically, it is equal to the function with parameter  $\psi_a^*$ . Pictures of semi-discrete optimal transports for  $k = 3$  are included in Fig. 2.

The proof of Gangbo and McCann (1996) required the cost function to be strictly convex and superlinear (Assumptions H1 to H3 in their paper), which are not satisfied by our  $\ell_1$  cost (Ambrosio and Pratelli, 2003). Therefore, for our simplex-vertex transportation problem under the  $\ell_1$  cost, we give a proof in Appendix D for the existence and uniqueness of the optimal transport in  $\mathcal{G}_k$  via analyzing its geometry.

**Our Implementation.** The optimal transports  $\mathcal{T}_{r_a \rightarrow \hat{q}_a}^*$  can be estimated via solving an extra set of optimization problems subsequent to obtaining the  $\hat{q}_a$ 's from LP. But curiously, is it possible to eliminate this step, and instead, extract a set of transport mappings directly from the solution  $\gamma_a^*$  to LP (equivalently,  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}}^*$ ) good enough for post-processing? Yes!

Algorithm 2 details our post-processing procedure for finite samples in the continuous case. We highlight Lines 6–9, where transport mappings  $\mathcal{T}_a$  are extracted from empirical transports  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}}^*$  returned from LP; a step-by-step illustration is provided in Fig. 3, and formal derivations are deferred to Appendix D, which arise from the geometric analysis of the optimal transport. Each  $\mathcal{T}_a$  has the property that it agrees with  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}}^*$  on all points in  $S_a$  that do not lie on the boundaries of  $\mathcal{T}_a$ . Since the boundaries are described by at most  $\binom{k}{2}$  hyperplanes, the number of disagreements is almost

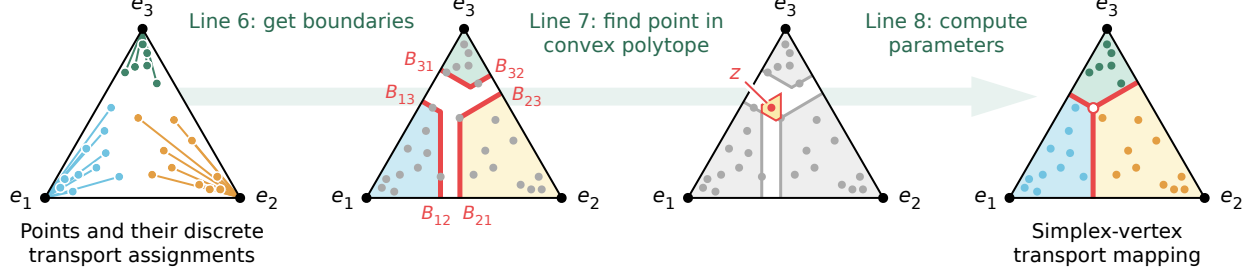


Figure 3: Extract a simplex-vertex transport  $\mathcal{T} \in \mathcal{G}_3$  that agrees with the discrete optimal transport (except for points that lie on the boundaries), corresponding to Lines 6–9 of Algorithm 2. For illustration, the discrete transport on the left does not split mass.

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**Algorithm 2** Post-Process Predictor for  $\alpha$ -DP (Finite Samples, Continuous Case)

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- 1: **Input:** unlabeled samples  $S_1, \dots, S_m$ , predictors  $f_1, \dots, f_m : \mathcal{X} \rightarrow \Delta_k$ , relaxation  $\alpha \in [0, 1]$
  - 2:  $\hat{r}_a := \frac{1}{|S_a|} \sum_{x \in S_a} \delta_{f_a(x)}, \forall a \in [m]$
  - 3:  $\gamma_1, \dots, \gamma_m \leftarrow$  minimizer of  $\text{LP}(\hat{r}_1, \dots, \hat{r}_m, \alpha)$   $\triangleright$  relaxed barycenter problem in finite case
  - 4:  $v_{ij} := e_j - e_i$
  - 5: **for**  $a = 1$  **to**  $m$  **do**  $\triangleright$  extract transports
  - 6:    $B_{ij} \leftarrow \max\{f_a(x)^\top v_{ij} + 1 : x \in S_a, \gamma_a(f_a(x), e_i) > 0\} \cup \{0\}$
  - 7:    $z \leftarrow$  point in  $\bigcap_{i \neq j} \{x \in \mathbb{R}^k : x^\top v_{ij} \geq B_{ij} - 1\}$   $\triangleright$  arbitrary; always exists
  - 8:    $\psi_i \leftarrow 2z^\top v_{i1}, \forall i \in [k]$
  - 9:    $\mathcal{T}_a \leftarrow (s \mapsto e_{\arg \min_{i \in [k]} (\|s - e_i\|_1 - \psi_i)})$
  - 10: **end for**
  - 11: **Return:**  $(x, a) \mapsto \mathcal{T}_a \circ f_a(x)$
- 

surely  $O(k^2)$ . And thanks to the low complexity of  $\mathcal{G}_k \ni \mathcal{T}_a$  (Theorem D.2), classifiers derived using Algorithm 2 have the following guarantees:

**Theorem 4.4** (Generalization, Continuous Case). *Let predictor  $f_a$ 's be given, and  $\alpha \in [0, 1]$ . Under Assumption 4.1, w.p. at least  $1 - \delta$  over the random draw of the samples, for the classifier  $\hat{h}$  returned from Algorithm 2,*

$$\Delta_{\text{DP}}(\hat{h}) \leq \alpha + O\left(\sqrt{\frac{k}{n} \ln\left(\frac{mk}{\delta}\right)} + \frac{k}{n}\right),$$

and additionally with Assumption 4.2,

$$\text{err}(\hat{h}) - \text{err}_{\alpha, f}^* \leq O\left(\sqrt{\frac{k}{n} \ln\left(\frac{nm}{k\delta}\right)} + \frac{k^2}{n}\right).$$

The first term in both expressions is from standard sample complexity analysis, and the second term is attributed to the aforementioned disagreements.

### 4.3 The General Case

For completeness, we briefly discuss post-processing in the general case where the  $r_a$ 's are neither finite nor purely continuous (i.e., they contain atoms) via distribution smoothing.

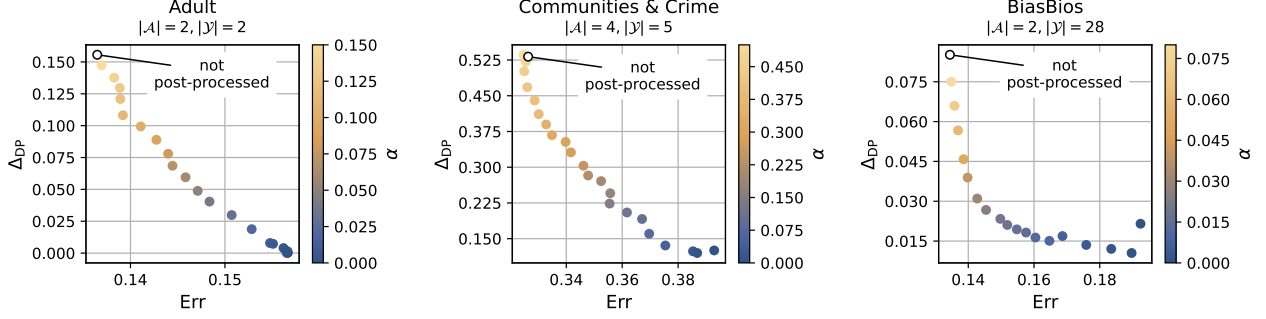


Figure 4: Group-balanced error rate (Eq. (4)) and DP fairness ( $\Delta_{\text{DP}}$ ; Definition 2.1) of classifiers post-processed using Algorithm 2, under varying settings for  $\alpha$ . The number of groups  $\mathcal{A}$  and classes  $\mathcal{Y}$  on each task are included.

Let  $\rho_s$  be a continuous distribution<sup>6</sup> with finite first moment (potentially depends on  $s$ ), and  $u_\rho$  a randomized function s.t.  $u_\rho(s) \sim s + N$  with  $N \sim \rho_s$  as i.i.d. random noise. Let  $q_a$ 's denote the minimizer of the relaxed barycenter problem in Eq. (5) on the  $r_a$ 's with  $\alpha$ , and  $\mathcal{T}_{\tilde{r}_a \rightarrow q_a}^*$  the optimal transport from  $\tilde{r}_a := u_\rho \# r_a$  to  $q_a$  (can be obtained with the method in Algorithm 2 if  $\text{supp}(\tilde{r}_a) \subseteq \Delta_k$ ). Then the classifier given by  $\bar{h}_\rho(x, a) := \mathcal{T}_{\tilde{r}_a \rightarrow q_a}^* \circ u_\rho \circ f_a(x)$  is  $\alpha$ -fair, and its suboptimality is controlled via the *bandwidth* of  $\rho_s$ :

**Theorem 4.5** (Error Propagation, Smoothing). *Let predictor  $f_a$ 's be given, and  $\alpha \in [0, 1]$ . Under Assumption 4.2, for the  $\alpha$ -fair classifier  $\bar{h}_\rho$  derived from above,*

$$0 \leq \text{err}(\bar{h}_\rho) - \text{err}_{\alpha, f}^* \leq \frac{1}{m} \sum_{a \in [m]} \mathbb{E}_{N \sim \rho_s, s \sim r_a} [\|N\|_1].$$

E.g., if  $\rho = \text{Laplace}(0, b \cdot I_k)$ , then  $\mathbb{E}[\|N\|_1] = kb$ , and the suboptimality attributed to smoothing is less than  $kb$ .

## 5 Experiments

To demonstrate the effectiveness of our post-processing procedure, we apply Algorithm 2 (LP is computed using linear program solvers) on three real-world benchmark datasets: the Adult (Kohavi, 1996) and Communities & Crime tabular datasets (Redmond and Baveja, 2002), and the BiasBios text dataset (De-Arteaga et al., 2019). The pre-trained attribute-aware predictors on which Algorithm 2 is applied are trained to minimize MSE of the one-hot class labels *without constraints*. We use linear predictors (learned via OLS) on the tabular datasets, and a fine-tuned BERT base neural language model on BiasBios (Devlin et al., 2019). The training data are split for pre-training and post-processing. Descriptions of the datasets, the classification tasks, and further experiment details are in Appendix E.

**Results.** Figure 4 presents the test set evaluation results of post-processed classifiers returned from Algorithm 2 under varying settings of  $\alpha$ . On all datasets, the post-processing procedure reduces the bias (i.e.  $\Delta_{\text{DP}}$ ) without significant increases to the error rate, and their tradeoff is effectively adjusted via  $\alpha$ . Note that almost precise control of  $\Delta_{\text{DP}}$  is achieved on the Adult dataset, which contains sufficient number of (unlabeled) training data for generalization.

Under strict DP ( $\alpha = 0$ ), near-zero  $\Delta_{\text{DP}}$  is attained on Adult (see Table 2 for numbers), but not on the other two datasets due to generalization error (Communities & Crime is a small dataset, and BiasBios has many classes) or potentially the violation of the continuous assumption required by Algorithm 2 (Section 4.2). The latter could be remedied by, e.g., the smoothing procedure discussed in Section 4.3; after smoothing with a Dirichlet distribution, we observed further improvements to  $\Delta_{\text{DP}}$  in Table 2 of Appendix E.3. Lastly, as discussed in Section 3.3—although not empirically explored here—lower error rates are possible if the predictors were calibrated prior to post-processing.

## 6 Further Related Work

Fairness criteria are generally categorized into individual fairness (Dwork et al., 2012; Sharifi-Malvajerdi et al., 2019), subgroup (Kearns et al., 2018), and group fairness (Zemel et al., 2013; Hardt et al., 2016; Kleinberg et al., 2017; Verma and Rubin, 2018). A predictive model is said to satisfy individual fairness if it treats *similar* individuals similarly; the practical challenge with this notion of fairness lies in the specification of the similarity measure, which needs to be application and context dependent. On the other hand, (sub)group fairness, to which demographic parity belongs, is defined on population-level statistics, e.g., true positive and/or negative rates (Hardt et al., 2016), predictive rates (Chouldechova, 2017; Berk et al., 2021; Zeng et al., 2022b), accuracy (Buolamwini and Gebru, 2018), etc.

For mitigating the bias in machine learning models under the fairness criteria, a variety of algorithms have been proposed. Besides post-processing, there are methods based on data pre-processing (Calmon et al., 2017; Song et al., 2019), constrained optimization (Kamishima et al., 2012; Zafar et al., 2017; Agarwal et al., 2019), and fair representation learning (Zemel et al., 2013; Madras et al., 2018; Zhao et al., 2020). There are also methods under other learning paradigms, such as unsupervised learning (Chierichetti et al., 2017; Backurs et al., 2019; Li et al., 2020), ranking (Zehlike et al., 2017), and sequential decision making (Joseph et al., 2016, 2017; Gillen et al., 2018; Chi et al., 2022).

## 7 Conclusion

In this paper, we characterized the inherent tradeoff of DP fairness on classification problems in the most general setting, and proposed a post-processing procedure with generalization guarantees. Our implementation uses linear program solvers; while they enjoy stability and consistent performance, a potential concern is scalability to larger numbers of classes or samples. It would be of practical value to analyze an implementation that uses more runtime-efficient optimization methods, e.g., gradient descent.

Technically, we studied the geometry of the optimal transport between distributions supported on the simplex and its vertices. A main result is that when the distributions are semi-discrete, the optimal transport is unique, and is given by the  $c$ -transform of the Kantorovich potential, including under the  $\ell_1$  cost. This result may be of independent theoretical interest to the community.

Our results add to the line of work that study the inherent tradeoffs of fairness criteria, which we believe would benefit practitioners in the design of fair machine learning systems, and contribute to a better understanding of the implications of fairness in machine learning.

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## A Additional Discussions on Theorem 3.2

This section contains deferred discussions on Theorem 3.2: the extension to arbitrarily group-weighted classification error (Appendix A.1), the reduction to TV-barycenter in the noiseless setting (Appendix A.2), and providing examples to the remarks (Appendix A.3).

### A.1 Group-Weighted Classification Error Rates

For clarity, in the main sections, we focused on group-balanced classification error. But our results apply generally to arbitrarily group-weighted error via an extension of Theorem 3.2.

Let  $w_1, \dots, w_m \geq 0$  denote a set of nonnegative weights assigned to each group, and define group-weighted classification error under  $w$  by

$$\text{err}_w(h) := \sum_{a \in [m]} w_a \mathbb{P}(h(X, A) \neq Y \mid A = a).$$

**Theorem A.1** (Full Version of Theorem 3.2). *Let  $\mu$  be given along with Bayes optimal predictor  $f_a^*$ 's,  $\alpha \in [0, 1]$ , and  $w_1, \dots, w_m \geq 0$ . Let  $r_a^* := f_a^* \# \mu_a^X$ ,  $\forall a \in [m]$ , then with  $W_1$  under the  $\ell_1$  metric,*

$$\min_{h: \Delta_{\text{DP}}(h) \leq \alpha} \text{err}_w(h) = \min_{\substack{q_1, \dots, q_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q_a - q_{a'}\|_\infty \leq \alpha}} \sum_{a \in [m]} w_a \cdot \frac{1}{2} W_1(r_a^*, q_a).$$

*Proof.* Lemma 3.1 implies that for each  $a \in [m]$  and fixed  $q_a \in \mathcal{Q}_k$ , the minimum error rate on group  $a$ , denoted by  $\text{err}_a$ , among randomized classifiers  $h_a : \mathcal{X} \rightarrow \mathcal{Y}$  whose output distribution equals to  $q_a$ , is given by

$$\min_{h_a: h_a \# \mu_a^X = q_a} \text{err}_a(h_a) := \min_{h_a: h_a \# \mu_a^X = q_a} \mathbb{P}(h_a(X) \neq Y \mid A = a) = \frac{1}{2} W_1(r_a^*, q_a).$$

Because of attribute-awareness, we can optimize each component of  $h : \mathcal{X} \times \mathcal{A} \rightarrow \mathcal{Y}$ ,  $h(\cdot, a) =: h_a$  for all  $a \in [m]$ , independently. So for any set of fixed  $q_1, \dots, q_m \in \mathcal{Q}_k$ ,

$$\min_{h: h_a \# \mu_a^X = q_a, \forall a} \text{err}_w(h) = \sum_{a \in [m]} w_a \cdot \min_{h_a: h_a \# \mu_a^X = q_a} \text{err}_a(h_a) = \sum_{a \in [m]} w_a \cdot \frac{1}{2} W_1(r_a^*, q_a).$$

Incorporating the  $\alpha$ -DP constraint, we get

$$\begin{aligned} \min_{h: \Delta_{\text{DP}}(h) \leq \alpha} \text{err}_w(h) &= \min_{\substack{q_1, \dots, q_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q_a - q_{a'}\|_\infty \leq \alpha}} \min_{h: h_a \# \mu_a^X = q_a, \forall a} \text{err}_w(h) \\ &= \min_{\substack{q_1, \dots, q_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q_a - q_{a'}\|_\infty \leq \alpha}} \sum_{a \in [m]} w_a \cdot \frac{1}{2} W_1(r_a^*, q_a). \end{aligned}$$

□

### A.2 Reduction to TV-Barycenter in Noiseless Setting

When the classification problem  $\mu$  is noiseless, i.e., the (unconstrained) Bayes error rate is zero,  $\min_h \text{err}(h) = 0$ , we show that Theorem 3.2 reduces to a relaxed TV-barycenter problem. For strict DP ( $\alpha = 0$ ), this result is previously established by Zhao and Gordon (2022) for the binary case of  $m = k = 2$ . Our reduction here holds for the general case.

Note that noiselessness means that there exist deterministic labeling functions  $y_a : \mathcal{X} \rightarrow \mathcal{Y}$  for each  $a \in [m]$  s.t.  $Y = y_A(X)$  almost surely. Therefore, the Bayes optimal predictors  $f_a^* = y_a$ , and we have

$$r_a^* = p_a^* := f_a^* \# \mu_a^X \quad \text{where} \quad p_a^*(e_i) = \mathbb{P}_\mu(Y = e_i \mid A = a).$$

**Theorem A.2** (Minimum Error Rate Under DP, Noiseless Setting). *Let noiseless  $\mu$  be given, and  $\alpha \in [0, 1]$ . Then*

$$\begin{aligned} \min_{h: \Delta_{\text{DP}}(h) \leq \alpha} \text{err}(h) &= \min_{\substack{q_1, \dots, q_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q_a - q_{a'}\|_\infty \leq \alpha}} \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a^*, q_a) \\ &= \min_{\substack{q_1, \dots, q_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q_a - q_{a'}\|_\infty \leq \alpha}} \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} \|p_a^* - q_a\|_1. \end{aligned}$$

This is due to  $\text{supp}(p_a^*) \subseteq \{e_1, \dots, e_k\}$  sharing the same finite support with any  $q_a \in \mathcal{Q}_k$ , whereby  $\frac{1}{2} W_1(r_a^*, q_a) = \frac{1}{2} W_1(p_a^*, q_a) = \frac{1}{2} \|p_a^* - q_a\|_1$ . Specifically, recall the fact that  $W_1$  under the 0-1 distance is equal to  $\frac{\|\cdot\|_1}{2}$ :

**Proposition A.3.** *Let  $p, q$  be probability measures on  $\mathcal{X}$  with metric  $d(x, y) = \mathbb{1}(x \neq y)$ , where  $\mathbb{1}(\cdot)$  denotes the indicator function. Then  $W_1(p, q) = \frac{1}{2} \|p - q\|_1$ .*

*Proof.* By definition, under the metric  $d(x, y) = \mathbb{1}(x \neq y)$ ,

$$\begin{aligned} W_1(p, q) &= \inf_{\gamma \in \Gamma(p, q)} \int_{\mathcal{X} \times \mathcal{X}} \mathbb{1}(x \neq y) d\gamma(x, y) \\ &= \left( 1 - \sup_{\gamma \in \Gamma(p, q)} \int_{\mathcal{X} \times \mathcal{X}} \mathbb{1}(x = y) d\gamma(x, y) \right) \\ &= 1 - \int_{\mathcal{X}} \min(p(x), q(x)) dx \\ &= \int_{\mathcal{X}} (p(x) - \min(p(x), q(x))) dx \\ &= \int_{\mathcal{X}} \max(0, p(x) - q(x)) dx \\ &= \frac{1}{2} \int_{\mathcal{X}} |p(x) - q(x)| dx, \end{aligned}$$

where line 3 is due to  $\gamma(x, x) \leq \min(p(x), q(x))$  for all  $\gamma \in \Gamma(p, q)$ , plus there always exists a coupling s.t.  $\gamma(x, x) = \min(p(x), q(x))$ , and line 5 to  $\int_{\mathcal{X}} p(x) - q(x) dx = 0$ .  $\square$

*Proof of Theorem A.2.* Because  $\text{supp}(r_a^*) = \text{supp}(p_a^*) \subseteq \{e_1, \dots, e_k\}$ , the  $\ell_1$  distance (in  $W_1$ ) between any  $s \in \text{supp}(r_a^*)$  and  $y \in \{e_1, \dots, e_k\}$  simplifies to  $\|s - y\|_1 = 2 \cdot \mathbb{1}(s \neq y)$ . The result then follows from Proposition A.3.  $\square$

Moreover, in this case, we have closed-form solution for the optimal fair classifier in Theorem 3.3:

**Theorem A.4** (Optimal Classifier Under DP, Noiseless Setting). *Let noiseless  $\mu$  be given along with the ground-truth labeling functions  $y_a$ , and let  $\alpha \in [0, 1]$ . Let  $q_1^*, \dots, q_m^*$  be a minimizer of Eq. (5), define*

$$d_a(e_i) := \frac{\max(0, q_a^*(e_i) - p_a^*(e_i))}{\sum_{j \in [k]} \max(0, q_a^*(e_j) - p_a^*(e_j))}, \quad s_a(e_i) := \frac{\max(0, p_a^*(e_i) - q_a^*(e_i))}{p_a^*(e_i)}, \quad \forall a \in [m], i \in [k],$$

and randomized functions  $\mathcal{T}_a : \mathcal{Y} \rightarrow \mathcal{Y}$  for each  $a \in [m]$  satisfying

$$\mathcal{T}_a(e_i) = \begin{cases} e_i & \text{w.p. } s_a(e_i)d_a(e_i) + (1 - s_a(e_i)), \\ e_j & \text{w.p. } s_a(e_i)d_a(e_j), \end{cases} \quad \forall j \in [m], j \neq i.$$

Then

$$(x, a) \mapsto \mathcal{T}_a \circ y_a(x) \in \arg \min_{h: \Delta_{\text{DP}}(h) \leq \alpha} \text{err}(h).$$

*Proof.* We first verify that  $(\mathcal{T}_a \circ y_a) \# \mu_a^X = q_a^*$ , which would imply  $\Delta_{\text{DP}}(h) \leq \alpha$  by the constraints in Eq. (5). For all  $e_i \in \mathcal{Y}$ ,

$$\begin{aligned} \mathbb{P}(\mathcal{T}_a \circ y_a(X) = e_i \mid A = a) &= p_a^*(e_i)(s_a(e_i)d_a(e_i) + (1 - s_a(e_i))) + d_a(e_i) \sum_{i \neq j} p_a^*(e_j)s_a(e_j) \\ &= p_a^*(e_i)(1 - s_a(e_i)) + d_a(e_i) \sum_{j \in [k]} p_a^*(e_j)s_a(e_j) \\ &= p_a^*(e_i) - \max(0, p_a^*(e_i) - q_a^*(e_i)) + \max(0, q_a^*(e_i) - p_a^*(e_i)) \\ &= q_a^*(e_i), \end{aligned}$$

where line 3 is because  $\sum_{i \in [k]} p_a^*(e_i) - q_a^*(e_i) = 0 \implies \sum_{i \in [k]} \max(0, p_a^*(e_i) - q_a^*(e_i)) = \sum_{i \in [k]} \max(0, q_a^*(e_i) - p_a^*(e_i))$ , and the last line is from case analysis.

Next, we compute the error rate on group  $a \in [m]$ . By construction, its accuracy conditioned on  $Y = y_a(X) = e_i$  is

$$\mathbb{P}(\mathcal{T}_a \circ y_a(X) = e_i \mid A = a, Y = e_i) = \begin{cases} 1 - s_a(e_i) & \text{if } d_a(e_i) = 0, \\ 1 = 1 - s_a(e_i) & \text{if } d_a(e_i) > 0 \iff s_a(e_i) = 0, \end{cases}$$

so the error rate is

$$\begin{aligned} \mathbb{P}(\mathcal{T}_a \circ y_a(X) \neq Y \mid A = a) &= \sum_{i \in [k]} p_a^*(e_i) \cdot (1 - \mathbb{P}(\mathcal{T}_a \circ y_a(X) = e_i \mid A = a, Y = e_i)) \\ &= \sum_{i \in [k]} p_a^*(e_i)s_a(e_i) \\ &= \sum_{i \in [k]} \max(0, p_a^*(e_i) - q_a^*(e_i)) \\ &= \frac{1}{2} \sum_{i \in [k]} |p_a^*(e_i) - q_a^*(e_i)|. \end{aligned}$$

We conclude by averaging the error on all groups and invoking Theorem A.2.  $\square$

### A.3 Two Examples in Remarks

In the remarks of Theorem 3.2, we discussed properties of the inherent tradeoff of error rate for DP fairness, which we illustrated here with two concrete examples.

It is discussed that the tradeoff could be zero even when the distribution of class probabilities  $r_a^* := f_a^* \# \mu_a^X$  differ, or equivalently,  $\mathbb{E}_\mu[Y \mid X, A] \not\perp A$ . This means that on certain problem instances, the Bayes error rate is simultaneously achieved by an unfair classifier and a fair one; in other words, the cost of DP fairness is zero. Such cases arise from the nonuniqueness of the optimal classifier. They would not occur on regression problems (with MSE), where the optimal regressor is always unique (namely,  $f_a^*(x) = \mathbb{E}_\mu[Y \mid X, A = a]$ ).

*Example A.5.* Consider the two-group binary classification problem given by

$$\begin{aligned}\mathbb{P}_{\mu_1}(Y = e_1 \mid X = x) &= 1 \quad \text{and} \\ \mathbb{P}_{\mu_2}(Y = e_1 \mid X = x) &= \mathbb{P}_{\mu_2}(Y = e_2 \mid X = x) = \frac{1}{2} \quad \text{for all } x \in \mathcal{X}.\end{aligned}$$

The optimal classifier on group 1 is the constant function  $x \mapsto e_1$ , and all classifiers on group 2 yield the same (hence optimal) error rate of  $\frac{1}{2}$ , including  $x \mapsto e_1$  which when combined with the optimal group 1 classifier achieves DP and the (group-balanced) Bayes error rate of  $\frac{1}{4}$ .

In (Zhao and Gordon, 2022), it is concluded that in the noiseless setting, the inherent tradeoff is zero if and only if the class marginal distributions are the same,  $p_a^*(e_i) = \mathbb{P}_\mu(Y = e_i \mid A = a)$  and  $r_a^* = p_a^* := f_a^* \# \mu_a^X$  in this case, or equivalently  $\mathbb{E}_\mu[Y \mid A] \perp\!\!\!\perp A$ . However, for the general case, this is no longer sufficient for the tradeoff to be zero (a sufficient condition here is  $\mathbb{E}_\mu[Y \mid X, A] \perp\!\!\!\perp A$ ).

*Example A.6.* Consider the two-group binary classification problem of two inputs,  $\mathcal{X} = \{1, 2\}$ , given by

$$\begin{aligned}\mathbb{P}_{\mu_1}(Y = e_1 \mid X = 1) &= 1, & \mathbb{P}_{\mu_1}(Y = e_1 \mid X = 2) &= 0, \\ \mathbb{P}_{\mu_1}(Y = e_2 \mid X = 1) &= 0, & \mathbb{P}_{\mu_1}(Y = e_2 \mid X = 2) &= 1, \quad \text{with} \\ \mathbb{P}_{\mu_1}(X = 1) &= \frac{1}{3}, & \mathbb{P}_{\mu_1}(X = 2) &= \frac{2}{3}, \quad \text{and} \\ \mathbb{P}_{\mu_2}(Y = e_1 \mid X = x) &= \frac{1}{3} \quad \text{for all } x \in \{1, 2\}.\end{aligned}$$

Note that the class marginal on both groups is  $(\frac{1}{3}, \frac{2}{3})$ . The unique optimal classifier on group 1 is  $x \mapsto e_x$ , and the unique optimal classifier on group 2 is the constant  $x \mapsto e_2$ , but this combination do not satisfy DP, since the output distribution on group 1 is  $(\frac{1}{3}, \frac{2}{3})$  but that on group 2 is  $(0, 1)$ . Since all other classifiers including the fair ones have strictly higher error rates, the tradeoff is nonzero.

## B Omitted Proofs from Section 3

To make our arguments rigorous, we provide a definition of randomized functions via the Markov kernel. These definitions will be frequently referred to in the proofs in this section, and that of Theorem 4.5.

**Definition B.1** (Markov Kernel). A Markov kernel from a measurable space  $(\mathcal{X}, \mathcal{S})$  to  $(\mathcal{Y}, \mathcal{T})$  is a mapping  $\mathcal{K} : \mathcal{X} \times \mathcal{T} \rightarrow [0, 1]$ , such that  $\mathcal{K}(\cdot, T)$  is  $\mathcal{S}$ -measurable  $\forall T \in \mathcal{T}$ , and  $\mathcal{K}(x, \cdot)$  is a probability measure on  $(\mathcal{Y}, \mathcal{T}) \forall x \in \mathcal{X}$ .

**Definition B.2** (Randomized Function). A randomized function  $f : (\mathcal{X}, \mathcal{S}) \rightarrow (\mathcal{Y}, \mathcal{T})$  is associated with a Markov kernel  $\mathcal{K} : \mathcal{X} \times \mathcal{T} \rightarrow [0, 1]$ , and for all  $x \in \mathcal{X}, T \in \mathcal{T}$ ,  $\mathbb{P}(f(x) \in T) = \mathcal{K}(x, T)$ .

**Definition B.3** (Push-Forward by Randomized Function). Let  $p$  be a measure on  $(\mathcal{X}, \mathcal{S})$  and  $f : (\mathcal{X}, \mathcal{S}) \rightarrow (\mathcal{Y}, \mathcal{T})$  a randomized function with Markov kernel  $\mathcal{K}$ . The push-forward of  $p$  under  $f$ , denoted by  $f \# p$ , is a measure on  $\mathcal{Y}$  given by  $f \# p(T) = \int_{\mathcal{X}} \mathcal{K}(x, T) dp(x)$  for all  $T \in \mathcal{T}$ .

Also, let blackboard bold  $\mathbf{1}$  denote the indicator function, where  $\mathbf{1}(E) = 1$  if the predicate  $E$  is true, else 0.

We provide the proofs to Lemma 3.1 and Theorems 3.3 and 3.4; a proof of Theorem 3.2 was provided in Appendix A.1. The proofs to these results and the ones in Section 4 all make use of the following rewriting of the error rate as an integral over a coupling:

**Lemma B.4.** Let  $\mu$  with  $|\mathcal{A}| = 1$  be given along with the Bayes optimal predictor  $f^*$ . Then for any randomized classifier  $h : \mathcal{X} \rightarrow \mathcal{Y}$ , its error rate can be written as

$$\text{err}(h) = \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \mathbb{P}(f^*(X) = s, h(X) = y) \, d(s, y) \equiv \frac{1}{2} \mathbb{E}[\|f^*(X) - h(X)\|_1].$$

Note that the joint distribution  $\mathbb{P}$  of  $(f^*(X), h(X))$  is a coupling belonging to  $\Gamma(f^* \# \mu^X, h \# \mu^X)$ .

*Proof.* The accuracy of  $h$  is

$$\begin{aligned} 1 - \text{err}(h) &= 1 - \mathbb{P}(h(X) \neq Y) = \mathbb{P}(h(X) = Y) \\ &= \int_{\Delta_k} \sum_{i \in [k]} \mathbb{P}(Y = e_i, h(X) = e_i, f^*(X) = s) \, ds \\ &= \int_{\Delta_k} \sum_{i \in [k]} \mathbb{P}(Y = e_i, h(X) = e_i \mid f^*(X) = s) \mathbb{P}_\mu(f^*(X) = s) \, ds \\ &= \int_{\Delta_k} \sum_{i \in [k]} \mathbb{P}_\mu(Y = e_i \mid f^*(X) = s) \mathbb{P}(h(X) = e_i \mid f^*(X) = s) \mathbb{P}_\mu(f^*(X) = s) \, ds \\ &= \int_{\Delta_k} \sum_{i \in [k]} s_i \mathbb{P}(f^*(X) = s, h(X) = e_i) \, ds, \end{aligned}$$

where line 4 follows from  $X \perp\!\!\!\perp Y$  given  $f^*(X)$ , since  $f^*(X) = \mathbb{E}_\mu[Y \mid X]$  fully specifies the pmf of  $Y$  conditioned on  $X$ . Next, because  $\mathbb{P}(f^*(X) = \cdot, h(X) = \cdot)$  is a probability measure,

$$\begin{aligned} \text{err}(h) &= \int_{\Delta_k} \sum_{i \in [k]} (1 - s_i) \mathbb{P}(f^*(X) = s, h(X) = e_i) \, ds \\ &= \frac{1}{2} \int_{\Delta_k} \sum_{i \in [k]} \|s - e_i\|_1 \mathbb{P}(f^*(X) = s, h(X) = e_i) \, ds \\ &\equiv \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \mathbb{P}(f^*(X) = s, h(X) = y) \, d(s, y) \\ &\equiv \frac{1}{2} \mathbb{E}[\|f^*(X) - h(X)\|_1], \end{aligned}$$

where the second equality is due to an identity stated in Eq. (9) between points in the simplex and its vertices.  $\square$

**Lemma B.5** (Full Version of Lemma 3.1). Let  $\mu$  with  $|\mathcal{A}| = 1$  be given along with the Bayes optimal predictor  $f^*$ , define  $r^* := f^* \# \mu^X$ , and fix  $q \in \mathcal{Q}_k$ . Then for any randomized classifier  $h : \mathcal{X} \rightarrow \mathcal{Y}$  with Markov kernel  $\mathcal{K}$  satisfying  $h \# \mu^X = q$ , the coupling  $\gamma \in \Gamma(r^*, q)$  given by

$$\gamma(s, y) = \int_{f^{*-1}(s)} \mathcal{K}(x, y) \, d\mu^X(x)$$

satisfies

$$\text{err}(h) = \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \, d\gamma(s, y). \quad (7)$$

Conversely, for any  $\gamma \in \Gamma(r^*, q)$ , the randomized classifier  $h$  with Markov kernel

$$\mathcal{K}(x, T) = \gamma(f^*(x), T) / \gamma(f^*(x), \mathcal{Y})$$

satisfies  $h \# \mu^X = q$  and Eq. (7).

*Proof.* We begin with the first direction. Let a randomized classifier  $h$  with Markov kernel  $\mathcal{K}$  satisfying  $h\sharp\mu^X = q$  be given. We verify that the coupling constructed above belongs to  $\Gamma(r^*, q)$ :

$$\begin{aligned} \int_{\mathcal{Y}} \gamma(s, y) \, dy &= \int_{\mathcal{Y}} \int_{f^{*-1}(s)} \mathcal{K}(x, y) \, d\mu^X(x) \, dy \\ &= \int_{f^{*-1}(s)} \int_{\mathcal{Y}} \mathcal{K}(x, y) \, dy \, d\mu^X(x) \\ &= \int_{f^{*-1}(s)} d\mu^X(x) \\ &= \mathbb{P}_{\mu^X}(f^*(X) = s) = r^*(s), \end{aligned}$$

where line 3 follows from Definition B.1 of Markov kernels, and line 5 from the definition of push-forward measures;

$$\begin{aligned} \int_{\Delta_k} \gamma(s, y) \, ds &= \int_{\Delta_k} \int_{f^{*-1}(s)} \mathcal{K}(x, y) \, d\mu^X(x) \, ds \\ &= \int_{\mathcal{X}} \mathcal{K}(x, y) \, d\mu^X(x) \\ &= \int_{\mathcal{X}} \mathbb{P}(h(X) = y \mid X = x) \, d\mu^X(x) \\ &= \mathbb{P}(h(X) = y) = q(y), \end{aligned}$$

where line 3 follows from Definition B.2 of randomized function, and line 5 is by assumption.

Next, by Lemma B.4 and the same arguments above,

$$\begin{aligned} \text{err}(h) &= \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \, \mathbb{P}(f^*(X) = s, h(X) = y) \, d(s, y) \\ &= \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \left( \int_{\mathcal{X}} \mathbb{P}(f^*(X) = s, h(X) = y, X = x) \, dx \right) \, d(s, y) \\ &= \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \left( \int_{f^{*-1}(s)} \mathbb{P}(h(X) = y, X = x) \, dx \right) \, d(s, y) \\ &= \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \left( \int_{f^{*-1}(s)} \mathbb{P}(h(X) = y \mid X = x) \, d\mu^X(x) \right) \, d(s, y) \\ &= \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \cdot \gamma(s, y) \, d(s, y) \end{aligned}$$

as desired, where line 3 is due to  $\mathbb{P}(f^*(X) = s, h(X) = y, X = x) = \mathbb{1}(f^*(x) = s) \mathbb{P}(h(X) = y, X = x)$  for all  $(s, y, x)$ .

For the converse, let a coupling  $\gamma \in \Gamma(r^*, q)$  be given. We show that the Markov kernel of the randomized classifier  $h$  constructed in the statement satisfies the equality  $\gamma(s, y) = \int_{f^{*-1}(s)} \mathcal{K}(x, y) \, d\mu^X(x)$ , then Eq. (7) will follow directly from the same arguments used in the previous part. Let  $s \in \Delta_k$



and  $y \in \mathcal{Y}$ , and  $x' \in f^{*-1}(s)$  arbitrary, then

$$\begin{aligned}
\gamma(s, y) &= \frac{\gamma(s, y)}{\gamma(s, \mathcal{Y})} \cdot \gamma(s, \mathcal{Y}) \\
&= \frac{\gamma(f^*(x'), y)}{\gamma(f^*(x'), \mathcal{Y})} \cdot \gamma(s, \mathcal{Y}) \\
&= \mathcal{K}(x', y) \cdot \gamma(s, \mathcal{Y}) \\
&= \mathcal{K}(x', y) \cdot r^*(s) \\
&= \mathcal{K}(x', y) \int_{x \in f^{*-1}(s)} d\mu^X(x) \\
&= \int_{x \in f^{*-1}(s)} \mathcal{K}(x', y) d\mu^X(x) \\
&= \int_{x \in f^{*-1}(s)} \mathcal{K}(x, y) d\mu^X(x),
\end{aligned}$$

where line 3 is by construction of  $\mathcal{K}$ , line 4 from  $\gamma \in \Gamma(r^*, q)$ , and the last line is because  $\mathcal{K}(x, y)$  is constant for all  $x \in f^{*-1}(s)$ , also by construction.  $\square$

*Proof of Theorem 3.3.* By construction, the Markov kernel of the randomized optimal fair classifier  $\bar{h}^*(x, a) := \mathcal{T}_{r_a^* \rightarrow q_a^*}^* \circ f_a^*(x)$  is

$$\mathcal{K}((x, a), y) = \frac{\gamma_a^*(f_a^*(x), y)}{\gamma_a^*(f_a^*(x), \mathcal{Y})}$$

where  $\gamma_a^* \in \Gamma(r_a^*, q_a^*)$  is the optimal transport between  $r_a^*$  and  $q_a^*$ .

We verify that the output distributions of  $\bar{h}^*$  equal  $q_1^*, \dots, q_m^*$ , thereby it is  $\alpha$ -DP because the  $q_a^*$ 's satisfy the constraint in Eq. (5), and its error rate achieves the minimum in Theorem 3.2.

First, for all  $y \in \mathcal{Y}$ ,

$$\begin{aligned}
\mathbb{P}(\bar{h}^*(X, A) = y \mid A = a) &= \int_{\mathcal{X}} \mathbb{P}(\bar{h}^*(x, a) = y) \mathbb{P}_\mu(X = x \mid A = a) dx \\
&= \int_{\mathcal{X}} \mathcal{K}((x, a), y) d\mu_a^X(x) \\
&= \int_{\mathcal{X}} \frac{\gamma_a^*(f_a^*(x), y)}{\gamma_a^*(f_a^*(x), \mathcal{Y})} d\mu_a^X(x) \\
&= \int_{\Delta_k} \frac{\gamma_a^*(s, y)}{\gamma_a^*(s, \mathcal{Y})} \left( \int_{f_a^{*-1}(s)} d\mu_a^X(x) \right) ds \\
&= \int_{\Delta_k} \frac{\gamma_a^*(s, y)}{\gamma_a^*(s, \mathcal{Y})} r_a^*(s) ds \\
&= \int_{\Delta_k} \gamma_a^*(s, y) ds = \gamma_a^*(\Delta_k, y) = q_a^*(y),
\end{aligned}$$

where line 3 is due to  $\gamma_a^*(f_a^*(x), y) = \gamma_a^*(s, y)$  being constant for all  $x \in f_a^{*-1}(s)$ .

Similarly, Lemma B.5 implies that the error rate on group  $a$ , denoted by  $\text{err}_a(\bar{h}^*)$ , is

$$\text{err}_a(\bar{h}^*) = \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 d\gamma_a(s, y),$$

where  $\gamma_a \in \Gamma(r_a^*, q_a^*)$  equals to

$$\begin{aligned}\gamma_a(s, y) &= \int_{f_a^{*-1}(s)} \mathcal{K}((x, a), y) d\mu_a^X(x) \\ &= \int_{f_a^{*-1}(s)} \frac{\gamma_a^*(f_a^*(x), y)}{\gamma_a^*(f_a^*(x), \mathcal{Y})} d\mu_a^X(x) \\ &= \frac{\gamma_a^*(s, y)}{\gamma_a^*(s, \mathcal{Y})} \int_{f_a^{*-1}(s)} d\mu_a^X(x) \\ &= \gamma_a^*(s, y).\end{aligned}$$

So  $\text{err}_a(\bar{h}^*) = \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 d\gamma_a^*(s, y) = \frac{1}{2} W_1(r_a^*, q_a^*)$  because  $\gamma_a^*$  is an optimal transport between  $r_a^*$  and  $q_a^*$ , and  $\text{err}(\bar{h}^*) = \frac{1}{m} \sum_{a \in [m]} \text{err}_a(\bar{h}^*) = \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a^*, q_a^*)$ , the minimum error rate under  $\alpha$ -DP.  $\square$

*Proof of Theorem 3.4.* The  $\alpha$ -fair classifier  $\bar{h}$  returned from Algorithm 1 on  $f_1, \dots, f_m$  is

$$\bar{h}(x, a) = \mathcal{T}_{r_a \rightarrow q_a}^* \circ f_a(x),$$

where  $q_1, \dots, q_m$  is the minimizer of Eq. (5) on  $r_a := f_a \# \mu_a^X$  and  $\alpha$ , and  $\mathcal{T}_{r_a \rightarrow q_a}^*$  is the optimal transport from  $r_a$  to  $q_a$ .

Denote the  $L^1$  error of  $f_a$  relative to  $f_a^*$  conditioned on  $A = a$  by

$$\mathcal{E}_a := \mathbb{E}_{\mu_a^X} [\|f_a(X) - f_a^*(X)\|_1],$$

and write  $\mathcal{E} := \frac{1}{m} \sum_{a \in [m]} \mathcal{E}_a$ .

For the upper bound, by Lemma B.4 and the triangle inequality,

$$\begin{aligned}\text{err}(\bar{h}) &= \frac{1}{2m} \sum_{a \in [m]} \mathbb{E} [\|\mathcal{T}_{r_a \rightarrow q_a}^* \circ f_a(X) - f_a^*(X)\|_1 \mid A = a] \\ &\leq \frac{1}{2m} \sum_{a \in [m]} (\mathbb{E} [\|\mathcal{T}_{r_a \rightarrow q_a}^* \circ f_a(X) - f_a(X)\|_1 \mid A = a] + \mathbb{E} [\|f_a(X) - f_a^*(X)\|_1 \mid A = a]) \\ &= \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a, q_a) + \frac{1}{2} \cdot \frac{1}{m} \sum_{a \in [m]} \mathcal{E}_a \\ &= \min_{\substack{q'_1, \dots, q'_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q'_a - q'_{a'}\|_\infty \leq \alpha}} \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a, q'_a) + \frac{\mathcal{E}}{2},\end{aligned}$$

where line 3 is because  $\mathcal{T}_{r_a \rightarrow q_a}^*$  is the optimal transport from  $r_a$  to  $q_a$  under the  $\ell_1$  cost, and line 4 because  $q_1, \dots, q_m$  is the minimizer. Let  $q_1^*, \dots, q_m^*$  denote the minimizer of Eq. (5) on the  $r_a^* := f_a^* \# \mu_a^X$  and  $\alpha$ , then by Theorem 3.2,

$$\begin{aligned}\text{err}(\bar{h}) - \text{err}_\alpha^* &\leq \frac{1}{2m} \left( \min_{\substack{q'_1, \dots, q'_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q'_a - q'_{a'}\|_\infty \leq \alpha}} \sum_{a \in [m]} W_1(r_a, q'_a) - \sum_{a \in [m]} W_1(r_a^*, q_a^*) \right) + \frac{\mathcal{E}}{2} \\ &\leq \frac{1}{2m} \left( \sum_{a \in [m]} W_1(r_a, q_a^*) - \sum_{a \in [m]} W_1(r_a^*, q_a^*) \right) + \frac{\mathcal{E}}{2} \\ &\leq \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a, r_a^*) + \frac{\mathcal{E}}{2} \leq \frac{1}{2} \cdot \frac{1}{m} \sum_{a \in [m]} \mathcal{E}_a + \frac{\mathcal{E}}{2} = \mathcal{E},\end{aligned}$$

where the last line is because for each  $a \in [m]$ ,  $W_1(r_a, r_a^*)$  is upper bounded by the transportation cost under the coupling given by the joint distribution of  $(f_a(X), f_a^*(X))$  conditioned on  $A = a$ : denote the coupling by  $\pi_a$ , then clearly  $\pi_a \in \Gamma(r_a, r_a^*)$ , and  $\int_{\Delta_k \times \Delta_k} \|s - s'\|_1 d\pi_a(s, s') = \int_{\mathcal{X}} \|f_a(x) - f_a^*(x)\|_1 d\mu_a^X(x) = \mathcal{E}_a$ .

For the lower bound, again by Lemma B.4,

$$\begin{aligned} \text{err}(\bar{h}) &= \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \mathbb{P}(f_a^*(X) = s, \mathcal{T}_{r_a \rightarrow q_a}^* \circ f_a(X) = y \mid A = a) d(s, y) \\ &\geq \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a^*, q_a) \geq \min_{\substack{q'_1, \dots, q'_m \in \mathcal{Q}_k \\ \max_{a, a'} \|q'_a - q'_{a'}\|_\infty \leq \alpha}} \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a^*, q'_a) = \text{err}_\alpha^*, \end{aligned}$$

where line 2 is because the joint distribution of  $(f_a^*(X), \mathcal{T}_{r_a \rightarrow q_a}^* \circ f_a(X))$  conditioned on  $A = a$  is a coupling belonging to  $\Gamma(r_a^*, q_a)$ , thereby the transportation cost represented by the quantity in the preceding line upper bounds  $W_1(r_a^*, q_a)$ .  $\square$

## C Omitted Proofs from Section 4

We provide proofs to the generalization results (Theorems 4.3 and 4.4) and the error propagation bound for smoothing (Theorem 4.5), in that order. We remark that Assumption 4.2 of the predictors to be post-processed being calibrated can be dropped by adding the error propagation of Theorem 3.4 (the  $L^1$  error w.r.t. the calibrated versions; via combining the proofs). A finite sample generalization bound for the general case procedure in Section 4.3 can also be obtained by combining Theorems 4.4 and 4.5, provided that the supports of the distributions after smoothing are contained in the simplex.

The generalization bound of the finite case uses an  $\ell_1$  (TV) convergence result of empirical distributions, which is obtained from the following vector concentration bound (Kohler and Lucchi, 2017, Lemma 18):

**Lemma C.1** (Vector Bernstein Inequality). *Let  $x_1, \dots, x_n \in \mathbb{R}^d$  be independent vector-valued random variables, satisfying  $\mathbb{E}[x_i] = 0$ ,  $\|x_i\|_2 \leq \mu$ , and  $\mathbb{E}[\|x_i\|_2^2] \leq \sigma^2$  for all  $i \in [n]$ . Then for all  $\alpha \in (0, \sigma^2/\mu)$ ,*

$$\mathbb{P}\left(\left\|\frac{1}{n} \sum_{i=1}^n x_i\right\|_2 \geq \alpha\right) \leq \exp\left(-\frac{n\alpha^2}{8\sigma^2} + \frac{1}{4}\right).$$

**Lemma C.2.** *Let  $p$  be a distribution over  $\mathcal{X}$  with finite support, and  $x_1, \dots, x_n \sim p$  be i.i.d. samples. Define the empirical distribution  $\hat{p}_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ . Then w.p. at least  $1 - \delta$  over the random draw of the samples,  $\|p - \hat{p}_n\|_1 \leq \sqrt{\frac{32|\mathcal{X}|}{n}} \left(\frac{1}{4} + \ln\left(\frac{1}{\delta}\right)\right)$ .*

*Proof.* By viewing each  $\delta_{x_i}$  as a vector in  $\Delta_{|\mathcal{X}|}$ , we have that  $p - \delta_{x_i}$  is contained in the  $|\mathcal{X}|$ -dimensional  $\ell_1$ -ball of width 2, whereby  $\|p - \delta_{x_i}\|_2^2 \leq \|p - \delta_{x_i}\|_1^2 \leq 4$  for all  $i$ . So by Lemma C.1, w.p. at least  $1 - \delta$ ,  $\|p - \frac{1}{n} \sum_{i=1}^n \delta_{x_i}\|_1 \leq \sqrt{|\mathcal{X}|} \|p - \frac{1}{n} \sum_{i=1}^n \delta_{x_i}\|_2 \leq \sqrt{\frac{32|\mathcal{X}|}{n}} \left(\frac{1}{4} + \ln\left(\frac{1}{\delta}\right)\right)$ .  $\square$

*Proof of Theorem 4.3.* We first bound the error rate, then the fairness.

**Error Rate.** Consider the classification problem  $\mu'$  derived from the original  $\mu$  under an input transformation given by the joint distribution of  $(f_A(X), A, Y)$ , as discussed in Section 3.3, on which

Id is the Bayes optimal predictor due to calibration of the  $f_a$ 's. Then by Lemma B.4 applied on  $\mu'$ ,

$$\begin{aligned}
\text{err}(\hat{h}) &= \frac{1}{2m} \sum_{a \in [m]} \sum_{s \in \mathcal{R}_a} \sum_{y \in \mathcal{Y}} \|s - y\|_1 \mathbb{P}(\text{Id}(X') = s, \mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(X') = y) \\
&= \frac{1}{2m} \sum_{a \in [m]} \sum_{s \in \mathcal{R}_a} \sum_{y \in \mathcal{Y}} \|s - y\|_1 \cdot r_a(s) \cdot \mathbb{P}(\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s) = y) \\
&\leq \frac{1}{2m} \sum_{a \in [m]} \sum_{s \in \mathcal{R}_a} \sum_{y \in \mathcal{Y}} \|s - y\|_1 \cdot (\hat{r}_a(s) + |r_a(s) - \hat{r}_a(s)|) \cdot \mathbb{P}(\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s) = y) \\
&\leq \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(\hat{r}_a, \hat{q}_a) + \frac{1}{m} \sum_{a \in [m]} \sum_{s \in \mathcal{R}_a} |r_a(s) - \hat{r}_a(s)|,
\end{aligned}$$

where line 4 uses the fact that each  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$  is an optimal transport from  $\hat{r}_a$  to  $\hat{q}_a$ . Let the  $q_a$ 's denote the minimizer of Eq. (5) on the  $r_a$ 's with  $\alpha$ , then

$$\begin{aligned}
\text{err}(\hat{h}) - \text{err}_{\alpha, f}^* &\leq \frac{1}{m} \sum_{a \in [m]} \left( \frac{1}{2} (W_1(\hat{r}_a, \hat{q}_a) - W_1(r_a, q_a)) + \sum_{s \in \mathcal{R}_a} |r_a(s) - \hat{r}_a(s)| \right) \\
&\leq \frac{1}{m} \sum_{a \in [m]} \left( \frac{1}{2} (W_1(\hat{r}_a, q_a) - W_1(r_a, q_a)) + \sum_{s \in \mathcal{R}_a} |r_a(s) - \hat{r}_a(s)| \right) \\
&\leq \frac{1}{m} \sum_{a \in [m]} \left( \frac{1}{2} W_1(\hat{r}_a, r_a) + \sum_{s \in \mathcal{R}_a} |r_a(s) - \hat{r}_a(s)| \right),
\end{aligned}$$

where line 2 is due to  $\hat{q}_a$  being the minimizer of Eq. (5) on the  $\hat{r}_a$ 's. Because  $\|s - s'\|_1 \leq 2 \cdot \mathbf{1}(s \neq s')$ , by Proposition A.3,  $W_1(\hat{r}_a, r_a) \leq \|\hat{r}_a - r_a\|_1$ , so it follows that

$$\text{err}(\hat{h}) - \text{err}_{\alpha, f}^* \leq \frac{3}{2m} \sum_{a \in [m]} \sum_{s \in \mathcal{R}_a} |r_a(s) - \hat{r}_a(s)| \leq \frac{1}{m} \sum_{a \in [m]} \sqrt{\frac{72|\mathcal{R}_a|}{n} \left( \frac{1}{4} + \ln\left(\frac{m}{\delta}\right) \right)}$$

w.p. at least  $1 - \delta$  from  $m$  applications of Lemma C.2 and a union bound.

**Fairness ( $\Delta_{\text{DP}}$ ).** In the finite case, we can get a stronger result in terms of the  $\ell_1$ -norm. Note that for all  $a \in [m]$  and  $y \in \mathcal{Y}$ ,

$$\begin{aligned}
&\sum_{y \in \mathcal{Y}} \left| \mathbb{P}(\hat{h}(X, A) = y \mid A = a) - \hat{q}_a(y) \right| \\
&= \sum_{y \in \mathcal{Y}} \left| \sum_{s \in \mathcal{R}_a} r_a(s) \mathbb{P}(\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s) = y) - \sum_{s \in \mathcal{R}_a} \hat{r}_a(s) \mathbb{P}(\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s) = y) \right| \\
&\leq \sum_{y \in \mathcal{Y}} \sum_{s \in \mathcal{R}_a} |r_a(s) - \hat{r}_a(s)| \mathbb{P}(\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s) = y) \\
&= \sum_{s \in \mathcal{R}_a} |r_a(s) - \hat{r}_a(s)| \\
&\leq \sqrt{\frac{32|\mathcal{R}_a|}{n} \left( \frac{1}{4} + \ln\left(\frac{mk}{\delta}\right) \right)}
\end{aligned}$$

w.p. at least  $1 - \delta$  from applications of Lemma C.2 and a union bound, where the first equality is because  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$  is a transport from  $\hat{r}_a$  to  $\hat{q}_a$ . Then an  $\ell_\infty$ -norm bound follows:

$$\begin{aligned} \max_{y \in \mathcal{Y}} \left| \mathbb{P}(\hat{h}(X, A) = y \mid A = a) - \hat{q}_a(y) \right| &\leq \sum_{y \in \mathcal{Y}} \left| \mathbb{P}(\hat{h}(X, A) = y \mid A = a) - \hat{q}_a(y) \right| \\ &= \sqrt{\frac{32|\mathcal{R}_a|}{n} \left( \frac{1}{4} + \ln \left( \frac{mk}{\delta} \right) \right)}. \end{aligned}$$

Lastly, because of the constraint in Eq. (5) that  $\max_{a, a' \in [m]} \|\hat{q}_a - \hat{q}_{a'}\|_\infty \leq \alpha$ ,

$$\begin{aligned} \Delta_{\text{DP}}(\hat{h}) &= \max_{\substack{a, a' \in [m] \\ y \in \mathcal{Y}}} \left| \mathbb{P}(\hat{h}(X, A) = y \mid A = a) - \mathbb{P}(\hat{h}(X, A') = y \mid A = a') \right| \\ &\leq \max_{\substack{a, a' \in [m] \\ y \in \mathcal{Y}}} |\hat{q}_a(y) - \hat{q}_{a'}(y)| \\ &\quad + \max_{\substack{a, a' \in [m] \\ y \in \mathcal{Y}}} \left( \left| \mathbb{P}(\hat{h}(X, A) = y \mid A = a) - \hat{q}_a(y) \right| + \left| \mathbb{P}(\hat{h}(X, A') = y \mid A = a') - \hat{q}_{a'}(y) \right| \right) \\ &\leq \alpha + \max_{a, a' \in [m]} \left( \sqrt{\frac{32|\mathcal{R}_a|}{n} \left( \frac{1}{4} + \ln \left( \frac{mk}{\delta} \right) \right)} + \sqrt{\frac{32|\mathcal{R}_{a'}|}{n} \left( \frac{1}{4} + \ln \left( \frac{mk}{\delta} \right) \right)} \right). \end{aligned}$$

The theorem then follows from a final application of union bound.  $\square$

The proof of the generalization bound in the continuous case uses the following uniform bounds with the VC dimension and the pseudo-dimension as the complexity measure. We omit the proofs, but refer readers to (Shalev-Shwartz and Ben-David, 2014, Theorem 6.8) and (Mohri et al., 2018, Theorem 11.8), respectively. We also need a characterization of the disagreement between the empirical transports  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}}^*$  and the transport mappings  $\mathcal{T}_a \in \mathcal{G}_k$  extracted from them in Lines 6–9 of Algorithm 2, (to be) stated in Lemma D.5.

**Theorem C.3.** *Let a class of binary functions  $\mathcal{H} \subset \{0, 1\}^{\mathcal{X}}$  be given, and  $\ell(\hat{y}, y) = \mathbb{1}(y \neq \hat{y})$  be the 0-1 loss. Let  $p$  be a distribution over  $\mathcal{X} \times \{0, 1\}$ , and  $(x_1, y_1), \dots, (x_n, y_n) \sim p$  be i.i.d. samples. Then w.p. at least  $1 - \delta$  over the random draw of the samples,  $\forall h \in \mathcal{H}$ ,*

$$\left| \mathbb{E}_{(X, Y) \sim p} [\ell(h(X), Y)] - \frac{1}{n} \sum_{i=1}^n \ell(h(x_i), y_i) \right| \leq \sqrt{\frac{C}{n} \left( d + \ln \left( \frac{1}{\delta} \right) \right)},$$

where  $C > 0$  is a universal constant, and  $d$  is the VC-dimension of  $\mathcal{H}$ .

**Theorem C.4.** *Let a class of real-valued functions  $\mathcal{H} \subset [0, 1]^{\mathcal{X}}$  be given, along with a non-negative loss function  $\ell$  that is upper bounded by  $B$ . Let  $p$  be a distribution over  $\mathcal{X} \times \mathbb{R}$ , and  $(x_1, y_1), \dots, (x_n, y_n) \sim p$  be i.i.d. samples. Then w.p. at least  $1 - \delta$  over the random draw of the samples,  $\forall h \in \mathcal{H}$ ,*

$$\mathbb{E}_{(X, Y) \sim p} [\ell(h(X), Y)] - \frac{1}{n} \sum_{i=1}^n \ell(h(x_i), y_i) \leq O \left( B \sqrt{\frac{1}{n} \left( d \ln \left( \frac{n}{d} \right) + \ln \left( \frac{1}{\delta} \right) \right)} \right),$$

where  $d$  is the pseudo-dimension of  $\{(x, y) \mapsto \ell(h(x), y) : h \in \mathcal{H}\}$ , the class of  $\ell$  associated to  $\mathcal{H}$ .

One highlight of our proof is that we avoided using the convergence of the empirical measure under Wasserstein distance in our arguments, which would have resulted in sample complexity that is exponential in the number of label classes  $k$  (Weed and Bach, 2019). Instead, we leveraged the existence and uniqueness of the semi-discrete simplex-vertex optimal transport in the low complexity function class  $\mathcal{G}_k$ , established in Theorems D.1 and D.2, whereby we can apply the above uniform bound to  $\mathcal{G}_k$  and achieve a rate that is only polynomial in  $k$ .

In addition, we remark that the  $O(k^2/n)$  term attributed to the disagreements between  $\mathcal{T}_a$  and  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$  on  $S_a$  could potentially be improved to  $O(k/n)$  if LP is assumed to return an extremal solution (Peyré and Cuturi, 2019), and  $\mathcal{G}_k$  is modified so that the output on points that lie on each boundary can be specified, rather than always tie-broken to the  $e_i$  with the largest index  $i$ .

*Proof of Theorem 4.4.* We first bound the error rate, followed by  $\Delta_{\text{DP}}$ . Recall that the classifier returned from Algorithm 2 is

$$\hat{h}(x, a) := \mathcal{T}_a \circ f_a(x),$$

where each  $\mathcal{T}_a \in \mathcal{G}_k$  is extracted from the empirical optimal transport  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$  by Algorithm 2, obtained from calling  $\text{LP}(\hat{r}_1, \dots, \hat{r}_m, \alpha)$ , where  $\hat{q}_1, \dots, \hat{q}_m$  is the minimizer of Eq. (5) on the  $\hat{r}_a$ 's with  $\alpha$ . We will use a complexity result of  $\mathcal{G}_k$  in terms of its pseudo-dimension when associated with  $\ell_1$  loss, and a VC bound of binarized versions of  $\mathcal{G}_k$  (to be defined in Eq. (18)), which are deferred to Theorem D.15 and Corollary D.16.

**Error Rate.** Consider the classification problem  $\mu'$  derived from the original  $\mu$  under an input transformation given by the joint distribution of  $(f_A(X), A, Y)$ , as discussed in Section 3.3, on which  $\text{Id}$  is the Bayes optimal predictor due to calibration of the  $f_a$ 's. Then by Lemma B.4 applied on  $\mu'$ ,

$$\begin{aligned} \text{err}(\hat{h}) &= \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 \mathbb{P}(\text{Id}(X') = s, \mathcal{T}_a(X') = y) \, d(s, y) \\ &= \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} \mathbb{E}_{S \sim r_a} [\|\mathcal{T}_a(S) - S\|_1]. \end{aligned}$$

Define  $s_{a,j} := f_a(x_{a,j})$ . By Theorems C.4 and D.15, and a union bound, we have w.p. at least  $1 - \delta$ , for all  $a \in [m]$ ,

$$\mathbb{E}_{S \sim r_a} [\|\mathcal{T}_a(S) - S\|_1] - \frac{1}{n} \sum_{j=1}^n \|\mathcal{T}_a(s_{a,j}) - s_{a,j}\|_1 \leq O\left(\sqrt{\frac{1}{n} \left(k \ln\left(\frac{n}{k}\right) + \ln\left(\frac{m}{\delta}\right)\right)}\right).$$

Because each  $\mathcal{T}_a$  is extracted from the empirical optimal transport  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$  using Line 6–9 of Algorithm 2, by the discussion in Appendix D and Lemma D.5, they both agree on all of  $S_a$  except for points that lie on the decision boundaries of  $\mathcal{T}_a$ . The boundaries are described by  $\binom{k}{2}$  hyperplanes, and because  $r_a$  is continuous, no two points in  $S_a$  lie on the same hyperplane almost surely, so the number of disagreements is at most  $\binom{k}{2} = k(k-1)/2$ , and

$$\begin{aligned} \left| \frac{1}{n} \sum_{j=1}^n \|\mathcal{T}_a(s_{a,j}) - s_{a,j}\|_1 - W_1(\hat{r}_a, \hat{q}_a) \right| &= \left| \frac{1}{n} \sum_{j=1}^n \|\mathcal{T}_a(s_{a,j}) - s_{a,j}\|_1 - \frac{1}{n} \sum_{j=1}^n \|\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s_{a,j}) - s_{a,j}\|_1 \right| \\ &\leq \frac{1}{n} \sum_{j=1}^n \|\mathcal{T}_a(s_{a,j}) - \mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s_{a,j})\|_1 \\ &= \frac{2}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_a(s_{a,j}) \neq \mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s_{a,j})) \leq O\left(\frac{k^2}{n}\right), \end{aligned}$$

where the first equality is because  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$  is the optimal transport from  $\hat{r}_a$  to  $\hat{q}_a$ . Therefore, we arrive at w.p. at least  $1 - \delta$ ,

$$\text{err}(\hat{h}) - \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(\hat{r}_a, \hat{q}_a) \leq O\left(\sqrt{\frac{1}{n} \left(k \ln\left(\frac{n}{k}\right) + \ln\left(\frac{m}{\delta}\right)\right)} + \frac{k^2}{n}\right) =: \mathcal{E}.$$

Continuing, let  $\mathcal{T}_{r_a \rightarrow q_a}^* \in \mathcal{G}_k$  denote the optimal transport from  $r_a$  to  $q_a$ , where the  $q_a$ 's denote the minimizer of Eq. (5) on the  $r_a$ 's with  $\alpha$ . The existence of this transport in  $\mathcal{G}_k$  is due to the problem being semi-discrete and Theorem D.1. Define  $q'_a(y) = \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_{r_a \rightarrow q_a}^*(s_{a,j}) = y)$ . It follows that

$$\begin{aligned} \text{err}(\hat{h}) - \text{err}_{\alpha, f}^* &\leq \mathcal{E} + \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} (W_1(\hat{r}_a, \hat{q}_a) - W_1(r_a, q_a)) \\ &= \mathcal{E} + \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} (W_1(\hat{r}_a, \hat{q}_a) - W_1(\hat{r}_a, q_a) + W_1(\hat{r}_a, q_a) - W_1(\hat{r}_a, q'_a) \\ &\quad + W_1(\hat{r}_a, q'_a) - W_1(r_a, q_a)) \\ &\leq \mathcal{E} + \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} ((W_1(\hat{r}_a, q_a) - W_1(\hat{r}_a, q'_a)) + (W_1(\hat{r}_a, q'_a) - W_1(r_a, q_a))) \\ &\leq \mathcal{E} + \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} (W_1(q_a, q'_a) + (W_1(\hat{r}_a, q'_a) - W_1(r_a, q_a))), \end{aligned}$$

where line 3 is due to  $\hat{q}_a$  being the minimizer of Eq. (5) on the  $\hat{r}_a$ 's

For the first term in the summand, because both distributions  $q_a, q'_a$  are supported on the vertices, so by Proposition A.3,  $W_1(q_a, q'_a) = \|q_a - q'_a\|_1$ , and w.p. at least  $1 - \delta$ , for all  $a \in [m]$ ,

$$\begin{aligned} \|q_a - q'_a\|_1 &= \sum_{i \in [k]} \left| \mathbb{E}_{S \sim r_a} [\mathbb{1}(\mathcal{T}_{r_a \rightarrow q_a}^*(S)_i = 1)] - \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_{r_a \rightarrow q_a}^*(s_{a,j})_i = 1) \right| \\ &= \left\| \mathbb{E}_{S \sim r_a} [\mathcal{T}_{r_a \rightarrow q_a}^*(S)] - \frac{1}{n} \sum_{j=1}^n \mathcal{T}_{r_a \rightarrow q_a}^*(s_{a,j}) \right\|_1 \\ &\leq O\left(\sqrt{\frac{k}{n} \ln\left(\frac{m}{\delta}\right)}\right), \end{aligned}$$

where the last line follows from applying Lemma C.1 using the same arguments in the proof of Lemma C.2, and a union bound over all  $a \in [m]$ .

For the second term, because then the joint probability of  $(\hat{S}, \mathcal{T}_{r_a \rightarrow q_a}^*(\hat{S}))$ ,  $\hat{S} \sim \hat{r}_a$ , is a coupling belonging to  $\Gamma(\hat{r}_a, q'_a)$ , the transportation cost of  $\mathcal{T}_{r_a \rightarrow q_a}^*$  on  $\hat{r}_a$  to  $q'_a$  upper bounds  $W_1(\hat{r}_a, q'_a)$ , whereby w.p. at least  $1 - \delta$ , for all  $a \in [m]$ ,

$$\begin{aligned} W_1(\hat{r}_a, q'_a) - W_1(r_a, q_a) &\leq \frac{1}{n} \sum_{j=1}^n \|\mathcal{T}_{r_a \rightarrow q_a}^*(s_{a,j}) - s_{a,j}\|_1 - \mathbb{E}_{S \sim r_a} [\|\mathcal{T}_{r_a \rightarrow q_a}^*(S) - S\|_1] \\ &\leq O\left(\sqrt{\frac{1}{n} \ln\left(\frac{m}{\delta}\right)}\right) \end{aligned}$$

by Hoeffding's inequality, because  $\|\mathcal{T}_{r_a \rightarrow q_a}^*(s_{a,j}) - s_{a,j}\|_1 \leq 2$ .

Hence, putting everything together, we conclude with a union bound that

$$\text{err}(\hat{h}) - \text{err}_{\alpha, f}^* \leq O\left(\sqrt{\frac{k}{n} \ln\left(\frac{nm}{k\delta}\right)} + \frac{k^2}{n}\right)$$

(assuming  $n \geq k$ , otherwise  $O(\sqrt{k/n \cdot \ln(nm/\delta)} + k^2/n)$ ).

**Fairness ( $\Delta_{\text{DP}}$ ).** By applying Theorem C.3 and Corollary D.16 to the artificial binary classification problem whose data distribution is the joint distribution of  $(S, 1)$ ,  $S \sim r_a$ , and a union bound, w.p. at least  $1 - \delta$ , for all  $i \in [k]$  and  $a \in [m]$ ,

$$\begin{aligned} & \left| \mathbb{P}(\hat{h}(X, A) = e_i \mid A = a) - \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_a(s_{a,j}) = e_i) \right| \\ &= \left| \mathbb{E}_{S \sim r_a, \mathcal{T}_a}[\mathbb{1}(\mathcal{T}_a(S)_i = 1)] - \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_a(s_{a,j})_i = 1) \right| \leq O\left(\sqrt{\frac{k}{n} \ln\left(\frac{mk}{\delta}\right)}\right). \end{aligned}$$

Now, the decision boundaries of the function  $s \mapsto \mathbb{1}(\mathcal{T}_a(s)_i = 1) \in \mathcal{G}_{k,i}$  (defined in Eq. (18)) are described by  $k$  hyperplanes, and  $\mathcal{T}_a$  is extracted from  $\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*$ , so by the discussion in Appendix D and Lemma D.5 and the same reasoning used previously, they both agree on all but  $k$  points in  $S_a$  almost surely, thereby

$$\begin{aligned} \left| \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_a(s_{a,j}) = e_i) - \hat{q}_a(e_i) \right| &= \left| \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_a(s_{a,j})_i = 1) - \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s_{a,j})_i = 1) \right| \\ &\leq \frac{1}{n} \sum_{j=1}^n \mathbb{1}(\mathcal{T}_a(s_{a,j})_i \neq \mathcal{T}_{\hat{r}_a \rightarrow \hat{q}_a}^*(s_{a,j})_i) \leq O\left(\frac{k}{n}\right). \end{aligned}$$

Therefore, we conclude that

$$\begin{aligned} \Delta_{\text{DP}}(\hat{h}) &= \max_{\substack{a, a' \in [m] \\ y \in \mathcal{Y}}} \left| \mathbb{P}(\hat{h}(X, A) = y \mid A = a) - \mathbb{P}(\hat{h}(X, a') = y \mid A = a') \right| \\ &\leq \max_{\substack{a, a' \in [m] \\ y \in \mathcal{Y}}} |\hat{q}_a(y) - \hat{q}_{a'}(y)| \\ &\quad + \max_{\substack{a, a' \in [m] \\ y \in \mathcal{Y}}} \left( \left| \mathbb{P}(\hat{h}(X, A) = y \mid A = a) - \hat{q}_a(y) \right| + \left| \mathbb{P}(\hat{h}(X, a') = y \mid A = a') - \hat{q}_{a'}(y) \right| \right) \\ &\leq \alpha + O\left(\sqrt{\frac{k}{n} \ln\left(\frac{mk}{\delta}\right)} + \frac{k}{n}\right). \end{aligned}$$

□

*Proof of Theorem 4.5.* Let the  $q_a$ 's denote the minimizer of Eq. (5) on the  $r_a$ 's with  $\alpha$ , then

$$\bar{h}_\rho(x, a) := \mathcal{T}_{\hat{r}_a \rightarrow q_a}^* \circ u_\rho \circ f_a(x)$$



where  $\tilde{r}_a := u_\rho \sharp r_a$ .

Denote the coupling associated with  $\mathcal{T}_{\tilde{r}_a \rightarrow q_a}^*$  by  $\gamma_a \in \Gamma(\tilde{r}_a, q_a)$ , then the Markov kernel of  $\mathcal{T}_{\tilde{r}_a \rightarrow q_a}^* \circ u_\rho$  is

$$\mathcal{K}(s, T) = \mathbb{E}_{N \sim \rho_s} \left[ \frac{\gamma_a(s + N, T)}{\gamma_a(s + N, \mathcal{Y})} \right] = \int_{\tilde{s} \in \mathbb{R}^k} \frac{\gamma_a(\tilde{s}, T)}{\gamma_a(\tilde{s}, \mathcal{Y})} d(\rho_s * \delta_s)(\tilde{s}) = \int_{\tilde{s} \in \mathbb{R}^k} \frac{\gamma_a(\tilde{s}, T)}{\tilde{r}_a(\tilde{s})} d(\rho_s * \delta_s)(\tilde{s}),$$

where  $*$  denotes convolution.

Consider the classification problem  $\mu'$  derived from the original  $\mu$  under an input transformation given by the joint distribution of  $(f_A(X), A, Y)$ , as discussed in Section 3.3, on which  $\text{Id}$  is the Bayes optimal predictor due to calibration of the  $f_a$ 's. Then by Lemma B.5 applied on  $\mu'$ , the error rate on group  $a$ , denoted by  $\text{err}_a(\bar{h}_\rho)$ , is

$$\text{err}_a(\bar{h}_\rho) = \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 d\gamma'_a(s, y), \quad (8)$$

where  $\gamma'_a \in \Gamma(r_a, q_a)$  equals to

$$\gamma'_a(s, y) = \int_{\text{Id}^{-1}(s)} \mathcal{K}(s', y) dr_a(s') = \mathcal{K}(s, y) \cdot r_a(s) = \int_{\mathbb{R}^k} \frac{\gamma_a(\tilde{s}, y)}{\tilde{r}_a(\tilde{s})} d(\rho_s * \delta_s)(\tilde{s}) \cdot r_a(s),$$

whereby

$$\begin{aligned} 2 \text{err}_a(\bar{h}_\rho) &= \sum_{y \in \mathcal{Y}} \int_{\Delta_k} \int_{\mathbb{R}^k} \|s - y\|_1 \frac{\gamma_a(\tilde{s}, y)}{\tilde{r}_a(\tilde{s})} \cdot (\rho_s * \delta_s)(\tilde{s}) r_a(s) d\tilde{s} ds \\ &\leq \sum_{y \in \mathcal{Y}} \int_{\Delta_k} \int_{\mathbb{R}^k} \|\tilde{s} - y\|_1 \frac{\gamma_a(\tilde{s}, y)}{\tilde{r}_a(\tilde{s})} \cdot (\rho_s * \delta_s)(\tilde{s}) r_a(s) d\tilde{s} ds \\ &\quad + \sum_{y \in \mathcal{Y}} \int_{\Delta_k} \int_{\mathbb{R}^k} \|s - \tilde{s}\|_1 \frac{\gamma_a(\tilde{s}, y)}{\tilde{r}_a(\tilde{s})} \cdot (\rho_s * \delta_s)(\tilde{s}) r_a(s) d\tilde{s} ds \\ &=: \sum_{y \in \mathcal{Y}} \int_{\mathbb{R}^k} \|\tilde{s} - y\|_1 \frac{\gamma_a(\tilde{s}, y)}{\tilde{r}_a(\tilde{s})} \cdot \left( \int_{\Delta_k} (\rho_s * \delta_s)(\tilde{s}) r_a(s) d\tilde{s} \right) d\tilde{s} \\ &\quad + \sum_{y \in \mathcal{Y}} \int_{\Delta_k} \int_{\mathbb{R}^k} \|n\|_1 \frac{\gamma_a(n - s, y)}{\tilde{r}_a(n - s)} \cdot (\rho_s * \delta_s)(n - s) r_a(s) dn ds \\ &= \sum_{y \in \mathcal{Y}} \int_{\mathbb{R}^k} \|\tilde{s} - y\|_1 \frac{\gamma_a(\tilde{s}, y)}{\tilde{r}_a(\tilde{s})} \cdot \tilde{r}_a(\tilde{s}) d\tilde{s} + \int_{\Delta_k} \int_{\mathbb{R}^k} \|n\|_1 d\rho_s(n) dr_a(s) \\ &= W_1(\tilde{r}_a, q_a) + \mathbb{E}_{N \sim \rho_s, s \sim r_a} [\|N\|_1], \end{aligned}$$

where line 3 involves a change of variable  $n := \tilde{s} - s$ . Then we have

$$\begin{aligned} \text{err}(\bar{h}_\rho) - \text{err}_{\alpha, f}^* &\leq \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} (W_1(\tilde{r}_a, q_a) - W_1(r_a, q_a)) + \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} \mathbb{E}_{N \sim \rho_s, s \sim r_a} [\|N\|_1] \\ &\leq \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(\tilde{r}_a, r_a) + \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} \mathbb{E}_{N \sim \rho_s, s \sim r_a} [\|N\|_1]. \end{aligned}$$

Now, we upper bound the first term. Consider the coupling  $\pi_a \in \Gamma(\tilde{r}_a, r_a)$  given by  $\pi_a(\tilde{s}, s) = \rho_s(\tilde{s} - s)r_a(s)$ , whereby

$$\begin{aligned}
W_1(\tilde{r}_a, r_a) &= \inf_{\gamma \in \Gamma(\tilde{r}_a, r_a)} \int_{\mathbb{R}^k \times \Delta_k} \|\tilde{s} - s\|_1 d\gamma(\tilde{s}, s) \\
&\leq \int_{\mathbb{R}^k \times \Delta_k} \|\tilde{s} - s\|_1 d\pi_a(\tilde{s}, s) \\
&= \iint \|\tilde{s} - s\|_1 \rho_s(\tilde{s} - s) r_a(s) d\tilde{s} ds \\
&=: \iint \|(s + n) - s\|_1 \rho_s(n) r_a(s) dn ds \\
&= \mathbb{E}_{N \sim \rho_s, s \sim r_a} [\|N\|_1].
\end{aligned}$$

Substituting this into the result above, we obtain the upper bound.

On the other hand, the lower bound follows from Eq. (8), where

$$\text{err}(\bar{h}_\rho) = \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} \int_{\Delta_k \times \mathcal{Y}} \|s - y\|_1 d\gamma'_a(s, y) \geq \frac{1}{m} \sum_{a \in [m]} \frac{1}{2} W_1(r_a, q_a) = \text{err}_{\alpha, f}^*.$$

□

## D Optimal Transport Between Simplex and Vertex Distributions

The  $(k - 1)$ -dimensional probability simplex is defined for  $k \geq 2$  by

$$\Delta_k := \left\{ x \in \mathbb{R}^k : x \geq 0, \sum_{i=1}^k x_i = 1 \right\},$$

and its  $k$  vertices are  $\{e_1, \dots, e_k\}$ . In this section, we study the optimal transport problem between distributions supported on the simplex and its vertices under the  $\ell_1$  cost, given by  $c(x, y) = \|x - y\|_1$ .

By extending each  $\Delta_k$  to infinity, we obtain a  $(k - 1)$ -dimensional affine space of

$$\mathbb{D}^k := \left\{ x \in \mathbb{R}^k : \sum_{i=1}^k x_i = 1 \right\} \supset \Delta_k.$$

Define vectors

$$v_{ij} := e_j - e_i, \quad \forall i, j \in [k],$$

and note that for each  $i \in [k]$ ,  $\{v_{ij} : j \neq i\}$  forms a basis for  $\mathbb{D}^k$ . Also, observe the following identity for the  $\ell_1$  distance between a point on the simplex and a point on the vertex:

$$\|x - e_i\|_1 = 1 - x_i + \sum_{j \neq i} x_j = 1 - 2x_i + \sum_j x_j = 2(1 - x_i), \quad \forall x \in \Delta_k, i \in [k] \quad (9)$$

(this identity is central to some of the upcoming results).

A main result of this section is that when the transportation problem is semi-discrete, the deterministic (Monge) optimal transport exists, and is unique:

**Theorem D.1.** Let  $p$  be a continuous probability measure on  $\Delta_k$ ,  $q$  a probability measure on  $\{e_1, \dots, e_k\}$ , and  $c(x, y) = \|x - y\|_1$ . Then the optimal transport from  $p$  to  $q$  is a Monge plan, and is unique up to sets of measure zero w.r.t.  $p$ .

Specifically, the optimal transport  $\mathcal{T}_{p \rightarrow q}^*$  in Theorem D.1 is given by the  $c$ -transform of the Kantorovich potential from the Kantorovich-Rubinstein dual formulation of the transportation problem. In other words, it belongs to the following parameterized class of deterministic functions:

$$\mathcal{G}_k := \left\{ x \mapsto e_{\arg \min_{i \in [k]} (\|x - e_i\|_1 - \psi_i)} : \psi \in \mathbb{R}^k \right\} \subset \{e_1, \dots, e_k\}^{\Delta_k} \quad (10)$$

(break ties to the tied  $e_i$  with the largest index  $i$ ).

This function class is therefore of particular interest to various analyses in this paper. For the generalization bounds in Section 4.2, we show that this function class has low complexity in terms of the Natarajan dimension (Definition D.12):

**Theorem D.2.**  $d_N(\mathcal{G}_k) = k - 1$ .

In addition, note that as illustrated in Fig. 2, we can equivalently characterize each  $g \in \mathcal{G}_k$  by the center point at which its  $k$  decision boundaries all intersect:

**Proposition D.3.** Define the function class  $\mathcal{G}'_k \subset \{e_1, \dots, e_k\}^{\Delta_k}$  parameterized by  $\mathbb{R}^k$  s.t. for each  $g_z \in \mathcal{G}'_k$  with parameter  $z \in \mathbb{R}^k$ ,

$$g_z(x) = e_i \quad \text{if} \quad x_j - x_i \leq z_j - z_i \iff x^\top v_{ij} \leq z^\top v_{ij}, \quad \forall j \neq i \quad (11)$$

(when multiple  $e_i$ 's are eligible, output the tied  $e_i$  with the largest index  $i$ ).

Then  $\forall g_\psi \in \mathcal{G}_k$ ,  $g_\psi = g_z \in \mathcal{G}'_k$  by setting

$$z_i = \frac{1}{k} + \frac{1}{2} \left( \frac{1}{k} \sum_{j=1}^k \psi_j - \psi_i \right), \quad \forall i \in [k] \quad (12)$$

(the choice of  $\sum_{i=1}^k z_i = 1$  s.t.  $z \in \mathbb{D}^k$  was arbitrary, due to an extra degree of freedom because the support of  $g$  is contained in  $\Delta_k$ ).

Conversely,  $\forall g_z \in \mathcal{G}'_k$ ,  $g_z = g_\psi \in \mathcal{G}_k$  by setting

$$\psi_i = 2(z_1 - z_i) = 2z^\top v_{i1}, \quad \forall i \in [k] \quad (13)$$

(again, the choice of  $\psi_1 = 0$  was arbitrary).

*Proof.* Let  $g_\psi \in \mathcal{G}_k$ , then for the  $g_z \in \mathcal{G}'_k$  constructed in Eq. (12), by Eq. (9),

$$\begin{aligned} g_z(x) = e_i \text{ is eligible} &\iff x_j - x_i \leq z_j - z_i, & \forall j \neq i \\ &\iff x_j - x_i \leq (\psi_i - \psi_j)/2, & \forall j \neq i \\ &\iff 2(x_j - x_i) \leq \psi_i - \psi_j, & \forall j \neq i \\ &\iff 2(1 - x_i) - \psi_i \leq 2(1 - x_j) - \psi_j, & \forall j \neq i \\ &\iff \|x - e_i\|_1 - \psi_i \leq \|x - e_j\|_1 - \psi_j, & \forall j \neq i. \end{aligned}$$

Conversely, let  $g_z \in \mathcal{G}'_k$ , then for the  $g_\psi \in \mathcal{G}_k$  constructed in Eq. (13),

$$\begin{aligned} g_\psi(x) = e_i \text{ is eligible} &\iff \|x - e_i\|_1 - \psi_i \leq \|x - e_j\|_1 - \psi_j, & \forall j \neq i \\ &\iff 2(x_j - x_i) \leq 2(z_1 - z_i) - 2(z_1 - z_j), & \forall j \neq i \\ &\iff x_j - x_i \leq z_j - z_i, & \forall j \neq i. \end{aligned}$$

□

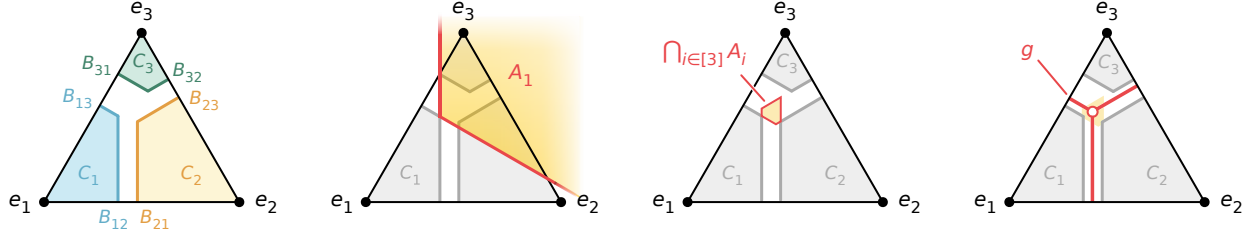


Figure 5: Illustration of the objects defined on Eqs. (15) and (16) for  $k = 3$ . See Fig. 6 for an example where the intersection is empty, when the underlying transport is not optimal.

We will often use this alternative characterization of  $\mathcal{G}_k$ .

The remaining proofs are deferred to Appendix D.2. Theorem D.1 is established via an analysis of the geometry of the simplex-vertex optimal transport, which we discuss in the next section.

## D.1 Geometry of Optimal Transport

Let  $p$  be an arbitrary distribution supported on  $\Delta_k$ , and  $q$  a (finite) distribution on  $\mathcal{Y} := \{e_1, \dots, e_k\}$ . We study the geometric properties of the optimal solution to the (Kantorovich) transportation problem between  $p, q$  under the  $\ell_1$  cost,

$$\sup_{\gamma \in \Gamma(p, q)} \int_{\Delta_k \times \mathcal{Y}} \|x - y\|_1 d\gamma(x, y), \quad (14)$$

and note that the supremum can be attained because the supports are compact.

First, given a simplex-vertex transport  $\gamma \in \Gamma(p, q)$ , we define the following geometric objects:

$$B_{ij} := \min \left\{ b \in \mathbb{R} : \gamma(\{x \in \Delta_k : x^\top v_{ij} \leq b - 1\}, e_i) = q(e_i) \right\} \cup \{0\}, \quad \text{and} \quad (15)$$

$$C_i := \bigcap_{j \neq i} \{x \in \Delta_k : x^\top v_{ij} \leq B_{ij} - 1\}.$$

For each  $i \in [k]$ ,  $B_{ij}$  defines the (smallest offset of the) halfspace in the  $v_{ij}$  direction in which all points that are transported by  $\gamma$  to  $e_i$  are contained, and  $C_i$  is formed by the intersections of these halfspaces, also containing all points transported to  $e_i$ . See Figs. 3 and 5 for illustrations.

Now, if  $\gamma^*$  is an optimal transport of Eq. (14), then intuition tells us that in order to achieve minimum cost, the halfspaces along each direction should not overlap (i.e.,  $B_{ij} + B_{ji} \leq 2$  for all  $i \neq j$ ), and the  $C_i$ 's should not intersect (except on a set of Lebesgue measure zero). We show that these intuitions regarding the geometry of  $\gamma^*$  are indeed valid, and they are implied by showing that the intersection of the following sets  $A_i$  is nonempty (see Fig. 5 for an illustration),

$$A_i := \bigcap_{j \neq i} \{x \in \mathbb{D}^k : x^\top v_{ij} \geq B_{ij} - 1\}. \quad (16)$$

**Proposition D.4.** *If  $\gamma^*$  is a minimizer of Eq. (14), then  $\bigcap_{i \in [k]} A_i \neq \emptyset$ .*

The proof is deferred to Appendix D.2. Note that  $\bigcap_{i \in [k]} A_i$  is exactly the set considered on Line 7 of Algorithm 2, and Proposition D.4 says that if  $\gamma^*$  is an optimal transport, then a point  $z \in \bigcap_{i \in [k]} A_i$  exists. The significance of this point is that, the function  $g_z \in \mathcal{G}_k$  with parameter  $z \in \mathbb{D}^k$  agrees with the transport  $\mathcal{T}_{p \rightarrow q}$  associated with  $\gamma^*$  only except for points that lie on the boundaries (which have Lebesgue measure zero):

**Lemma D.5.** *Let  $p, q$  be probability measures on  $\Delta_k$  and  $\{e_1, \dots, e_k\}$ , respectively. If  $\gamma^* \in \Gamma(p, q)$  is a minimizer of Eq. (14), then  $\exists \mathcal{T} \in \mathcal{G}_k$  with parameters  $z \in \mathbb{D}^k$  satisfying*

$$\gamma(x, \mathcal{T}(x)) = p(x), \quad \forall x \in \text{supp}(p) \setminus \bigcup_{i \neq j} \{x \in \mathbb{D}^k : x^\top v_{ij} = z^\top v_{ij}\}.$$

This result underlies many discussions throughout our presentation: (1) the construction used in its proof led to Lines 6–9 of Algorithm 2 for extracting post-processing functions from the empirical optimal transports, (2) it embodies the argument used in the proof of Theorem 4.4 regarding the disagreements between the extracted functions and the empirical transports, and (3) the existence part of Theorem D.1 is a direct consequence, since the set on which disagreements may occur always has measure zero when  $p$  is continuous.

*Proof.* Let  $z \in \bigcap_{i \in [k]} A_i$ , which exists due to Proposition D.4. Then let  $\mathcal{T} \in \mathcal{G}_k$  with parameter  $z$ , which we show agrees with  $\gamma^*$  on all  $x \in \text{supp}(p) \setminus \bigcup_{i \neq j} \{x \in \mathbb{D}^k : x^\top v_{ij} = z^\top v_{ij}\}$ : suppose  $\mathcal{T}(x) = e_i$ , then  $\mathcal{T}(x) = e_i \iff x^\top v_{ij} \leq z^\top v_{ij}$  by construction. Furthermore, by the definition of  $A_i$  in Eq. (16) of  $\gamma^*$ ,  $x^\top v_{ij} < z^\top v_{ij} \leq B_{ij} - 1$  for all  $j \neq i$ , so we must have that  $\gamma^*(x, e_j) = 0$ ,  $\forall j \neq i \implies \gamma^*(x, e_i) = p(x)$ . Otherwise, it would contradict the definition of  $B_{ij}$  in Eq. (15).  $\square$

## D.2 Omitted Proofs from Section D

*Proof of Theorem D.1.* For existence, Lemma D.5 provides a  $\mathcal{T} \in \mathcal{G}_k$  that agrees with the optimal transport almost everywhere, since the set of points lying on the boundaries has measure zero w.r.t.  $p$  by continuity.

Next, we prove uniqueness. Let  $\gamma, \gamma' \in \Gamma(p, q)$  be two optimal transports, and  $\mathcal{T}, \mathcal{T}' \in \mathcal{G}_k$  mappings provided by Lemma D.5 that agree with  $\gamma, \gamma'$  a.e. We will show that  $\mathcal{T} = \mathcal{T}'$  a.e., and so is  $\gamma = \gamma'$ .

Denote the parameter (i.e. center of the decision boundaries) of  $\mathcal{T}$  (analogously for  $\mathcal{T}'$ ) by  $z \in \mathbb{D}^k$ , the decision boundaries by  $B_{ij} := z^\top v_{ij} + 1$ , and the decision regions by  $C_i := \bigcap_{j \neq i} \{x \in \Delta_k : x^\top v_{ij} \leq B_{ij} - 1\}$ . By definition of  $\mathcal{G}_k$ ,  $\Delta_k = \bigsqcup_{i=1}^k C_i$ , and for all  $x \in \Delta_k$ ,  $\mathcal{T}(x) = e_i \iff x \in C_i$  almost surely, therefore,  $\gamma(C_i, e_i) = q(e_i)$  because  $\mathcal{T}$  agrees with the transport  $\gamma$  a.e.

Define the difference in the boundaries between  $\mathcal{T}$  and  $\mathcal{T}'$  by  $d_{ij} := B'_{ij} - B_{ij}$ , and note that

$$d_{ij} = d_{nj} - d_{ni} \quad \text{with} \quad d_{\ell\ell} := 0, \quad \forall i, j, n, \ell \in [k], \quad (17)$$

which follows from the observation that

$$B_{ij} = z^\top (v_{nj} - v_{ni}) + 1 = B_{nj} - B_{ni} + 1 \quad \text{with} \quad B_{\ell\ell} := 0, \quad \forall i, j, n, \ell \in [k].$$

Construct a directed graph of  $k$  nodes where  $(i, j)$  is an edge iff  $d_{ij} > 0$ . Note that this graph is acyclic: first, it cannot contain cycles of length 2, otherwise,  $(i, j), (j, i) \in E \implies d_{ij} + d_{ji} > 0$  contradicts the fact that  $d_{ij} + d_{ji} = 0$  by definition; next, consider the shortest cycle, and let  $(i, j), (n, i)$ ,  $j \neq n$  denote two edges contained in it. It follows that  $d_{ij}, d_{ni} > 0$ , and  $d_{nj} \leq 0$ , or it is not the shortest cycle. Then by Eq. (17),  $0 < d_{ij} = d_{nj} - d_{ni} < 0$ , which is a contradiction.

Now, we show by strong induction on the reverse topological order of the graph nodes that for all  $i \in [n]$ ,  $p(C_i \oplus C'_i) = 0$  where  $\oplus$  denotes the symmetric difference of the sets. For the base case, let  $i$  denote a sink node in the graph, then we have that  $d_{ij} \leq 0$  for all  $j$ , meaning that  $C'_i \subseteq C_i$ . Then  $q(e_i) = \gamma'(C'_i, e_i) = p(C'_i) \leq p(C_i) = \gamma(C_i, e_i) = q(e_i)$ . If the inequality is strict, then it is a contradiction; otherwise, combining the equality with  $\mathcal{T}(x) = e_i \iff x \in C_i$  a.s. (and  $\mathcal{T}'$

analogously) implies  $p(C_i \oplus C'_i) = p(C_i \setminus C'_i) = 0$ . For the inductive case, let  $i$  denote a node, and  $J \subseteq [n] \setminus \{i\}$  the set of nodes directed to from  $i$ , then by construction  $\bigsqcup_{j \in J \cup \{i\}} C'_j \subseteq \bigsqcup_{j \in J \cup \{i\}} C_j$ . Let  $F_i := C_i \cap C'_i$ , and note that for all  $x \in C'_i \setminus F_i$ ,  $\mathcal{T}'(x) = e_i$  and  $\mathcal{T}(x) \in \{e_j : j \in J \setminus \{i\}\}$ . Therefore,  $C'_i \setminus F_i \in \bigcup_{j \in J} (C_j \oplus C'_j)$ , and by the inductive hypothesis,  $p(C'_i \setminus F_i) \leq 0$ . It then follows that  $p(C'_i) \leq p(C_i)$ , and subsequently  $p(C_i \oplus C'_i) = p(C_i \setminus C'_i) = 0$  by the same arguments used in the base case.

Therefore,  $p(\{x : \mathcal{T}(x) \neq \mathcal{T}'(x)\}) \leq \sum_{i=1}^k p(C_i \oplus C'_i) = 0$ , so  $\mathcal{T} = \mathcal{T}'$  a.e.  $\square$

The proof of Proposition D.4 needs the following technical result, which at a high-level states that if a collection of  $v_{ij}$ -aligned convex sets do not intersect, then they cannot cover the entire space:

**Proposition D.6.** *Let  $B \in \mathbb{R}^{k \times k}$  arbitrary, and define  $S_i := \bigcap_{j \neq i} \{x \in \mathbb{D}^k : x^\top v_{ij} \leq B_{ij} - 1\}$  for each  $i \in [k]$ , then  $\bigcap_{i \in [k]} S_i = \emptyset \implies \bigcup_{i \in [k]} S_i \neq \mathbb{D}^k$ .*

While this could be proved with elementary arguments, for clarity, we use known results from algebraic topology in the final steps of our proof. The tools and concepts that we use include homotopy equivalence and homology groups (we omit the definition for the latter, but refer readers to (Spanier, 1981) for a textbook). The definitions are provided below for completeness; readers may skip to the main proof.

**Definition D.7** (Homotopy). Let  $\mathcal{X}, \mathcal{Y}$  be topological spaces, and  $f, g : \mathcal{X} \rightarrow \mathcal{Y}$  two continuous functions. A homotopy between  $f$  and  $g$  is a continuous function  $h : \mathcal{X} \times [0, 1] \rightarrow \mathcal{Y}$ , such that  $h(x, 0) = f(x)$  and  $h(x, 1) = g(x)$  for all  $x \in \mathcal{X}$ . We say  $f, g$  are homotopic if there exists a homotopy between them.

**Definition D.8** (Homotopy Equivalence). Let  $\mathcal{X}, \mathcal{Y}$  be topological spaces. If there exist continuous maps  $f : \mathcal{X} \rightarrow \mathcal{Y}$  and  $g : \mathcal{Y} \rightarrow \mathcal{X}$  such that  $g \circ f$  is homotopic to the identity map  $\text{Id}_{\mathcal{X}}$  on  $\mathcal{X}$ , and  $f \circ g$  is homotopic to  $\text{Id}_{\mathcal{Y}}$ , then  $\mathcal{X}$  and  $\mathcal{Y}$  are homotopy equivalent, denoted by  $\mathcal{X} \cong \mathcal{Y}$ .

**Fact D.9** (Homology). (See (Spanier, 1981) for a textbook).

1. The homology groups of  $\mathbb{R}^d$ , denoted by  $H_n(\mathbb{R}^d)$  for  $n \in \{0, 1, 2, \dots\}$ , are

$$H_n(\mathbb{R}^d) = \begin{cases} \mathbb{Z} & \text{if } n = 0 \\ \{0\} & \text{else.} \end{cases}$$

2. The homology groups of the  $d$ -dimensional simplex,  $\Delta_{d+1}$ , are

$$H_n(\Delta_{d+1}) = \begin{cases} \mathbb{Z} & \text{if } n = 0 \\ \{0\} & \text{else.} \end{cases}$$

3. The homology groups of the  $d$ -dimensional simplex without its interior,  $\partial\Delta_{d+1}$ , are

$$H_n(\partial\Delta_{d+1}) = \begin{cases} \mathbb{Z} & \text{if } n = 0 \text{ or } d - 1 \\ \{0\} & \text{else.} \end{cases}$$

4. If  $\mathcal{X} \cong \mathcal{Y}$ , then  $H_n(\mathcal{X}) = H_n(\mathcal{Y})$  for all  $n$ .

Clearly, the affine space  $\mathbb{D}^k \cong \mathbb{R}^{k-1}$  via a rotation and a translation. We also cite the Nerve theorem (Bauer et al., 2022, Theorem 3.1):

**Theorem D.10** (Nerve). *Let  $\mathcal{S} = \{S_1, \dots, S_n\}$  be a finite collection of sets, and define its nerve by*

$$\text{Nrv}(\mathcal{S}) = \left\{ J \subseteq [n] : \bigcap_{i \in J} S_i \neq \emptyset \right\}.$$

*If the sets  $S_i$ 's are convex closed subsets of  $\mathbb{R}^d$ , then  $\text{Nrv}(\mathcal{S}) \cong \bigcup_{i \in [n]} S_i$ .*

*Proof of Proposition D.6.* We prove the contrapositive statement of  $\bigcup_{i \in [k]} S_i = \mathbb{D}^k \implies \bigcap_{i \in [k]} S_i \neq \emptyset$  by strong induction on the dimensionality  $k$ . For the base case of  $k = 2$ , observe that  $S_1 \cup S_2 = \{x : x^\top v_{12} \leq B_{12} - 1 \text{ or } x^\top v_{12} \geq 1 - B_{21}\}$ , so  $S_1 \cup S_2 = \mathbb{D}^2$  if and only if  $B_{12} - 1 \geq 1 - B_{21}$ , in which case the point  $(1 - B_{12}/2, B_{12}/2) \in S_1 \cap S_2$ , thereby the intersection is nonempty.

For  $k > 2$ , suppose  $\bigcup_{i \in [k]} S_i = \mathbb{D}^k$ . Our goal is to show that for all  $J \subset [k]$ ,  $\bigcap_{j \in J} S_j \neq \emptyset$ . Recall that

$$S_i = \bigcap_{j \in [k], j \neq i} \{x \in \mathbb{D}^k : x^\top v_{ij} \leq B_{ij} - 1\},$$

and we define for any  $J \subset [k]$  and  $i \in [k]$

$$S'_{J,i} := \bigcap_{j \in J, j \neq i} \{x \in \mathbb{D}^k : x^\top v_{ij} \leq B_{ij} - 1\},$$

(we will drop the subscript  $J$  as the discussions below will focus on a single  $J$ ).

We first show that  $\bigcap_{i \in J} S_i \neq \emptyset$  for any  $J \subset [k]$  with  $|J| \leq k-1$ . By assumption,  $\mathbb{D}^k = \bigcup_{i \in [k]} S_i \subset \bigcup_{i \in [k]} S'_{J,i}$ , and we argue that  $\bigcup_{i \in J} S'_i = \mathbb{D}^k$ . Suppose not, then let  $z \notin \bigcup_{i \in J} S'_i$ , and consider the line

$$L := \left\{ z + a \sum_{i \notin J, j \in J} v_{ij} : a \in \mathbb{R} \right\}.$$

First, no part of this line is contained in  $\bigcup_{i \in J} S'_i$ , because it does not contain the point  $z \in L$ , and  $L$  runs parallel to and hence never intercepts any of the halfspaces defining each  $S'_i$  for  $i \in J$ : let  $i, j \in J$ ,  $i \neq j$ , then

$$v_{ij}^\top \sum_{n \notin J, m \in J} v_{nm} = \sum_{n \notin J, m \in J} (e_j^\top e_m - e_j^\top e_n - e_i^\top e_m + e_i^\top e_n) = 1 - 0 - 1 + 0 = 0.$$

Second, this line is partially not contained any  $S'_i = \bigcap_{j \in J} \{x \in \mathbb{D}^k : x^\top v_{ij} \leq B_{ij} - 1\}$  for  $i \notin J$ : let  $i \notin J$  and  $j \in J$ , then

$$v_{ij}^\top \sum_{n \notin J, m \in J} v_{nm} = \sum_{n \notin J, m \in J} (e_j^\top e_m - e_j^\top e_n - e_i^\top e_m + e_i^\top e_n) = 1 - 0 - 0 + 1 = 2;$$

so points on  $L$  with sufficiently large  $a$ 's are not contained in  $\bigcup_{i \notin J} S'_i$ , contradicting the assumption that  $\bigcup_{i \in [k]} S'_i = \mathbb{D}^k$ .

Back to proving that  $\bigcap_{i \in J} S_i \neq \emptyset$  for any  $J \subset [k]$  with  $|J| \leq k-1$ . Since  $\bigcup_{i \in J} S'_i = \mathbb{D}^k$ , by applying the inductive hypothesis to a  $|J|$ -dimensional instance derived from  $\{S'_i : i \in J\}$  by removing the axes  $\{e_i : i \notin J\}$ , we get  $\exists z' \in \bigcap_{i \in J} S'_i$ . Using similar arguments above, it can be shown that the line  $L' := \{z' + a \sum_{i \notin J, j \in J} v_{ij} : a \in \mathbb{R}\}$  is entirely contained in  $\bigcap_{i \in J} S'_i$  and partially in  $\bigcap_{i \in J} S_i = (\bigcap_{i \in J} S'_i) \cap (\bigcap_{i \notin J, j \in J} \{x \in \mathbb{D}^k : x^\top v_{ij} \leq B_{ij} - 1\})$ , so the intersection is nonempty.

We have thus established that any intersection of the strict subset of  $\{S_i\}_{i \in [k]}$  is nonempty, and we will conclude with the Nerve theorem. We have  $\forall J \subset [k]$ ,  $1 \leq |J| \leq k-1$ ,  $J \in$

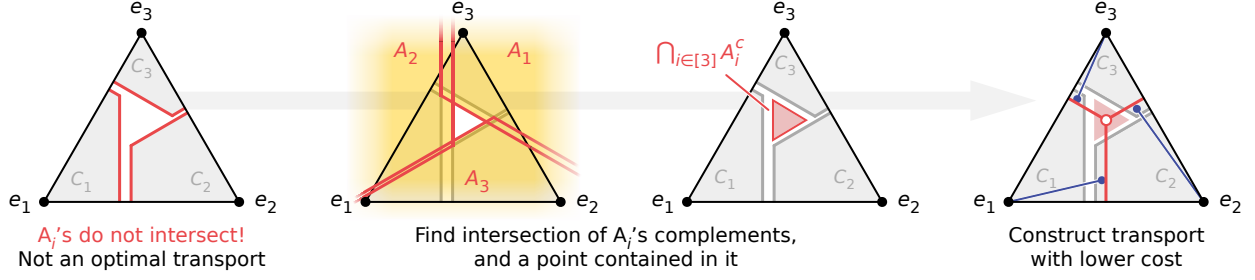


Figure 6: Illustration of the construction in the proof of Proposition D.4 for  $k = 3$ .

$\text{Nrv}(\{S_1, \dots, S_k\})$ . Because we assumed in the beginning that  $\bigcup_{i \in [k]} S_i = \mathbb{D}^k$ , it must follow that  $[k] \in \text{Nrv}(\{S_1, \dots, S_k\})$  as well. Otherwise, the nerve is a  $(k-1)$ -dimensional simplex (each  $n$ -face is represented by its  $n-1$  vertices) without its interior (represented by  $[k]$ ), whose homology differs from that of  $\mathbb{D}^k$ , then  $\bigcup_{i \in [k]} S_i \cong \text{Nrv}(\{S_1, \dots, S_k\}) \not\cong \mathbb{D}^k$  by Theorem D.10, which contradicts our assumption that  $\bigcup_{i \in [k]} S_i = \mathbb{D}^k$ . Hence the nerve contains  $[k]$ , meaning  $\bigcap_{i \in [k]} S_i \neq \emptyset$ .  $\square$

*Proof of Proposition D.4.* Recall the definitions of the objects  $B_{ij}$ ,  $C_i$  and  $A_i$  in Eqs. (15) and (16) of  $\gamma^*$ . Suppose  $\bigcap_{i \in [k]} A_i = \emptyset$ , then  $\exists z \in \bigcap_{i \in [k]} (\mathbb{D}^k \setminus A_i)$  by Proposition D.6. It then follows by definition that  $\forall i \in [k]$ ,  $\exists j \neq i$  s.t.  $z^\top v_{ij} < B_{ij} - 1$ . Let  $u : [k] \rightarrow [k]$  denote a mapping s.t. the pairs  $(i, u(i))$  satisfy this relation for all  $i \in [k]$ ; note that there exists a nonempty  $J \subseteq [m]$  s.t. the undirected edges  $\{(i, u(i)) : i \in J\}$  form a cycle because  $u(i) \neq i$ . Also, there exist  $m > 0$  and measurable sets  $F_i \subset \{x : x^\top v_{iu(i)} > z^\top v_{iu(i)}\} \subset C_i$  s.t.  $\gamma^*(F_i, e_i) := m_i \geq m$ .

We show that the coupling  $\gamma' \in \Gamma(p, q)$  given by

$$\gamma'(B, e_i) = \begin{cases} \gamma^*(B, e_i) & \text{if } i \notin J, \\ \gamma^*(B \cap (\Delta_k \setminus F_i), e_i) + \frac{m_i - m}{m_i} \gamma^*(B \cap F_i, e_i) + \frac{m}{m_{u^{-1}(i)}} \gamma^*(B \cap F_{u^{-1}(i)}, e_{u^{-1}(i)}) & \text{else} \end{cases}$$

has a lower transportation cost than  $\gamma^*$  (see Fig. 6 for an illustration):

$$\begin{aligned} \int_{\Delta_k \times \mathcal{Y}} \|x - y\|_1 d(\gamma^* - \gamma')(x, y) &= \sum_{i \in J} \frac{m}{m_i} \int_{F_i} (\|x - e_i\|_1 - \|x - e_{u(i)}\|_1) d\gamma^*(x, e_i) \\ &= \sum_{i \in J} \frac{2m}{m_i} \int_{F_i} x^\top v_{iu(i)} d\gamma^*(x, e_i) \\ &> \sum_{i \in J} \frac{2m}{m_i} \int_{F_i} z^\top v_{iu(i)} d\gamma^*(x, e_i) \\ &= 2m \sum_{i \in J} z^\top v_{iu(i)} \\ &= 2m \sum_{i \in J} (z_{u(i)} - z_i) = 0, \end{aligned}$$

where line 2 follows from Eq. (9).  $\square$

Finally, we consider the complexity of the function class  $\mathcal{G}_k$  defined in Eq. (10). First, recall the (multiclass-generalized) definition of shattering, based on which the Natarajan dimension is defined (Shalev-Shwartz and Ben-David, 2014, Definitions 29.1 and 29.2):



**Definition D.11** (Shattering). Let  $\mathcal{H} \subset \{1, \dots, k\}^{\mathcal{X}}$  be a class of multiclass functions.  $\mathcal{H}$  is said to shatter a set  $S \subset \mathcal{X}$  if there exist  $f_0, f_1 : S \rightarrow \{1, \dots, k\}$  satisfying  $f_0(x) \neq f_1(x)$  for all  $x \in S$ , such that  $\forall S_0, S_1 \subset S$  that partition  $S$ ,  $\exists h \in \mathcal{H}$ ,

$$\begin{aligned} h(x) &= f_0(x), \quad \forall x \in S_0, \quad \text{and} \\ h(x) &= f_1(x), \quad \forall x \in S_1. \end{aligned}$$

**Definition D.12** (Natarajan Dimension). The Natarajan dimension of a class of multiclass functions  $\mathcal{H} \subset \{1, \dots, k\}^{\mathcal{X}}$ , denoted by  $d_N(\mathcal{H})$ , is the largest number  $n$  s.t.  $\exists S \subset \mathcal{X}$  of cardinality  $n$  that is shattered by  $\mathcal{H}$ .

*Proof of Theorem D.2.* We associate  $e_i$  with the label  $i$ ,  $\forall i \in \{1, \dots, k\}$ . We first show that  $d_N(\mathcal{G}_k) \geq k - 1$  by constructing a set of cardinality  $k - 1$  that is shattered by  $\mathcal{G}_k$ , then show that  $d_N(\mathcal{G}_k) < k$  by contradiction.

**Lower Bound.** Consider the set  $S = \{e_1, e_2, \dots, e_{k-1}\}$  and let  $f_0(e_j) = j$  and  $f_1(e_j) = k$  for all  $j \in [k - 1]$ , which satisfy  $f_0 \neq f_1$  on all  $x \in S$ . Let  $S_0 \sqcup S_1 = S$  be arbitrary, and define

$$\iota(j) := \begin{cases} \mathbb{1}(e_j \in S_1) & \text{if } j \in [k - 1] \\ 0 & \text{if } j = k. \end{cases}$$

Consider  $g_z \in \mathcal{G}_k$  with parameters

$$z = \frac{1}{k} \cdot \mathbf{1}_k - \sum_{j=1}^{k-1} \iota(j) \sum_{\ell \neq j} v_{j\ell},$$

where boldface  $\mathbf{1}_k \in \mathbb{R}^k$  denotes the vector of all ones. Observe that

$$\begin{aligned} z^\top v_{nm} &= - \sum_{j=1}^{k-1} \iota(j) \sum_{\ell \neq j} v_{j\ell}^\top v_{nm} \\ &= - \sum_{j=1}^{k-1} \iota(j) \sum_{\ell \neq j} (e_\ell^\top e_m - e_\ell^\top e_n - e_j^\top e_m + e_j^\top e_n) \\ &= \sum_{j=1}^{k-1} \iota(j) (\mathbb{1}(n \neq j) - \mathbb{1}(m \neq j)) + (k - 1) \sum_{j=1}^{k-1} \iota(j) (e_j^\top e_m - e_j^\top e_n) \\ &= (k - 1)(\iota(m) - \iota(n)) + (\iota(m) - \iota(n)) \\ &= k(\iota(m) - \iota(n)). \end{aligned}$$

Recall from Eq. (11) that for all  $i, n \in [k]$ ,

$$g_z(e_i) = e_n \text{ is eligible} \iff e_i^\top v_{nm} \leq z^\top v_{nm}, \quad \forall m \neq n;$$

so in our case, it follows that for all  $i \in [k - 1]$  and  $j \neq i$ ,

$$g_z(e_i) = e_i \text{ is eligible} \iff -1 \leq k(\iota(m) - \iota(i)), \quad \forall m \neq i,$$

and

$$g_z(e_i) = e_j \text{ is eligible} \iff 1 \leq k(\iota(i) - \iota(j)) \quad \text{and} \quad 0 \leq k(\iota(m) - \iota(j)), \quad \forall m \neq i$$

(also, recall  $\iota(k) := 0$ ).

Observe that for any  $i \in [k - 1]$ , if  $\iota(i) = 0$ , then  $g_z(e_i) = e_j$  is ineligible for all  $j \neq i$ , then we must have  $g_z(e_i) = e_i$ . Otherwise, if  $\iota(i) = 1$ , then  $e_k$  is always eligible, so  $g_z(e_i) = e_k$  due to the tie-breaking rule. Therefore,  $g_z$  is a witness function, and we conclude that  $\mathcal{G}_k$  shatters  $S$ .

**Upper Bound.** Let  $S = (x_1, \dots, x_k)$  be given, along with  $f_0, f_1 : S \rightarrow [k]$  satisfying  $f_0(x) \neq f_1(x)$  for all  $x \in S$ . Suppose  $\mathcal{G}_k$  shatters  $S$ . Let  $g_z \in \mathcal{G}_k$  denote a witness function for the partitioning of  $S_0 = S$  and  $S_1 = \emptyset$ , and  $g_{z'} \in \mathcal{G}_k$  that for the partitioning of  $S'_0 = \emptyset$  and  $S'_1 = S$ .

We will reuse an argument from an earlier proof. Denote the decision boundaries of  $g_z$  (analogously for  $g_{z'}$ ) by  $B_{ij} := z^\top v_{ij} + 1$ , and the decision regions by  $C_i := \bigcap_{j \neq i} \{x \in \Delta_k : x^\top v_{ij} \leq B_{ij} - 1\}$ . By definition of  $\mathcal{G}_k$ ,  $x \in C_i \implies g_z(x) = e_i$  is eligible. Then, define the difference in the boundaries between  $g_z$  and  $g_{z'}$  by  $d_{ij} := B'_{ij} - B_{ij}$ . Construct a directed graph of  $k$  nodes where  $(i, j)$  is an edge iff  $d_{ij} > 0$ , which is acyclic as shown in the proof of Theorem D.1.

First, consider the case where  $\exists x, x' \in S$  s.t.  $\{f_0(x), f_1(x)\} = \{f_0(x'), f_1(x')\}$ . W.l.o.g., assume  $i := f_0(x_1) = f_1(x_2)$  and  $j := f_1(x_2) = f_0(x_1)$ , then we have

$$\begin{aligned} g_z(x_1) = e_i, g_{z'}(x_1) = e_j &\implies d_{ji} > 0, \\ g_z(x_2) = e_j, g_{z'}(x_2) = e_i &\implies d_{ij} > 0 \end{aligned}$$

(after taking into account of the tie-breaking rule), however, this would imply a cycle in the graph, which is a contradiction.

Next, if  $\{f_0(x), f_1(x)\}$  differs for all  $x \in S$ , then we may assume w.l.o.g.  $f_0(x_i) = e_i$  and  $f_1(x_i) = e_{i+1}$  for all  $i \in [k]$  (where the index of  $k+1$  means 1). Then

$$g_z(x_i) = e_i, g_{z'}(x_i) = e_{i+1} \implies d_{i+1,i} > 0, \quad \forall i \in [k];$$

again, this would imply a cycle in the graph, hence a contradiction. Therefore, we conclude that  $\mathcal{G}_k$  cannot shatter any  $S \subset \Delta_k$  of cardinality  $k$ .  $\square$

In addition, on data distributions that satisfy  $X = Y$ ,  $X \in \Delta_k$ , applying the  $\ell_1$  loss of  $\ell(\hat{y}, y) := \|\hat{y} - y\|_1$  to  $\mathcal{G}_k$  yields a function class with pseudo-dimension of  $k - 1$ :

**Definition D.13** (Pseudo-Shattering). Let  $\mathcal{H} \subset [0, 1]^\mathcal{X}$  be a class of real-valued functions.  $\mathcal{H}$  is said to pseudo-shatter a set  $\{x_1, \dots, x_n\} \subset \mathcal{X}$  if  $\exists r_1, \dots, r_n \in \mathbb{R}$  such that  $\forall y_1, \dots, y_n \in \{0, 1\}$ ,  $\exists h \in \mathcal{H}$  satisfying  $\mathbb{1}(h(x_i) \geq r_i) = y_i$  for all  $i \in [n]$ .

**Definition D.14** (Pseudo-Dimension). The pseudo-dimension of a class of real-valued functions  $\mathcal{H} \subset [0, 1]^\mathcal{X}$ , denoted by  $d_P(\mathcal{H})$ , is the largest number  $n$  s.t.  $\exists S \subset \mathcal{X}$  of cardinality  $n$  that is pseudo-shattered by  $\mathcal{H}$ .

**Theorem D.15.** Define  $\mathcal{H}_k := \{x \mapsto \|g(x) - x\|_1 : g \in \mathcal{G}_k\}$ , then  $d_P(\mathcal{H}_k) = k - 1$ .

*Proof.* The proof shares the same arguments as that of Theorem D.2. We will only show the upper bound, and remark that the lower bound can be established using a similar construction of that in Theorem D.2.

Let  $x_1, \dots, x_k$  be given, and suppose there exists thresholds  $r_1, \dots, r_k$  s.t.  $\mathcal{H}_k$  shatters the set of points. It follows that  $\exists g_z, g_{z'} \in \mathcal{G}_k$  s.t.  $\|g_{z'}(x_i) - x_i\|_1 < r_i \leq \|g_z(x_i) - x_i\|_1$  for all  $i$ , which means that  $g_z(x_i) \neq g_{z'}(x_i)$ . But by the arguments in the proof of the upper bound of Theorem D.2, such  $(g_z, g_{z'})$  pair does not exist, contradicting the shattering assumption.  $\square$

Finally, for all  $i \in \{1, \dots, k\}$ , define the label- $i$ -versus-all binarization of  $\mathcal{G}_k$  by

$$\mathcal{G}_{k,i} := \{x \mapsto \mathbb{1}(g(x) = e_i) : g \in \mathcal{G}_k\} \subset \{0, 1\}^{\Delta_k}. \quad (18)$$

Clearly, its *VC dimension*, the binary class reduction of the Natarajan dimension (Definition D.12), denoted by  $d_{VC}(\mathcal{G}_{k,i})$ , is upper bounded by  $d_N(\mathcal{G}_k)$ :

**Corollary D.16.**  $d_{VC}(\mathcal{G}_{k,i}) \leq d_N(\mathcal{G}_k) = k - 1$ .

## E Experiment Details

### E.1 Datasets and Tasks

We provide descriptions of each dataset and the tasks they entail. Statistics of the datasets are included in Tables 3 to 5, where the numbers indicate the proportion (%) of examples belonging to the classes in each group.

**Adult** (Kohavi, 1996). This binary classification task decides whether the annual income of an individual is over or below \$50k per year ( $|\mathcal{Y}| = 2$ ) given attributes including gender, race, age, education level, etc. The data are collected from the 1994 US Census. We consider gender to be the sensitive attribute ( $|\mathcal{A}| = 2$  from the dataset).

The tabular dataset is pre-processed by normalizing numerical attributes and converting categorical attributes into one-hot representation. The training set of 30,162 examples is split in half for training the predictor and performing post-processing.

**Communities & Crime** (Redmond and Baveja, 2002). The Communities & Crime tabular dataset contains the socioeconomic and crime data of communities in 46 US states, and the task is to predict the number of violent crimes per 100k population given attributes ranging from the racial composition of the community, their income and background, and law enforcement resource. The data come from the 1990 US Census, 1990 LEMAS survey, and 1995 FBI Uniform Crime Reporting program. We bin the rate of violent crime into five classes ( $|\mathcal{Y}| = 5$ ), and we treat race as the sensitive attribute by the presence of minorities ( $|\mathcal{A}| = 4$ ): a community does not have a significant presence of minorities if White makes up more than 95% of the population, otherwise the largest minority group is considered to have a significant presence (Asian, Black, or Hispanic).

The pre-processing is the same as that on Adult. Because of the small dataset size of 1,994, results are averaged with 10-fold cross validation (using the folds provided by the dataset).

**BiasBios** (De-Arteaga et al., 2019). The task is to determine the occupation ( $|\mathcal{Y}| = 28$ ) of female and male individuals ( $|\mathcal{A}| = 2$ ) by their raw text biographies. The data are mined from the Common Crawl corpus. In this dataset, gender is the sensitive attribute, and is observed to correlate with certain occupations such as software engineer and nurse.

We use the version of BiasBios compiled and hosted by Ravfogel et al. (2020), which is reshuffled and split into 295,067 training and 98,356 test examples. We split the training set further by 95%/5% for training the predictor and performing post-processing, respectively.

This experiment is of particular interest because of the increasing popularity of large language models and the fairness concerns regarding their usage. In particular, the uncensored corpora (e.g., crawled from the internet) on which the language models are pre-trained may contain historical social bias, and empirical investigations have shown that such bias could be propagated and amplified in downstream applications (Bolukbasi et al., 2016; Zhao et al., 2018; Abid et al., 2021).

### E.2 Experiment Setup

On each dataset, we first train attribute-aware predictors via minimizing the MSE w.r.t. the one-hot class labels without constraints (Eq. (6)), then post-process the predictors using Algorithm 2, and also the smoothing procedure in Section 4.3 (Appendix E.3). Note that our post-processing procedure is also applicable to models trained with other losses, e.g., cross-entropy loss, but the performance may be suboptimal without model calibration as discussed in Section 3.3.

Table 2: Group-balanced error rate (Eq. (4)) and DP fairness ( $\Delta_{\text{DP}}$ ; Definition 2.1) of classifiers post-processed using Algorithm 2 and the smoothing procedure of Section 4.3 under strict DP ( $\alpha = 0$ ). The number of groups  $\mathcal{A}$  and classes  $\mathcal{Y}$  on each task are included.

Dataset	$ \mathcal{A} $	$ \mathcal{Y} $	Method	err	$\Delta_{\text{DP}}$
Adult	2	2	Not post-processed	0.1365	0.1556
			Algorithm 2	0.1566	0.00009
			Alg. 2 w/ smoothing	0.1566	0.00006
Communities & Crime	4	5	Not post-processed	0.3264	0.5321
			Algorithm 2	0.3929	0.1253
			Alg. 2 w/ smoothing	0.3836	0.1135
BiasBios	2	28	Not post-processed	0.1344	0.0852
			Algorithm 2	0.1924	0.0215
			Alg. 2 w/ smoothing	0.2072	0.0070

We use linear models on the Adult and Communities & Crime tabular datasets (learned via OLS), and a neural language model fine-tuned from the BERT base (uncased) checkpoint with 110 million parameters on the BiasBios text dataset (Devlin et al., 2019). Recall that Algorithm 2 requires the outputs of the predictor to be contained in the simplex  $\Delta_k$ ; we do not enforce this constraint during training, and instead project the outputs to the simplex during post-processing and inference. For simplex projection, we use the implementation by Blondel et al. (2014).

**BERT Hyperparameters.** To fine-tune BERT base (uncased) pre-trained language model on BiasBios, we add a new linear layer on the output embedding of the [CLS] token, and train the model end-to-end for three epochs using the AdamW optimizer. We set the batch size to 32, learning rate to  $2\text{e-}5$ , use a linearly decaying learning rate schedule with a warmup ratio of 0.1,  $L^2$  weight decay rate of 0.01, and clip the norm of the gradients to 1. The PyTorch implementation is included in our code,<sup>2</sup> which uses the Hugging Face Transformers library (Wolf et al., 2020).

### E.3 Results with Smoothing Procedure

Since it is possible that the continuity assumption on the  $r_a$ ’s required by Algorithm 2 is violated in our experiment setup (for instance, due to the simplex projection of raw model outputs), we explore whether further performance gains could be obtained from applying the remedy described in Section 4.3 of smoothing the distributions by a continuous noise.

For the continuous noise, we use a distribution based on the Dirichlet distribution, with point-wise scaling to ensure roughly equal variance on each input point (we refer readers to our code<sup>2</sup> for the implementation). Using the Dirichlet distribution ensures that the perturbed points always stay inside the simplex, hence we can apply the procedure used in Algorithm 2 to find the optimal transport from the smoothed  $\tilde{r}_a$  to each  $\hat{q}_a$ , the latter of which are estimated from calling  $\text{LP}(\hat{r}_1, \dots, \hat{r}_m, \alpha)$  (note that it is not called on the smoothed versions of the empirical distributions, which would be denoted by  $\hat{\tilde{r}}_a$ ).

Each example is perturbed 10 times for post-processing, and 1000 times during inference. The results under  $\alpha = 0$  are presented in Table 2, where we observe that smoothing achieves significant further improvements to  $\Delta_{\text{DP}}$ .

#### E.4 Finding Feasible Point in Intersection of Halfspaces

Line 7 of Algorithm 2 involves finding a feasible point in the intersection of halfspaces, which can be obtained with the following linear program:

$$\min_{z \in \mathbb{R}^k} 0 \quad \text{s.t.} \quad z^\top v_{ij} \leq B_{ij} - 1, \quad \forall i, j \in [k], i \neq j.$$

As illustrated in Fig. 3, the point  $z$  that is returned determines the center of the boundaries of the extracted transport maps  $\mathcal{T}_a \in \mathcal{G}_k$ . Because of the machine learning folklore that classifiers with larger margin enjoy better generalization properties, we instead use the follow quadratic program (of a least-squares problem) that maximizes the margins in our experiments for point-finding:

$$\min_{z \in \mathbb{R}^k} \sum_{i \neq j} \frac{\|z^\top v_{ij} - (B_{ij} - 1)\|_2^2}{(2 - B_{ij} - B_{ji})^2} \quad \text{s.t.} \quad z^\top v_{ij} \leq B_{ij} - 1, \quad \forall i, j \in [k], i \neq j.$$

Although comparisons are not included, our preliminary experiments showed that using the quadratic program for point-finding led to better post-processing performance with Algorithm 2 than using the linear program, both in terms of the error rate and  $\Delta_{\text{DP}}$  during inference.

Table 3: Dataset statistics of Adult (%).

Class \ Group	Female	Male
$\leq 50k$	89.07	69.62
$> 50k$	10.93	30.38
Count	14423	22732

Table 4: Dataset statistics of Communities &amp; Crime (%).

Class \ Group	Asian	Black	Hispanic	White
[0.0, 0.2]	76.87	34.06	41.73	92.21
(0.2, 0.4]	15.66	27.97	36.75	6.08
(0.4, 0.6]	3.20	18.59	13.12	1.22
(0.6, 0.8]	2.85	9.22	4.99	0.24
(0.8, 1.0]	1.42	10.16	3.41	0.24
Count	562	640	381	411

Table 5: Dataset statistics of BiasBios (%).

Class \ Group	Female	Male
Accountant	1.14	1.69
Architect	1.32	3.65
Attorney	6.86	9.52
Chiropractor	0.38	0.90
Comedian	0.33	1.04
Composer	0.50	2.22
Dentist	2.83	4.41
Dietitian	2.03	0.14
DJ	0.12	0.60
Filmmaker	1.27	2.22
Interior Designer	0.65	0.13
Journalist	5.42	4.77
Model	3.41	0.61
Nurse	9.47	0.82
Painter	1.95	1.98
Paralegal	0.82	0.13
Pastor	0.33	0.91
Personal Trainer	0.36	0.37
Photographer	4.77	7.40
Physician	10.75	8.98
Poet	1.89	1.69
Professor	29.26	30.67
Psychologist	6.25	3.27
Rapper	0.07	0.60
Software Engineer	0.60	2.75
Surgeon	1.08	5.35
Teacher	5.36	3.04
Yoga Teacher	0.77	0.12
Count	182102	211321