OPTIMAL TRANSPORT OF BINARY CLASSIFIERS TO FAIRNESS

A PREPRINT

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ABSTRACT

Much of the past work on fairness in machine learning has focused on forcing the predictions of classifiers to have similar statistical properties for individuals of different demographics. Yet, such methods often simply perform a rescaling of the classifier scores and ignore whether individuals of different groups have similar features. Our proposed method, Optimal Transport to Fairness (OTF), applies Optimal Transport (OT) to take this similarity into account by quantifying unfairness as the smallest cost of OT between a classifier and any score function that satisfies fairness constraints. For a flexible class of linear fairness constraints, we show a practical way to compute OTF as an unfairness cost term that can be added to any standard classification setting. Experiments show that OTF can be used to achieve an effective trade-off between predictive power and fairness.

Keywords fairness, machine learning, optimal transport, constraints, classification

1 Introduction

Machine learning methods are increasingly being deployed to perform automated decision making due to the potential benefits in terms of efficiency and effectiveness. Yet, there are clear risks in using machine learning to make automated decisions about people, as evidenced by more and more cases of undesirable algorithmic discrimination [22, 9, 7] with respect to the protected traits of individuals. While it is straightforward to avoid direct discrimination by simply not using such sensitive information in the machine learning model’s decisions, the main concern is with the remaining indirect discrimination where a model still disproportionately affects certain groups, even though the decisions are made in an apparently neutral way [29].

The research field of fairness in machine learning [23] therefore studies ways in which a model’s indirect discrimination with respect to a person’s sensitive features can be reduced or removed. Many notions to mathematically define fairness for binary classification tasks have been proposed [28]. Popular examples such as demographic parity and equalized odds [17] are represented in the form of equality constraints between groups of individuals in the dataset. For instance, by considering the gap between the mean predicted probabilities for each sensitive group, we can quantify the unfairness of the classifier that produced these probabilities [4].

Motivation A fairness-adjustment method that plans to equalize mean probabilities between groups usually requires that the scores for an undervalued group increase overall while the scores for the overvalued group decrease overall. However, by only considering such statistical properties of the classifier’s output, the input features for which those scores were computed are ignored. Yet, when quantifying the unfairness of a classifier, weighing the similarities between the features of people is important, because classifiers are already designed to map input features to scores as accurately as possible. It may thus be easier to make the classifier satisfy fairness constraints by minimizing score discrepancies between similar individuals that belong to different sensitive groups. With the goal of adjusting the classifier for fairness, we therefore aim to quantify unfairness as the amount of work that is minimally required to make the classifier fair.

To this end, we apply Optimal Transport (OT) theory [25] to assign a value to how different score distributions are, while expressing the desire to move scores between similar inputs through a cost function defined over the input
Optimal Transport of Binary Classifiers to Fairness

Our proposed method, referred to as Optimal Transport to Fairness (OTF), is defined as the smallest cost of OT between the score function of a classifier and any fair score function over the same data.

Contributions

- We present OTF as an OT-based quantification of unfairness that is flexible in how fairness is defined. In particular, we study linear fairness notions, i.e. notions of fairness that can be represented as a set of linear constraints over the classifier’s output. This class of constraints allows us to minimize unfairness with respect to multiple sensitive variables that can be categorical or continuous.

- To make the OTF method easier to differentiate, we add entropic regularization and sketch a way to efficiently compute this regularized OTF cost. By adding an adjustment term, we also make sure that the cost of the regularized OTF is zero for fair models.

- In experiments, our method shows its benefit of increased flexibility over other OT methods. It also achieves a trade-off between predictive power and (linear) fairness that is significantly more effective for conditional notions of fairness such as equalized odds.

Outline

In Sec. 2 we recall the standard context of fair binary classification, discuss the practical use of linear fairness notions and introduce the OT problem. With these preliminaries, we gradually construct the OTF method in Sec. 3. We compare with related work in Sec. 4 and end with experiment results in Sec. 5.

Notation

- \( Z \triangleq \mathcal{X} \times S \times \{0, 1\} \): the sample space, with \( \mathcal{X} \subset \mathbb{R}^{d_X} \) the input feature space and \( S \subset \mathbb{R}^{d_S} \) the sensitive feature space.

- \( Z \triangleq (X, S, Y) \): a random sample, with \( X \) the input features, \( S \) the sensitive features and \( Y \) the output label.

- \([d_S]\): the set of integers \( \{0, \ldots, d_S - 1\} \).

- \( S_k \): feature at index \( k \in [d_S] \) in \( S \). Categorical values in \( S \) are one-hot encoded.

- \( Y_l \): value at index \( l \in \{0, 1\} \) in the one-hot encoding of \( Y \).

- \( \hat{Y} \in \{0, 1\} \): the predicted output of the classifier \( h \).

- \( h: \mathcal{X} \to [0, 1] \): the score function corresponding with the classifier \( h \) via \( h(X) \triangleq \mathbb{P}(\hat{Y} = 1 \mid X) \).

- \( f: \mathcal{X} \to [0, 1] \): a generic score function.

- \( \mathcal{F} \): the set of fair score functions.

- \( g(Z): Z \to \mathbb{R}^{d_F} \) and \( \gamma \in [0, 1]^{d_F} \): the vector-valued function and constants that define a linear fairness notion with \( d_F \) constraints.

- \( \mathcal{D} \): the dataset of \( n \) data points sampled from \( Z \).

- \( P \in \mathbb{R}^{n \times n} \): the matrix of coupling values \( P_{ij} = \pi(x_i, x_j) \).

- \( C \in \mathbb{R}^{n \times n} \): the matrix of cost function values \( C_{ij} = c(x_i, x_j) \).

- \( G \in \mathbb{R}^{n \times d_F} \): the matrix of \( g \) values \( G_{jc} = g(x_j)_c \).

- \( f, h \in \mathbb{R}^n \): the vectors of score function values \( f_i = f(x_i) \) and \( h_i = h(x_i) \)

- \( \langle C, P \rangle = \sum_{ij} C_{ij} P_{ij} \).

- \( 1_n \): the \( n \)-dimensional vector of ones.

2 Background

Our discussion on Optimal Transport to Fairness (OTF) involves three notational contexts. First, we introduce notation relating to fair binary classifiers in Sec. 2.1. Second, we elaborate on some popular ways in which fairness is defined through fairness constraints in Sec. 2.2. Third, we sketch the background on Optimal Transport (OT) problems in Sec. 2.2.
2.1 Fair Binary Classification

We start the construction of our framework by considering the context of binary classification. Let \( Z \triangleq X \times S \times \{0, 1\} \) denote the sample space, from which we draw samples \( Z \triangleq (X, S, Y) \) and try to predict the binary output label \( Y \in \{0, 1\} \) from input features \( X \in \mathcal{X} \), without discriminating with respect to sensitive features \( S \in \mathcal{S} \). It is further assumed that \( \mathcal{X} \subset \mathbb{R}^{d_X} \) and \( \mathcal{S} \subset \mathbb{R}^{d_S} \) where \( d_X \) and \( d_S \) are the dimensionality of \( \mathcal{X} \) and \( \mathcal{S} \).

In this setting, we can find classifiers that provide binary predictions \( \hat{Y} \in \{0, 1\} \), where a positive classification has probability \( h(X) \triangleq P(\hat{Y} = 1 \mid X) \). Each classification model is therefore linked with a score function \( h : \mathcal{X} \rightarrow [0, 1] \). In what follows, we will interchangeably use the notation \( h \) to refer to a classifer, its score function or the measure corresponding with that score function (discussed in Sec. 2.3.1). Our general goal in fair classification is to minimize a loss function \( \mathcal{L}_Y(h) \), in our case the cross-entropy between \( \hat{Y} \) and \( Y \), while also improving the fairness of \( h \).

2.2 Fairness Constraints

Statistical definitions of group fairness are concerned with enforcing some notion of a (conditional) independence measurement [23]. The most common examples of such definitions are demographic parity and equalized odds, which we describe first. Afterwards, we discuss linear independence: a notion of fairness that extends demographic parity to continuous sensitive attributes. With minor adjustments, we also show how linear independence can be used for conditional forms of demographic parity.

2.2.1 Demographic Parity

Let \( \mathcal{S} \) consist of a single, categorical feature. A classic fairness notion is then demographic parity, which requires that the average predicted label \( \hat{Y} \) for every sensitive group \( S \) in \( \mathcal{S} \) is equal:

\[
P(\hat{Y} = 1 \mid S) = P(\hat{Y} = 1).
\]

For future convenience, we will represent the categorical values in \( \mathcal{S} \) as their one-hot encoding, e.g. if there is only one sensitive feature and it has two categories, then \( \mathcal{S} = \{[1, 0], [0, 1]\} \) with \( |\mathcal{S}| = d_S = 2 \). With the distribution of \( Y \) characterized by the score function \( h : \mathcal{X} \rightarrow [0, 1] \), we can rewrite demographic parity as

\[
\forall k \in [d_S] : \frac{1}{p_k} \mathbb{E}_Z [f(X)S_k] = \mathbb{E}[h(X)]
\]

with \( S_k \in \{0, 1\} \) the one-hot encoded features of the category \( S \), with \( p_k = P(S_k = 1) \) and \( [d_S] = \{0, ..., d_S - 1\} \).

2.2.2 Equalized Odds

A common criticism of demographic parity is that it enforces equal average probabilities for every group, i.e. \( P(\hat{Y} = 1 \mid S) = P(\hat{Y} = 1) \), regardless of whether every group is labeled positive at the same rate. If the latter is not the case for a justifiable reason, e.g. \( P(Y = 1 \mid S) \neq P(Y = 1) \), then it may be better to condition the constraint on \( Y \), which is referred to as equalized odds [17].

By also using a one-hot encoding of \( Y \), we retrieve the following expression for equalized odds:

\[
\forall l \in \{0, 1\}, \forall k \in [d_S] : \frac{1}{p_{k,l}} \mathbb{E}_Z [h(X)S_kY_l] = \mathbb{E}[h(X)Y_l].
\]

2.2.3 Linear (Conditional) Independence

Traditional group fairness constraints such as demographic parity assume that the sensitive features consist of discrete categories that an individual belongs to. However, some sensitive information, like age, is inherently continuous. In our formulation, we therefore allow for a mix of multiple categorical and continuous sensitive attributes by considering them as different dimensions in \( \mathcal{S} \). Categorical attributes then have as many dimensions as there are categories, while continuous attributes like age each consist of one dimension in \( \mathcal{S} \).

For such a collection of sensitive features, we could instead enforce linear independence, which we consider achieved when the covariance between \( h(X) \) and each dimension of \( \mathcal{S} \) equals zero:

\[
\forall k \in [d_S] : \mathbb{E}_Z [h(X)S_k] - \mathbb{E}_Z [h(X)] \mathbb{E}_Z [S_k] = 0.
\]
Observe that the constraint in Eq. \((3)\) is exactly the demographic parity constraint in Eq. \((1)\) since \(E_Z[S_k] = p_k\) for categorical \(S\).

The notation in Eq. \((3)\) is easily extended to linear conditional independence by conditioning on \(Y\):

\[
\forall \{0, 1\}, \forall k \in [d_S] : E_Z[h(X)S_k | Y] = E_Z[h(X) | Y]E_Z[S_k | Y] = 0.
\] (4)

By setting \(\gamma_k = E_Z[h(X)Y_l]\) in Eq. \((4)\), we similarly retrieve equalized odds in Eq. \((2)\). While out of scope for this paper, note that in Eq. \((4)\) we could have also conditioned on any other categorical variable.

### 2.2.4 Linear Fairness Notions

More generally, we are interested in all fairness notions that can be enforced through such linear constraints.

**Definition 2.1** (linear fairness notion). A notion of fairness is a linear fairness notion when the non-empty set \(\mathcal{F}\) of all score functions \(f\) that satisfy it is given by

\[
\mathcal{F} \triangleq \{ f : X \rightarrow [0, 1] : E_Z[f(X)g(Z)] = \gamma \}
\] (5)

with \(g(Z) : Z \rightarrow \mathbb{R}^{d_F}\) a vector-valued function not affected by \(f(X)\) and \(\gamma \in [0, 1]^{d_F}\) a vector of constants. Together, they define the linear fairness notion as \(d_F\) constraints.

Indeed, linear conditional independence can be achieved by setting \(g(Z)_{k+l:d_S} = \frac{S_kY_l}{E_Z[S_kY_l]}\) and \(\gamma_{k+l:d_S} = E(h(X)Y_l)\), making it, and all notions so far, linear fairness notions.

Similar characterizations of linear fairness constraints have been made in the past \([11]\). They are practical because they can be evaluated efficiently. Moreover, when multiple linear fairness notions are compatible, i.e. the intersection of their \(\mathcal{F}\) sets remains non-empty, their respective \(g\) function and \(\gamma\) constants can simply be stacked to retrieve a new linear fairness notion. Furthermore, the set of score functions \(\mathcal{F}\) is convex, which greatly helps in the search of \(\mathcal{F}\) for interesting models.

However, we do note that the linearity of the constraints means that non-linear dependence between a score function \(f(X)\) and sensitive attributes \(S\) can remain undetected. Also, some well-known fairness notions are not linear, e.g. enforcing predictive parity involves conditioning on \(f(X)\), which means that \(f(X)\) also shows up in the \(g(Z)\) function.

### 2.3 Optimal Transport

Optimal Transport \([24]\) (OT) theory considers the problem of moving a mass from one measure to another at the smallest possible cost. However, our aim is to transport mass between score functions, from which several kinds of measures could be constructed. We therefore address this discrepancy before applying the traditional OT problem.

#### 2.3.1 Tying Score Functions to Measures

A score function \(f : \mathcal{X} \rightarrow [0, 1]\) is involved in two domains: it operates on elements from the input space \(\mathcal{X}\), but then produces a probability for value 1 in the output space \(\{0, 1\}\). In some prior work on OT for classifiers, \([13, 20]\), the OT problem was posed using measures and a cost function over the output space. Yet, our intention is to avoid transports between inputs that are highly dissimilar. We therefore tie classifiers to measures over the input space \(\mathcal{X}\) endowed with the Borel \(\sigma\)-algebra:

\[
\phi_f(E) \triangleq \sum_{x \in D_X} f(x)\delta_x(E)
\] (6)

with \(E \subseteq \mathcal{X}\), \(\delta_e\) the Dirac measure (i.e. \(\delta_e(E) = 1\) if \(e \in E\), else \(\delta_e(E) = 0\)) and \(D_X\) all input features of samples in the dataset \(D\), gathered from the sample space \(Z\). Note that the input space measure \(\phi_f\) is not normalized (i.e. \(\phi_f(\mathcal{X}) \neq 1\)), though this is not necessary to apply OT theory.

In what follows, we use Eq. \((6)\) to implicitly consider the score functions \(h\) and \(f\) as their corresponding input space measures \(\phi_h\) and \(\phi_f\) when used in the OT problem.

#### 2.3.2 Transporting Classifiers

For a dataset \(D\) with \(n\) samples, we vectorize the notation in Sec. \([24]\) by having \(h\) and \(f\) denote the \(n\)-dimensional vectors of score function values for all data points, i.e. \(h_i = h(x_i)\) and \(f_i = f(x_i)\). Furthermore, for a non-negative cost function \(c\) defined over \(\mathcal{X} \times \mathcal{X}\), let \(C \in \mathbb{R}^{n \times n}_+\) represent the matrix of cost terms, i.e. \(C_{ij} = c(x_i, x_j)\). Similarly,
with \( \pi(x_i, x_j) \) the coupling that reflects how much score mass was transported from \( x_i \) to \( x_j \), define the matrix \( P \in \mathbb{R}^{n \times n} \) with \( P_{ij} = \pi(x_i, x_j) \). The OT cost is then simplified to

\[
\text{OT}(h, f) = \min_{P \in \Pi(h, f)} \langle C, P \rangle
\]

with

\[
\Pi(h, f) = \{ P \in \mathbb{R}^{n \times n} : P1_n = h, P^T1_n = f \}.
\]

where \( 1_n \) is the \( n \)-dimensional vector of ones.

Though the optimization in Eq. \( 7 \) is a linear programming problem, the OT cost is not directly differentiable with respect to the score functions \( h \) and \( f \).

A well-known trick to smoothen the OT problem is to also maximize (a variant \(^1\) of) the entropy \( H(P) \) of the coupling matrix \( 25 \):

\[
H(P) = -\sum_{ij} P_{ij} \left( \log(P_{ij}) - 1 \right).
\]

This results in the following formulation for OT (without fairness):

\[
\text{OT}_{\varepsilon}(h, f) = \min_{P \in \Pi(h, f)} \langle C, P \rangle - \varepsilon H(P)
\]

with \( \varepsilon > 0 \) a hyperparameter that regulates the strength of regularization. An interesting consequence of adding \( H(P) \) to the objective is that the entropy term excludes any coupling with non-positive elements, thus the problem only admits \( P \) matrices that are positive.

### 3 Optimal Transport to Fairness

Fairness constraints as in Sec. \( 2.2 \) can be applied to a classifier’s score function \( h \) to test whether the scores satisfy our notion of fairness. If \( h \) is shown to be unfair, however, there are many ways to quantify this unfairness. To motivate our proposed definition of unfairness, we set up the following thought experiment. Assume that a set \( F \) is available that denotes exactly all score functions which satisfy the required notion of fairness. If a classifier’s score function \( h \) is unfair, then it ought to be replaced by a fair score function \( f \in F \). Arguably, the most suitable \( f \) for this purpose is the projection of \( h \) onto \( F \), i.e. the \( f \in F \) that is closest to \( h \). However, replacing \( h \) by its fair projection may come at a cost, e.g. because the latter may not be as accurate in predicting the data as \( h \) was. The unfairness of \( h \) can thus be quantified at any point by measuring how far it is from its fair projection at that point.

We propose to measure the distance between score functions as the OT cost between \( h \) and \( f \), as it allows us to assign a higher unfairness to an \( h \) that needs to transport scores between highly dissimilar individuals in order to reach a fair function \( f \in F \). Thus, we propose to quantify unfairness as the cost of Optimal Transport to Fairness (OTF), i.e. the cost of the OT-based projection of \( h \) onto \( F \):

\[
\text{OTF}(h) = \min_{f \in F} \text{OT}(h, f).
\]

In what follows, we expand on the OTF method by constructing it in three steps.

1. In Sec. \( 3.1 \) we directly express the OTF(\( h \)) objective as a linear programming problem by making the assumption that \( F \) is defined by a linear fairness notion as in Def. \( 2.1 \).
2. In Sec. \( 3.2 \) we add entropic regularization to OTF(\( h \)) as was done in Eq. \( 8 \), thereby making the regularized OTF\( _\varepsilon \)(\( h \)) cost differentiable and efficient to compute.
3. In Sec. \( 3.3 \) we address the fact that due to this regularization, OTF\( _\varepsilon \)(\( h \)) does not necessarily equal zero for a fair \( h \). To this end, we subtract OT\( _\varepsilon \)(\( h, h \)), i.e. the cost of transporting a score function onto itself, resulting in the adjusted OTF\( _0 \)(\( h \)) cost.

After having fully constructed the adjusted, regularized OTF cost, we finally propose how this measure of unfairness can be minimized with respect to a classifier’s score function \( h \) in Sec. \( 3.4 \).

\(^1\)The total sum of \( P \) is subtracted to simplify later derivations.
3.1 Optimal Transport to Linear Fairness

To compute the minimization in Eq. (9), first note that in the OT(h, f) cost in Eq. (7), f only shows up in the constraint \( P^T 1_n = f \) on the column marginals of coupling matrix \( P \). It therefore suffices to weaken this constraint to \( P^T 1_n \in F \). Next, recall that for a linear fairness notion (see Definition 2.1), fairness can be enforced through a vector of constraints on the expectation of \( f(X)g(Z) \). For a dataset \( D \) with \( n \) samples, let \( G_{jc} = g(z_j)c \), i.e. \( G \in \mathbb{R}^{n \times d_F} \) is the constraints matrix with a row for every data point and a column for every constraint. Together, \( G \) and \( \gamma \), define the linear fairness notion for the dataset.

**Definition 3.1 (OTF).** For a linear fairness notion expressed through constraints matrix \( G \) and vector \( \gamma \) for \( n \) samples, and with non-negative cost matrix \( C \), the **Optimal Transport to Fairness** cost for score function \( h: \mathcal{X} \rightarrow [0, 1] \) is computed as

\[
\text{OTF}(h) = \min_{P \in \Pi^F(h)} \langle C, P \rangle
\]

with

\[
\Pi^F(h) = \{ P \in \mathbb{R}^{n \times n} : P 1_n = h, 1_n^T P G = \gamma \}.
\]

The optimal coupling computed for OTF(h) implicitly transports the scores of \( h \) to the fair vector \( f \) given the coupling’s column marginals (i.e. \( f = P^T 1_n \)). Note that for any coupling matrix that satisfies the first constraint (\( P 1_n = h \)), we have that \( h^T 1_n = 1_n^T P^T 1_n = f^T 1_n \), meaning that \( h \) and this implicitly found vector \( f \) sum to the same value. Scores of \( h \) are therefore only transported to a fair score function and no extra scores are created or destroyed.

For a constant \( G \) and \( \gamma \) and with \( P_{ij} > 0 \), the optimization problem in Eq. 10 can be solved through linear programming. However, its solution coupling is sparse, since it is optimal to meet the linear constraint by greedily transporting scores from data point \( x_i \) to \( x_j \) where \( C_{ij} \) is lowest until the budget given by \( h_i \) at index \( i \) runs out. Moreover, the solution is not directly differentiable with respect to the score function \( h \).

3.2 Entropic Regularization

Like the OT(h, f) cost in Sec. 2.3.2, the optimization of OTF(h) can be smoothened through entropic regularization.

**Definition 3.2 (OTF).** For a linear fairness notion expressed through constraints matrix \( G \) and vector \( \gamma \) for \( n \) data points, and with non-negative cost matrix \( C \), the **regularized OTF** cost with regularization strength \( \epsilon > 0 \) for score function \( h: \mathcal{X} \rightarrow [0, 1] \) is computed as

\[
\text{OTF}_\epsilon(h) = \min_{P \in \Pi^F(h)} \langle C, P \rangle - \epsilon H(P)
\]

with

\[
\Pi^F(h) = \{ P \in \mathbb{R}^{n \times n} : P 1_n = h, 1_n^T P G = \gamma \}.
\]

The use of the entropy term \( H(P) \) in the objective Eq. 11 requires some justification, since in contrast to the setting where the entropy regularization term is commonly used, we do not assume \( h \) to represent a normalized probability distribution (i.e. sum to one). Therefore, \( P \) also does not represent a normalized joint distribution. However, the \( H(P) \) term maintains the practical advantage that it only admits couplings with \( P_{ij} > 0 \). Together with the marginalization constraint \( P 1_n = h \), we thus still have that \( P_{ij} \leq 1 \), since \( h_i \leq 1 \).

A further advantage of using entropic regularization is that the overall OTF\(_\epsilon\) problem in Def. 3.2 remains convex. Under the assumption that there exists a score function \( f \in F \) with the same total score as \( h \), \( \Pi^F(h) \) is non-empty. The OTF\(_\epsilon\) problem for linear fairness notions therefore enjoys strong duality. Furthermore, the total number of constraints is \( n + d_F \), with \( n \) the number of samples and \( d_F \) the number of linear fairness constraints, which is usually far lower than the \( n^2 \) variables that make up the coupling in the primal problem. For these reasons, we will derive and then maximize the dual function instead.

3.2.1 The Dual Problem

The Lagrangian of the OTF\(_\epsilon\) problem in Def. 3.2 is given by

\[
\Lambda(P, \lambda, \mu) = \sum_{ij} C_{ij} P_{ij} - \sum_i \lambda_i \left( \sum_j P_{ij} - h_i \right) - \sum_c \mu_c \left( \sum_{ij} P_{ij} G_{jc} - \gamma_c \right) + \epsilon \sum_{ij} P_{ij} \left( \log P_{ij} - 1 \right).
\]

where \( \lambda \) and \( \mu \) denote the dual variable vectors for the marginalization and the fairness constraints respectively.
Setting $\frac{\partial \Lambda(P, \lambda, \mu)}{\partial P_{ij}} = 0$, we get:

$$P^*_{ij}(\lambda, \mu) = \exp \left( \frac{1}{\epsilon} \left[ -C_{ij} + \lambda_i + \sum_c \mu_c G_{jc} \right] \right).$$

(12)

This results in the dual function

$$L(\lambda, \mu) = \sum_i \lambda_i h_i + \sum_c \mu_c \gamma_c - \epsilon \sum_{ij} P^*_{ij}(\lambda, \mu).$$

(13)

The $\lambda$ and $\mu$ variables that maximize $L(\lambda, \mu)$ can, due to strong duality, be plugged into Eq. (12) to retrieve the optimal coupling $P$.

### 3.2.2 Optimization

Though Eq. (13) could be maximized directly, we follow standard OT approaches [25] and perform our optimization with coordinate ascent. This strategy is particularly useful here, because the $\lambda_i$ variable that maximizes $L(\lambda, \mu)$ while $\mu$ is fixed, is found independently of other variables in $\lambda$. All variables in $\lambda$ can therefore be updated at the same time:

$$\lambda_i \leftarrow \epsilon \log h_i - \epsilon \log \sum_j \exp \left( \frac{1}{\epsilon} \left[ -C_{ij} + \sum_c \mu_c G_{jc} \right] \right)$$

(14)

where we can use the stabilized log-sum-exp operation.

Unfortunately, there is no closed form expression for the $\mu_c$ that maximizes $L(\lambda, \mu)$. Instead, we preprocess $L(\lambda, \mu)$ and numerically solve for each $\mu_c$:

$$\mu_c \leftarrow \arg \max_{\mu_c} \mu_c \gamma_c - \epsilon \sum_j \eta_j(\lambda) \exp \left( \frac{1}{\epsilon} \sum_{k\neq c} \mu_k G_{jk} \right) \exp \left( \frac{1}{\epsilon} \mu_c G_{jc} \right)$$

(15)

with $\eta_j(\lambda) = \sum_i \exp \left( \frac{1}{\epsilon} [-C_{ij} + \lambda_i] \right)$.

### 3.2.3 Complexity

The dual function in Eq. (13) involves two variable vectors. First, $\lambda$ with length $n$ the dataset size that OTF is computed for. Second, $\mu$ with length $d_F$ the number of linear fairness constraints. It is often the case that $d_F << n$, because even when multiple sensitive features are composed, each is either categorical with a limited number of possible values (i.e. distinguished groups) or continuous and then only has a dimensionality of 1 in our setting. This is in contrast with the traditional OTF problem, where the dual problem involves two dual variable vectors of length $n$.

In terms of computational complexity, each $\lambda_i$ update is $O(n + d_F)$, making the update of the full $\lambda$ vector $O(n(n + d_F))$. However, we again note that the $\lambda_i$ can be updated in parallel. When keeping the $\lambda$ vector fixed, we can perform a $O(n^2)$ operation to precompute the $\eta_j(\lambda)$ values for the entire $\mu$ update. This latter update is more complicated due to the lack of a closed form solution to the maximization problem of each $\mu_c$. Still, using a precomputed $\eta$ vector this maximization only has complexity $O(n + d_F)$ and should only be performed for $d_F$ variables. Under the assumption that the computational complexity of a full maximization is far less than the $O(n^2)$ need to precompute $\eta$, the update of all $\mu$ will not have a greater order of computational complexity than $\lambda$. By permitting a high tolerance on the convergence of $\lambda$, the number of updates needed is also limited. In practice we found that a single update is often already enough.

In terms of memory complexity, we can achieve a theoretical complexity of $O(n + d_F)$, since the entire computation of OTF can be written in terms of individual scalars. However, being able to precompute and store the cost matrix $C$ and the fairness constraints matrix $G$ allows us to perform efficient matrix computations, e.g. the parallel update of $\lambda$. The memory required for practical use is therefore $O(n(n + d_F))$.

### 3.3 Adjusted OTF

A cause for concern with the regularized OTF cost is that, as opposed to the unregularized OTF, it does not necessarily equal zero if $h$ is already a fair score function. Indeed, while it may be feasible to achieve $\langle C, P \rangle = 0$, it is generally the case that the entropy $H(P) > 0$.

Therefore, again inspired by solutions for such problems for OT, [14][12], we propose an adjusted variant of OTF($h$) where we subtract OT($h, h$), i.e. the cost of transporting $h$ onto itself.
**Definition 3.3 (OTF\textsubscript{0}).** For a score function \( h : \mathcal{X} \to [0, 1] \), the adjusted OTF\textsubscript{0} cost is computed as

\[
\text{OTF}_0^\epsilon(h) = \text{OTF}_\epsilon(h) - \text{OT}_\epsilon(h, h)
\]  

(16)

In each definition so far, the only assumption we made about the cost function \( c \) (and its matrix \( C \)) is that it is non-negative. More strongly, we can assert that \( c \) is a semimetric, i.e. \( c : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+ \) with \( x = x' \iff c(x, x') = 0 \) and \( c(x, x') = c(x', x) \). With such a score function, we have the following result.

**Proposition 1.** For a semimetric cost matrix \( C \) and score function \( h : \mathcal{X} \to [0, 1] \), an optimal coupling for \( \text{OTF}_\epsilon(h, h) \) is symmetric. Moreover, an optimal coupling can be found without the constraint on the column marginals of the coupling, now referred to as \( \kappa \).

**Proof.** We aim to prove that the constraint on the column marginals of the coupling (i.e. \( P^T 1_n = h \)) is redundant to find the optimal coupling for \( \text{OTF}_\epsilon(h, h) \). Let \( \zeta(P) = \langle C, P \rangle - \epsilon H(P) \). We have that \( \zeta(P) = \zeta(P^T) \) due to the symmetry of \( C \). Because \( \zeta \) is also convex, we then have by Jensen’s inequality that \( \zeta \left( \frac{P + P^T}{2} \right) \leq \frac{1}{2} \zeta(P) + \frac{1}{2} \zeta(P^T) \).

Therefore, an optimal coupling \( P \in \Pi(h) \) for Eq. (17) must be symmetric. Due to this symmetry, the constraint on the row marginals \( (P 1_n = h) \) implies the constraint on the column marginals \( (P^T 1_n = h) \), making the latter redundant. \( \square \)

**Proposition 2.** For a linear fairness notion, \( h \in \mathcal{F} \implies \text{OTF}_0^\epsilon(h) = 0 \)

**Proof.** If \( h \) is already a fair model, i.e. \( h \in \mathcal{F} \), then an optimal coupling that optimizes \( \text{OTF}_\epsilon(h, h) \) is per Def. 3.2 also a valid coupling for \( \text{OTF}_\epsilon(h) \). From Prop. 1, it follows that this coupling is already optimal for a variant of the \( \text{OTF}_\epsilon(h) \) problem without column constraints. Taken together, we therefore have that \( \text{OTF}_\epsilon(h, h) \) and \( \text{OTF}_\epsilon(h) \) have the same optimal couplings. Their objective terms are thus the same, implying that \( \text{OTF}_0^\epsilon(h) = \text{OTF}_\epsilon(h) - \text{OTF}_\epsilon(h, h) = 0 \). \( \square \)

Proposition 1 allows us to solve the dual problem as was done in Sec. 3.2 yet this time without the \( \mu \) variables. The remaining dual variables for the constraint over the row marginals of the coupling, now referred to as \( \kappa \) to avoid confusion, could already be computed independently from each other. Consequently, the \( \kappa^* \) values that maximize the dual function \( L(\kappa) \) can be computed directly:

\[
\kappa^* = \epsilon \log h_i - \epsilon \log \sum_j \exp \left( \frac{-C_{ij}}{\epsilon} \right).
\]

(18)

### 3.4 Minimising Unfairness

Given an efficient way to compute the parameters of the adjusted, regularized \( \text{OTF}_0^\epsilon(h) \) cost, we can now jointly minimize the classifier’s error and the unfairness cost with respect to \( h \).

Let \( \mathcal{L}_Y(h) \) denote the cross entropy loss of \( h(X) \) for the output labels \( Y \). To add our \( \text{OTF}_0^\epsilon(h) \) cost to this objective, we can pose the following optimization problem:

\[
\min_h \left( 1 - \alpha \right) \mathcal{L}_Y(h) + \alpha \text{OTF}_0^\epsilon(h)
\]

(19)

with \( 0 \leq \alpha \leq 1 \) a hyperparameter that denotes the strength of the \( \text{OTF}_\epsilon \) term.

Though we forgo a rigorous analysis here, we take inspiration from prior work \( [25] \) on \( \text{OTF}_\epsilon \) to approximate the derivative of \( \text{OTF}_0^\epsilon(h) \) with respect to \( h \). Let \( \lambda^*, \mu^* \) and \( \kappa^* \) denote the fully converged dual variables. Then

\[
\frac{\partial}{\partial h} \text{OTF}_0^\epsilon(h) = \frac{\partial}{\partial h} \left( \text{OTF}_\epsilon(h) - \text{OT}_\epsilon(h, h) \right) = \frac{\partial}{\partial h} \left( L(\lambda^*, \mu^*) - L(\kappa^*) \right) = \frac{\partial}{\partial h} \sum_i (\lambda_i^* - \kappa_i^*) h_i.
\]

(20)

Here, \( \kappa^* \) can be computed directly from Eq. (13). Being a fixed point, the \( \lambda^* \) vector is given by the update Eq. (14). By assuming convergence and computing both with an automatic differentiation tool such as PyTorch\(^2\) to evaluate Eq. (19).
After a logistic regression classifier $h$ was trained on the Adult dataset without unfairness in mind (i.e. $\alpha = 0$ in Eq. (19)), the adjusted $\text{OTF}_0^0$ cost was optimized for 25 epochs with $\alpha = 1$. The $\text{OTF}_0(h)$ and $\text{OT}_0(h, h)$ terms quickly converged to the same values (shown on the left axis) as evidenced by the $\text{OTF}_0^0(h)$ values (shown on the right axis) that exponentially decrease to zero. [20], we can backpropagate through the OTF optimization. Even if we did not update $\lambda$ and $\mu$ until convergence, we can still use intermediate values to approximate the true gradient.

We further approximate the true $\text{OTF}_0^0(h)$ cost by allowing the optimization to be performed on a subset of the dataset, e.g. when batching is already used to optimize $\mathcal{L}_\gamma(h)$. The $\text{OTF}_0^0(h)$ can be optimized on a batch by only using the $C_{ij}$ values belonging to the data points of that batch, and by adjusting the $G$ matrix and $\gamma$ vector that make up the linear fairness notion. For example, for linear independence it is then necessary to compute $\mathbb{E}_Z[f(X)S_k]$, $\mathbb{E}_Z[f(X)]$, and $\mathbb{E}_Z[S_k]$ only over the data points in the batch. However, for small batch sizes this may lead to an underestimation of the unfairness in the data. At worst, batches of a single element will then not detect any unfairness.

Though we jointly minimize $\mathcal{L}_\gamma(h)$ and $\text{OTF}_0^0(h)$ in our experiments, we visualize the use of our cost term as a post-processing approach in Fig. 1. The fact that $\text{OTF}_0^0(h)$ is minimized towards zero empirically confirms Prop. 2.

### 4 Related Work

Fairness in machine learning literature is commonly understood in two (extreme) ways [23]. First, there is the concept of individual fairness, which states that similar individuals should be treated similarly [11]. Second, a notion of fairness where on as a group, e.g. as defined by membership to demographics, people are treated equally. The primary goal of our work is to achieve group fairness by measuring the distance of a score function to a set of group-fair functions. Yet, to an extent we also incorporate individual fairness because our unfairness takes the cost of transporting each individual’s features to the fair score function into account. By appropriately choosing the cost function to do this in a more unbiased way, it may be possible to further improve upon individual fairness in future work.

Other methods that aim to improve fairness can be categorized into three types: those that perform preprocessing where the data is made more fair [21] [5], as opposed to those that do postprocessing where the model’s predictions are modified to fit a notion of fairness [17]. Our work fits clearly in the class of inprocessing methods, i.e where the machine learning model or its training is directly altered to reduce unfairness [5] [31] [30] [4].

Our work draws inspiration from two kinds of inprocessing methods. First, the line of research concerned with explicitly projecting a (still unfair) model to a set of fair models defined by fairness constraints. In this direction, a popular definition of distance between models is the Kullback-Leibler divergence [2] [18] [3]. Second, our work is of course related to the literature on Optimal Transport (OT) [25]. Several works in recent years have applied OT to fairness, though they almost all do so by utilizing barycenters [27]: measures that are ‘equally far’ from the measures belonging to each demographic. This type of method has been applied to preprocessing [15], classification [19] [22] and regression [8] [16], with the overarching goal being to move each group’s measure closer to the barycenter. While this idea is intuitive for a limited amount of groups, it requires fairness notions to be encoded in this format of explicit equality between groups. It is not flexible in allowing for more complex constraints such as those involving continuous or multiple sensitive attributes, and makes the strong assumption that the cost function is a distance metric.
Our proposed method instead combines the idea of projecting the model to a fairness-constrained set and the use of OT to measure the cost of this projection. In this manner, our work is most similar to [26], which computes the (unregularized) OT projection onto such a fair set. However, they only use the method as a group fairness test and do not propose an efficient cost term.

5 Experiments

Our experiments were performed on two datasets from the UCI repository [10] which are discussed in Sec. 5.1. On these datasets, we compare our proposed OTF method to two other fairness cost terms that serve as baselines. First, the FairTorch method which implements the traditional group fairness setting. Second, the Barycenter method that uses OT to achieve linear independence. All evaluated methods are detailed in Sec. 5.2. The manner of their evaluation, described in Sec. 5.3, is designed to analyze the trade-off between predictive power and fairness. Our results are presented in Sec. 5.4 through a visualization of this trade-off.

5.1 Datasets

We experimented on two staple datasets from fair classification literature: the UCI Adult Census Income dataset and the UCI Bank Marketing dataset. The datasets were chosen due to the difference in characteristics of their sensitive attributes.

In the Adult dataset, the task is to predict whether an individual earns more than $50K/yr. We followed the default data preprocessing implemented by the AI Fairness 360 framework, which retains 45222 samples. The sensitive features are simplified to two binary sensitive attributes: SEX (with values {male, female}) and RACE (with values {white, non-white}).

In the Bank dataset, the target is whether a client will subscribe to a product offered by a bank. For the 41188 data samples of individuals, the sensitive attribute is the age of the clients, which is traditionally converted to a categorical value by dividing the age into a limited number of bins. As sensitive attributes, we study both the original continuous AGE values and the quantized version based on the median age of 38, i.e. AGE_BINNED (with values {< 38, ≥ 38}).

5.2 Methods

All experiments were performed using a logistic regression model without regularization, with three different fairness cost terms that are jointly optimized with the cross-entropy loss as in Eq. (19). These cost terms are referred to as OTF, FairTorch and Barycenter. The method optimized without such a cost term is referred to as Unfair.

Our proposed OTF cost term was evaluated using its adjusted variant discussed in Sec. 3.3, with the entropy regularization strength of $\epsilon = 10^{-3}$ chosen from $\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}\}$. The cost matrix $C$ was computed from the Euclidean distance between the non-protected features of all pairs of samples in each batch. We made a full abstraction of the OTF cost and wrapped it as a PyTorch loss function that can be directly minimized with respect to any binary classification model. For the Adult dataset, both sensitive features were included in the OTF computation at the same time by concatenating their respective $G$ matrices and $\gamma$ vectors. For the Bank dataset two OTF costs were computed: one using the continuous AGE values and one using the binned AGE_BINNED attribute. The latter method is referred to as OTF (binned).

As a first baseline, we used the two cost functions from the FairTorch library. While not as polished or firmly established as fairness frameworks such as AI Fairness 360, it can easily be added to a conventional classification loss in PyTorch. The framework is based on [11], which converts the linear fairness constraints into a Lagrangian cost term that is directly added to the optimization objective of the classifier. In theory, their framework can therefore handle any set of linear fairness notions just like our OTF method. From what we could find however, only FairTorch implemented a suitable cost term for this approach and only for categorical sensitive attributes. We therefore use their demographic parity and equalized opportunity loss terms, but not on the continuous version of the AGE attribute. For the Adult dataset, we sum over the loss terms for both the SEX and RACE attributes.
For our second baseline we employed an implementation of an OT Barycenter\cite{20} approach\cite{20}. This implementation directly minimizes the OT cost between the score distributions of two sensitive groups. Implicitly, both score distributions are then transported to their barycenter. The implementation can only minimize demographic parity, however, and does not admit a composition of linear fairness notions or continuous attributes. We therefore only minimize unfairness with respect to sex and age. All fairness cost terms were tested for strengths $\alpha \in \{0.01, 0.05, 0.1, 0.2, 0.3, 0.5\}$ (see Eq. (19)), yet the results for $\alpha \in \{0.01, 0.05, 0.5\}$ were omitted from our analysis for the Bank dataset as they introduced clutter in the visualization and did not entail diverging insights. All methods were trained for 100 epochs, used a learning rate of $10^{-3}$ and employed a batch size of 1000. No method included sensitive features in the input of its logistic regression model, and so does not require sensitive information at evaluation time.

5.3 Evaluation

To measure the predictive power of the methods, the ROC AUC score for binary classification was measured. Their unfairness is quantified with regard to linear independence (LI), as the maximal absolute Pearson correlation between the predictions $h(X)$ and each dimension of the sensitive attributes $S_k$. With regard to linear conditional independence (LCI), the violation is computed as the maximal LI violation for predictions of each one-hot encoded output label $Y_l$. These measures mirror the requirements in Eq. (3) and Eq. (4) that the covariances ought to equal zero, though we choose the Pearson correlation instead such that the violation is normalized between 0 and 1.

Each configuration for each method (i.e. each $\alpha$ value and fairness notion) was tested for five train-test splits with proportions 80/20 and with different random seeds. We report the mean scores and show the confidence interval ellipse corresponding with the first standard deviation. In our analysis we omit fairness scores for fairness notions that were not directly optimized in that configuration. Since the Barycenter implementation does not provide a way to achieve linear conditional independence, no results are reported for that notion for Barycenter.

5.4 Results

We start our analysis by considering the results on the Adult dataset in Fig. 2. For LI with respect to sex, the OTF method makes a similar trade-off between AUC and fairness as the baselines for various $\alpha$ values. In minimizing LI with respect to race, our method appears to lose AUC slightly faster than FairTorch. However, OTF clearly outperforms FairTorch for both sensitive attributes when they are trained to minimize LCI, especially in the lower violation range. This advantage may be due to the fact that OTF has the incentive to achieve fairness by exchanging classifier scores between similar individuals. Conditioning on the output label rewards such exchanges, as individuals with similar labels can be expected to have similar features.

Recall that OTF transports the classifier’s score function to a score function that is LCI-fair with respect to both sensitive attributes at the same time. While we replicated multiple fairness notions for FairTorch by using multiple cost terms, we did not provide such an adaptation for Barycenter. Without the race attribute in mind, the latter’s scores are worse on LI with respect to race for stronger fairness strengths, thus showing that group fairness for one group does not imply the same for another. Our proposed OTF method therefore displays an advantage in not only an effective AUC-fairness trade-off, but also in a flexible capacity for group fairness.

For our analysis of the results on the Bank dataset shown in Fig. 3, we recall that it includes only one sensitive attribute: age. The OTF method can effectively minimize either the LI or LCI with respect to the continuous age attribute. Yet, Barycenter can only minimize the OT cost between a limited number of score distributions belonging to protected groups. It thus lacks the capacity to deal with continuous attributes in the same way as OTF. Other methods that can minimize with respect to linear fairness notions such as FairTorch could theoretically have the same capacity, yet implementations of this capacity are scarcely available. Still, we also trained a variant of OTF which minimized fairness with respect to the binned version of age. We then see similar results as for the Adult dataset: our method is on par with the baselines for LI, but clearly outperforms the FairTorch baseline for LCI.

6 Conclusion

In this paper, we proposed the Optimal Transport to Fairness (OTF) method, which combines the advantages of flexible linear fairness constraints with Optimal Transport theory, thereby taking non-protected similarities between individuals into account. By adding entropic regularization, we make the OTF cost differentiable and efficient to compute in its dual form. Afterwards, we add an adjustment term such that the overall cost can again be minimized to zero. In

7 Retrieved from https://github.com/deepmind/wasserstein_fairness
Figure 2: Train and test set results of all methods on the Adult dataset. ROC AUC is measured over predictions of the respective data splits. Violation of LI and LCI is computed as the maximal absolute Pearson correlation between the predictions (conditioned on the output labels) and each sensitive attribute. Here, LI and LCI correspond to demographic parity and equalized odds respectively.

In the future, we hope to further investigate the properties of OT-based fairness, inspired by its clear advantage in achieving equalized odds. Though our method was only applied to linear fairness notions, OT may provide an opportunity to better achieve non-linear notions of fairness, e.g. through a creative choice of the cost function that directs the transport of classifier scores.
Figure 3: Train and test set results of all methods on the Bank dataset. ROC AUC is measured over predictions of the respective data splits. Violation of LI and LCI are computed as the maximal absolute Pearson correlation between the predictions (conditioned on the output labels) and the continuous $\text{AGE}$ attribute or the categorical $\text{AGE}_\text{Binned}$ attribute. For the latter, LI and LCI correspond to demographic parity and equalized odds respectively.

Acknowledgements

The research leading to these results has received funding from the European Research Council under the European Union’s Seventh Framework Programme (FP7/2007-2013) (ERC Grant Agreement no. 615517), and under the European Union’s Horizon 2020 research and innovation programme (ERC Grant Agreement no. 963924), from the Flemish Government under the “Onderzoeksprogramma Artificiële Intelligentie (AI) Vlaanderen” programme, from the Special Research Fund (BOF) of Ghent University (reference no. BOF20/DOC/144), and from the FWO (project no. G091017N, G0F9816N, 3G042220).
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