

Using optimal transport to mitigate unfair predictions and quantify counterfactual fairness

Arthur Charpentier

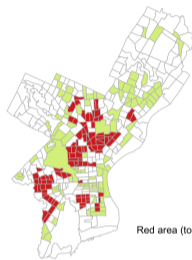
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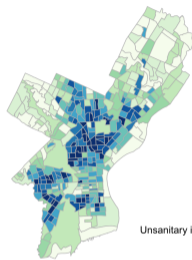
“Technology is neither good nor bad; nor is it neutral.”

(Fictitious maps, inspired by Home Owners’ Loan Corporation map, 1937, “redlining”)



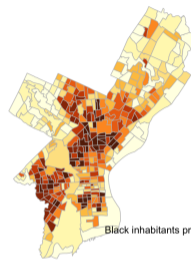
Red area (too risky)

decision y



Unsanitary index (0-100)

legitimate ratemaking variable x




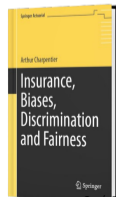
Black inhabitants proportion (%)

sensitive attribute a

Direct (intentional) discrimination / indirect (statistical) discrimination / neutrality

“Machine learning won’t give you anything like gender neutrality ‘for free’ that you didn’t explicitly ask for,” Kearns and Roth (2019)

Charpentier (2024) Insurance: Biases, Discrimination and Fairness. 



Agenda

Optimal Transport

- The setting
- The Gaussian case
- The discrete case
- The univariate case
- Optimal Transport with Pictures

Machine Learning Terminology

Group Fairness

- Some Definitions and Concepts
- Wasserstein Distance & Discrimination
- Wasserstein Barycenter & Mitigation
- Mitigating discrimination

Counterfactual Fairness

- Individual Fairness and Potential Outcomes
- Transport on a Probabilistic Graphical Model
- Transport on the Simplex

Optimal Transport, the Setting

Consider measures μ_0 and μ_1 on Z_0, Z_1 , compact subsets of \mathbb{R}^d .

There exists T such that $\mu_1 = T \# \mu_0$, where μ_0 is atomless ($T \# \mu_0(B) = \mu_0(T^{-1}(B))$).

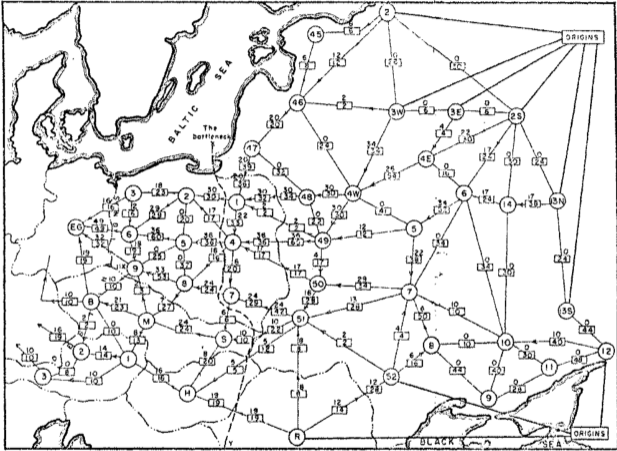
As shown in [Villani \(2003\)](#) and [Santambrogio \(2015\)](#), we can be interested in “optimal” mappings, satisfying Monge problem, from [Monge \(1781\)](#), i.e., solutions of

$$T \# \mu_0 = \mu_1 \quad \inf_{T: Z_0 \rightarrow Z_1} \int_{Z_0} c(\mathbf{z}_0, T(\mathbf{z}_0)) \mu_0(d\mathbf{z}_0), \quad (1)$$

for some positive ground cost function $c: Z_0 \times Z_1 \rightarrow \mathbb{R}_+$. If μ_0 and μ_1 are not absolutely continuous (with respect to Lebesgue measure), there might not be such deterministic mapping T . This limitation motivates a relaxation of Monge’s problem, as considered in [Kantorovich \(1942\)](#),

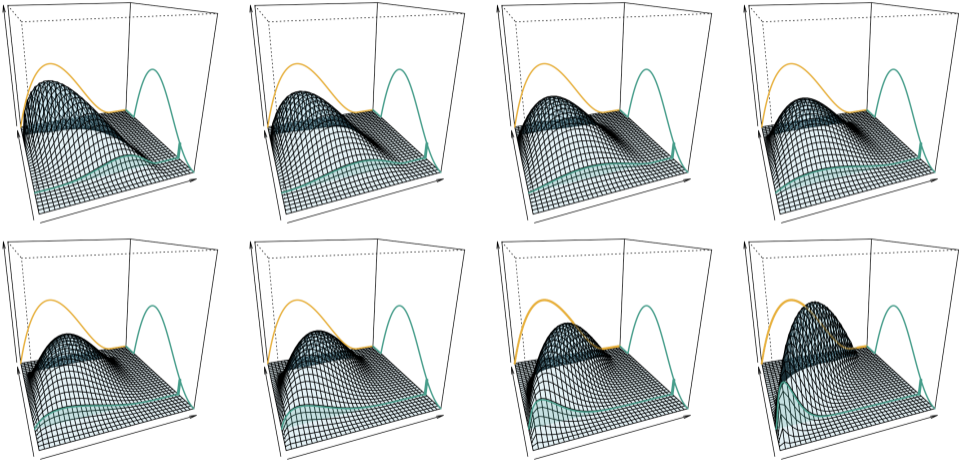
$$\inf_{\Pi(\mu_0, \mu_1)} \int_{Z_0 \times Z_1} c(\mathbf{z}_0, \mathbf{z}_1) (\mu_0 \otimes \mu_1)(d\mathbf{z}_0, d\mathbf{z}_1), \quad (2)$$

Optimal Transport, the Setting



(flow on networks, via Harris and Ross (1955))

Optimal Transport, the Setting



Optimal Transport, the Gaussian case

With a quadratic cost (and Euclidean distance in \mathbb{R}^d) and absolutely continuous measures, the optimal Monge map T is unique, and it is the gradient of a convex function, $T = \nabla \phi$, see [Brenier \(1991\)](#).

If $\mu_j \sim N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$,

$$\mathbf{z}_1 = T(\mathbf{z}_0) = \boldsymbol{\mu}_1 + \mathbf{M}(\mathbf{z}_0 - \boldsymbol{\mu}_0),$$

where \mathbf{M} is a symmetric positive matrix that satisfies $\mathbf{M}\boldsymbol{\Sigma}_0\mathbf{M} = \boldsymbol{\Sigma}_1$, which has a unique solution given by $\mathbf{M} = \boldsymbol{\Sigma}_0^{-1/2} \boldsymbol{\Sigma}_0^{1/2} \boldsymbol{\Sigma}_1 \boldsymbol{\Sigma}_0^{1/2} \boldsymbol{\Sigma}_0^{-1/2}$, where $\mathbf{M}^{1/2}$ denotes the square root of the square (symmetric) positive matrix \mathbf{M} based on the Schur decomposition ($\mathbf{M}^{1/2}$ is a positive symmetric matrix), as described in [Higham \(2008\)](#).

In the univariate case

$$z_1 = T(z_0) = \mu_1 + \frac{\sigma_1}{\sigma_0}(z_0 - \mu_0),$$

that is a linear non-decreasing mapping $\mathbb{R} \rightarrow \mathbb{R}$.

Optimal Transport, the discrete case

Consider two samples in the \mathbb{R}^d , $\{\mathbf{z}_{0,1}, \dots, \mathbf{z}_{0,n_0}\}$ and $\{\mathbf{z}_{1,1}, \dots, \mathbf{z}_{1,n_1}\}$. The discrete version of the Kantorovich problem (Equation 2) is

$$\min_{P \in U(n_0, n_1)} \sum_{i=1}^{n_0} \sum_{j=1}^{n_1} P_{i,j} C_{i,j} = \min_{P \in U(n_0, n_1)} \{ P, C \} \quad (3)$$

where, as in [Brualdi \(2006\)](#), $U(n_0, n_1)$ is the set of $n_0 \times n_1$ matrices corresponding to the convex transportation polytope

$$U(n_0, n_1) = \{ P : P \mathbf{1}_{n_1} = \mathbf{1}_{n_0} \text{ and } P \mathbf{1}_{n_0} = \frac{n_0}{n_1} \mathbf{1}_{n_1} \},$$

and where C denotes the $n_0 \times n_1$ cost matrix, $C_{i,j} = c(\mathbf{z}_i, \mathbf{z}_j)$, associated with cost c .

Optimal Transport, the discrete case

	7	8	9	10	11	12
1	0.41	0.55	0.22	0.64	0.04	0.25
2	0.28	0.24	0.73	0.22	0.64	0.80
3	0.28	0.47	0.32	0.52	0.16	0.37
4	0.28	0.62	0.81	0.25	0.64	0.85
5	0.41	0.37	0.89	0.25	0.81	0.97
6	0.66	0.76	0.21	0.89	0.22	0.14

argmin P, C
 $P \in U(\mathbf{1}_n, \mathbf{1}_n)$

over the set of **permutation matrices**.

minimal cost 0.2116

	7	8	9	10	11	12		
1	1	.	1	11
2	.	1	2	8
3	.	.	1	.	.	.	3	9
4	1	4	7
5	.	.	.	1	.	.	5	10
6	1	6	12

Optimal Transport, the discrete case

	7	8	9	10	11	12	13	14	15	16
1	0.41	0.55	0.22	0.64	0.04	0.25	0.24	0.77	0.74	0.55
2	0.28	0.24	0.73	0.22	0.64	0.80	0.76	0.76	0.12	0.10
3	0.28	0.47	0.32	0.52	0.16	0.37	0.27	0.68	0.63	0.45
4	0.28	0.62	0.81	0.25	0.64	0.85	0.58	0.32	0.51	0.48
5	0.41	0.37	0.89	0.25	0.81	0.97	0.91	0.81	0.05	0.25
6	0.66	0.76	0.21	0.89	0.22	0.14	0.33	0.96	0.99	0.79

	7	8	9	10	11	12	13	14	15	16		
1	.	.	1/5	.	3/5	.	1/5	.	.	.	1	{9,11,13}
2	.	2/5	3/5	2	{8,16}
3	3/5	2/5	.	.	.	3	{7,13}
4	.	.	.	2/5	.	.	.	3/5	.	.	4	{10,14}
5	.	1/5	.	1/5	3/5	.	5	{8,10,15}
6	.	.	2/5	.	.	3/5	6	{9,12}

Optimal Transport, the discrete case

	7	8	9	10	11	12
1	0.41	0.55	0.22	0.64	0.04	0.25
2	0.28	0.24	0.73	0.22	0.64	0.80
3	0.28	0.47	0.32	0.52	0.16	0.37
4	0.28	0.62	0.81	0.25	0.64	0.85
5	0.41	0.37	0.89	0.25	0.81	0.97
6	0.66	0.76	0.21	0.89	0.22	0.14

	7	8	9	10	11	12
1	.	.	0.35	.	0.59	0.06
2	0.12	0.82	.	0.07	.	.
3	.	.	0.55	.	0.41	0.04
4	0.85	.	.	0.14	.	.
5	0.03	0.18	.	0.79	.	.
6	.	.	0.10	.	.	0.90

$$\operatorname{argmin}_{P \in U(\mathbf{1}_{n_0}, \mathbf{1}_{n_1})} P, C - \lambda \cdot \text{entropy}(P)$$

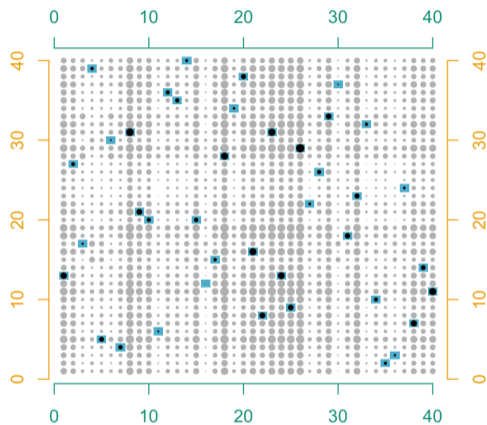
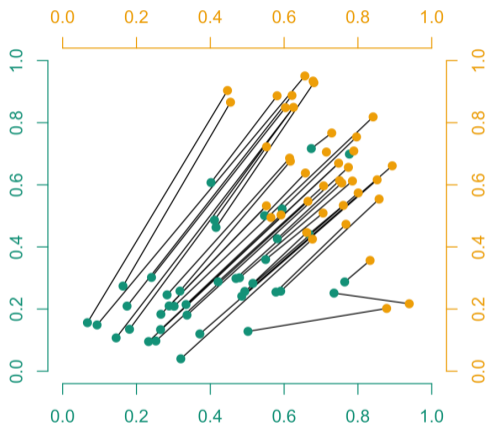
(**regularization** via Sinkhorn algorithm, associated to “Matrix Scaling Problem” in Sinkhorn (1962)) or

$$\operatorname{argmin}_{P \in U(\mathbf{1}_{n_0}, \mathbf{1}_{n_1})} P, C + \lambda \cdot d_{\text{KL}}(P // \mathbf{1}_{n_0} \mathbf{1}_{n_1})$$

minimal cost 0.2189 (> 0.2116)

1 11 + ...
 2 8 + ...
 3 9 + ...
 4 7 + ...
 5 10 + ...
 6 12 + ...

Optimal Transport, the discrete case



Discrete matching, $n_0 = n_1 = 40$ individuals in two groups, $\{z_i, s_i = 0\}$ and $\{z_i, s_i = 1\}$, with matrices C ($C_{ij} = \cdot$) and P (if $P_{ij} = 1$)

Optimal Transport, the univariate case

Wasserstein distance is defined as the optimal transportation cost, when c is the k distance, for $k \geq 1$, [Wasserstein \(1969\)](#),

$$W_k(\mu_0, \mu_1)^k := \inf_{T: \mathbb{R} \rightarrow \mathbb{R}} \int \mu_0(dz_0) \|z_0 - T(z_0)\|^k = \int_0^1 |Q_1(u) - Q_0(u)|^k du$$

i.e., the optimal mapping T (if $k > 1$) is non-decreasing, i.e.,

$$z_1 = T(z_0) = Q_1(F_0(z_0)) \text{ where } \begin{cases} F_j(z) = \mu_j(-\infty, z] \\ Q_j(u) = F_j^{-1}(u) = \inf\{t \in \mathbb{R} : F_j(t) \geq u\} \end{cases}$$

$T := Q_1 \circ F_0$ is a non-decreasing mapping $\mathbb{R} \rightarrow \mathbb{R}$.

In higher dimension, some multivariate extensions of quantiles can be introduced to keep this construction, see [Hallin et al. \(2021\)](#), [Hallin and Konen \(2024\)](#)

Optimal Transport, the univariate case

Given $x_1 \dots x_n$ and $y_1 \dots y_n$ n pairs of ordered real numbers, and some supermodular function $\Phi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$, for every permutation σ of $\{1, 2, \dots, n\}$,

$$\sum_{i=1}^n \Phi(x_i, y_{n+1-i}) \geq \sum_{i=1}^n \Phi(x_i, y_{\sigma(i)}) \geq \sum_{i=1}^n \Phi(x_i, y_i),$$

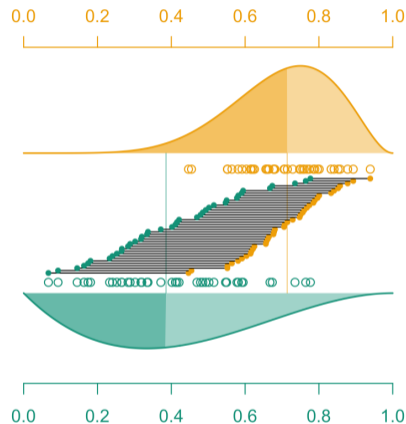
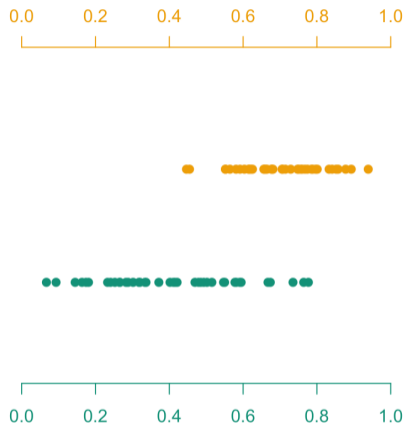
while if $\Phi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is submodular,

$$\sum_{i=1}^n \Phi(x_i, y_i) \geq \sum_{i=1}^n \Phi(x_i, y_{\sigma(i)}) \geq \sum_{i=1}^n \Phi(x_i, y_{n+1-i}).$$

see [Hardy et al. \(1952\)](#).

See related work on risk measures, [Denuit et al. \(2006\)](#), [Galichon \(2016\)](#), [Carlier et al. \(2016\)](#).

Optimal Transport with Pictures, the univariate case



Univariate predictions for n individuals in two groups, $\{z_i, s_i = 0\}$ and $\{z_i, s_i = 1\}$, or measures μ_0 and μ_1 . $T(\cdot) = Q_1 \circ F_0(\cdot)$.

Optimal Transport with Pictures, the univariate case

Univariate predictions for individuals in two groups, $T^*(\cdot) = Q_1 \# F_0(\cdot)$.

Optimal Transport with Pictures, the univariate case

Multivariate observations for individuals in two groups, μ_0 and μ_1 (densities).

Optimal Transport with Pictures, the univariate case

Bivariate observations for individuals in two groups $\{z_i; s_i = 0\}$ and $\{z_i; s_i = 1\}$.

Optimal Transport with Pictures, the univariate case

Discrete matching, n individuals in two groups $\{z_i; s_i = 0\}$ and $\{z_i; s_i = 1\}$.

Optimal Transport with Pictures, the univariate case

Optimal transport with Gaussian joint distributions $N(\mu_0; \sigma_0)$ and $N(\mu_1; \sigma_1)$.

Machine learning, supervised model

Consider some data $(Y; X)$, and a "model" for Y , and some loss,

$$m^* := \operatorname{argmin}_{m \in \mathcal{G}} R(m) ; \text{ where } R(m) := E \left[\ell(Y; m(X)) \right] :$$

e.g. if $\ell(y; m) = (y - m)^2$ and \mathcal{M} the set of all measurable functions,

$$m^* := \operatorname{argmin}_{m \in \mathcal{M}} R(m) \text{ is } m^*(x) := E[Y | X = x] ;$$

corresponding to the "regression function", or "Bayes regressor".

For a subclass of models \mathcal{G} , the excess of risk of class \mathcal{G} is

$$E(\mathcal{G}) = \min_{m \in \mathcal{G}} R(m) - \min_{m \in \mathcal{M}} R(m) = \min_{m \in \mathcal{G}} R(m) - R(m^*)$$

Machine learning, supervised model

In fairness problems, we still have the quantity of interest, but among covariates,

$$\begin{cases} X = (X_1; \dots; X_k) & \text{are legitimate authorized variables} \\ A = (A_1; \dots; A_j) & \text{are proscribed protected attributes} \end{cases}$$

Let $m(x; a)$ denotes a model

- | $\pi_a(m)$ is the conditional measure of $m(X; A)$ given $A = a$
- | $F_{m|a}(u) := P(m(X; A) \leq u | A = a)$ and,
with an abuse of notation $F_{m|a}(u) := P(m(X; A) \leq u | A = a)$
their cumulative distribution function (CDF);
- | $Q_{m|a}(v) := \inf \{ u \in \mathbb{R} : F_{m|a}(u) \geq v \}$ and,
with an abuse of notation, $Q_{m|a}(v) := \inf \{ u \in \mathbb{R} : F_{m|a}(u) \geq v \}$
their associated quantile functions.

Machine learning, supervised model

$F_{m|a=0}(\cdot)$, $F_{m|a=1}(\cdot)$ and $F_m(\cdot)$ on the left, $Q_{m|a=0}(\cdot)$, $Q_{m|a=1}(\cdot)$ and $Q_m(\cdot)$ on the right

Group Fairness

A model m satisfies the **independence property** if $m(X; A) \perp A$, with respect to the distribution P of the triplet $(X; A; Y)$

For binary classifiers, **demographic parity** w.r.t. A is defined as

$$\begin{aligned} & P(\psi = 1 | A = a) = P(\psi = 1) \quad \forall a \\ & P(m(X; A) > t | A = a) = P(m(X; A) > t) \quad \forall a \end{aligned}$$

and a measure of (weak) discrimination would be

$$\begin{aligned} & \delta \\ & \geq \max_{a \in \mathcal{A}} P(\psi = 1 | A = a) - P(\psi = 1) \\ & \geq \max_{a \in \mathcal{A}} P(m(X; A) > t | A = a) - P(m(X; A) > t) \end{aligned}$$

for some threshold t .

Group Fairness & Wasserstein Distance

A model m satisfies the **independence property** if $m(X; A) \perp A$, with respect to the distribution P of the triplet $(X; A; Y)$

More generally, define a (strong) discrimination measure $U(m) := \max_{a \in A} d(m; m_{j|a})$, for some distance d , to quantify discrimination w.r.t. A .

E.g., total variation:

$$U_{TV, A}(m) := \max_{a \in A} \sup_{I \subseteq \mathcal{R}} |P(m(X; A) \in I | A = a) - P(m(X; A) \in I)|;$$

E.g., Wasserstein based measure:

$$U_{W_k, A}(m) := \max_{a \in A} W_k(m; m_{j|a})^k = \max_{a \in A} \int_{u \in [0;1]} |Q_m(u) - Q_{m_{j|a}}(u)|^k du;$$

Group Fairness & Wasserstein Distance

Possibly multi-attributes measure $U_{W_k, A}(m) = U_{W_k, A_1}(m) + \dots + U_{W_k, A_j}(m)$

Let M denote the set of all measurable models.

Let G denote a set of models

$$G_{\text{fair}} := \{m \in G \text{ s.t. } m(X; A) \stackrel{?}{=} A\} = \{m \in G \text{ s.t. } U(m) = 0\}$$

price of fairness : $E(G_{\text{fair}}) := \min_{m \in G_{\text{fair}}} R(m) - \min_{m \in M} R(m) \geq 0$

We can also consider r -fairness for class G

$$G^r_{\text{fair}} := \{m \in G \text{ s.t. } U(m) \leq r \cdot U(\cdot)\} \text{ and } G^r_{\text{fair}} \subseteq G \subseteq G_{\text{fair}} \subseteq M$$

Barycenters

Recall that the barycenter of a set of points $\{z_i\}$ in \mathbb{R}^n with weights λ_i is

$$\arg\min_{z \in \mathbb{R}^n} \sum_{i=1}^n \lambda_i \|z - z_i\|^2$$

that can be extended to any metric space $(E; d)$, with n -barycenters,

$$\arg\min_{z \in E} \sum_{i=1}^n \lambda_i d(z, z_i) \quad \text{or} \quad \arg\min_{z \in E} \int d(z, z) \, \mu(dz)$$

for some probability measure on $(E; d)$.

The existence is related to geodesics. A complete metric space $(E; d)$ is said to be geodesic if $\forall x, y \in E, \exists z \in E$ such that

$$d(x; z) = d(y; z) = \frac{1}{2}d(x; y)$$

Barycenters

The p -barycenter of any probability measure on a locally compact geodesic space, with finite moments of order p , exists.

Given a metric space $(E; d)$, consider the Wasserstein distance

$$W_k(\mu_0; \mu_1)^k = \inf_{Z} \int_{E \times E} d(z_0; z_1)^k (dz_0; dz_1);$$

for two probability measures on $(E; d)$. Let $\mathcal{P}_k(E)$ denote the set of all measures $(E; d)$ for which moments of order k are finite.

The Wasserstein space $\mathcal{P}_k(E; W_k)$ of E is a complete geodesic space $(\mathcal{P}_k(E); W_k)$.

If $(E; d)$ be a separable locally compact geodesic space. Then any set of probability measures $\mathcal{P}_k(E; W_k)$ has a barycenter, when $k \geq 1$.

Barycenters

Barycenter of univariate distributions μ_0 and μ_1 and weights $\lambda \in [0, 1]$, and of two Gaussian distributions $N(\mu_0; \sigma_0^2)$ and $N(\mu_1; \sigma_1^2)$.

Barycenters

Price of projection and (almost) Wasserstein Barycenter

Write $\pi_A(X) := E(Y | X; A)$. From Pythagoras' theorem

$$E(Y - \pi_A(X))^2 + E(\pi_A(X) - m(X; A))^2 = E(Y - m(X; A))^2$$

$$E(\pi_A(X) - m(X; A))^2 = E(Y - m(X; A))^2 - E(Y - \pi_A(X))^2$$

therefore

$$\inf_{m \in \mathcal{G}} E \left(E(\pi_A(X) - m(X; A))^2 \mid A \right) = \inf_{m \in \mathcal{G}} E(Y - m(X; A))^2 - E(Y - \pi_A(X))^2$$

\uparrow
 $E(G)$

Barycenters

Thus

$$E \int_A (X - m(X; A))^2 dA = a \quad W_2(a(\cdot); a(m))^2$$

from the definition of Wasserstein-2 distance (optimal coupling)

$$W_2(\mu_0; \mu_1)^2 := \inf_{Z \sim (\mu_0; \mu_1)} \int |x - y|^2 dZ = \inf_{(Z_0; Z_1) \sim (\mu_0; \mu_1)} E |Z_0 - Z_1|^2$$

i.e.,

$$E \int_A (X - m(X; S))^2 dA = E W_2(A(\cdot); A(m))^2$$

and

$$\inf_{m \in G} E (Y - m(X; A))^2 = E (Y - A(X))^2 = \inf_{m \in G} E W_2(A(\cdot); A(m))^2$$

↑ $E(G)$

Barycenters

If μ is absolutely continuous (w.r.t. the Lebesgue measure),

$$E(G) = \inf_{m \in G} E W_2(\mu; \mu(m))^2 = \inf_{m \in G} \int_a^X P[A = a] W_2(\mu_a; \mu(m))^2$$

see [Gouic et al. \(2020\)](#). Heuristically, for any a there exists $T_a : \mathbb{R} \rightarrow \mathbb{R}$ s.t.

$$W_2(\mu_a; \mu(m))^2 = E |T_a(X) - m|^2$$

Set $h : (x; a) \mapsto T_a(x)$. If $h \in G$

$$E W_2(\mu; \mu(m))^2 = E |h(X; A) - m|^2 \leq \inf_{g \in G} E |g(X; A) - m|^2$$

(satisfied if G is "prole complete", [Gouic et al. \(2020\)](#)), i.e., the inequality is an equality.

Barycenters

Price of fairness and Wasserstein Barycenter

$$E(G_{\text{fair}}) = \inf_{m \in \mathcal{G}_{\text{fair}}} \sum_a P[A = a] W_2(a(\cdot); a(m))^2 = \inf_{2P} \sum_a P[A = a] W_2(a(\cdot); \cdot)^2$$

We recognize on the right the barycenter, with weights $P[A = a]$ and Wasserstein-2 distance, see [Chzhen et al. \(2020\)](#) and [Gouic et al. \(2020\)](#).

[Hu et al. \(2023b\)](#) considered [constraints on the set of distributions](#), i.e.,

$$G_{\text{fair}}^P = \{m \in \mathcal{G}_{\text{fair}} \text{ s.t. } m \in P\}$$

on-going work on [constraints on the set of models](#) which is not "pro le complete"

Mitigating discrimination

See Supreme Court Justice Harry Blackmun stated, in 1978, “In order to get beyond racism, we must first take account of race. There is no other way. And in order to treat some persons equally, we must treat them differently,” Knowlton (1978), cited in Lippert-Rasmussen (2020)

In the case of a binary sensitive attribute,

$$\begin{cases} m^?(x; a = 0) = P[A = 0] m(x; a = 0) + P[A = 1] Q_{mj1} F_{mj0} m(x; a = 0) \\ m^?(x; a = 1) = P[A = 0] Q_{mj0} F_{mj1} m(x; a = 1) + P[A = 1] m(x; a = 1) \end{cases}$$

or more generally
$$m^?(x; a) = \sum_{2A} P[A =] Q_{mj} F_{mja} m(x; a)$$

See Hu et al. (2023a) and Charpentier et al. (2023b).

Mitigating discrimination

Fair score, obtained as barycenter of two univariate distributions of score m_0 and m_1 and weights $\frac{1}{2}$ (similar to $n_0 = n_1$).

Mitigating discrimination

“God said: there will be white men, there will be black men, there will be tall men, there will be short men, there will be handsome men and there will be ugly men, and all will be equal; but it won't be easy... And then he added: there will even be some who will be black, short and ugly, and for them, it will be very hard! ,” Coluche (1975)

The use of barycenters is interesting when we consider multiple sensitive attributes $A = (A_1; \dots; A_j)$

Barycenters are associative.

See [Hu et al. \(2024\)](#)
and [Fernandes Machado et al. \(2025c\)](#).

Individual Fairness and Potential Outcomes

We have **counterfactual fairness** if “had the protected attributes (e.g., race) of the individual been different, other things being equal, the decision would have remained the same,” **Kusner et al. (2017)**

If the protected variable is considered as the treatment, individual fairness is close to measuring **treatment effect**.

What does “**other things being equal**” really mean?

It is possible to suppose that the protected attribute could affect some explanatory variables X in a non-discriminatory way, **Kilbertus et al. (2017)** (concept of **evolving variable**”).

- | two groups, distribution of height (cm) with **women** and **men** (in the U.S.)
- | two groups, distribution of baby weight (g) with **non-black** and **black** mothers, delivering babies (in the U.S.)

Individual Fairness and Potential Outcomes

Individual Fairness and Potential Outcomes

$$P[\psi = \text{yes} \mid A = \text{white}; X = x] \stackrel{?}{=} P[\psi = \text{yes} \mid A = \text{black}; X = x] + 8x$$

The diagram illustrates a sensitivity analysis of a probability difference. The left term is $P[\psi = \text{yes} \mid A = \text{white}; X = x]$ and the right term is $P[\psi = \text{yes} \mid A = \text{black}; X = x] + 8x$. A red box highlights the event $\psi = \text{yes}$ in both terms. A green arrow labeled "sensitive" points to the word "white" in the left term. A yellow arrow labeled "sensitive" points to the word "black" in the right term. A red arrow labeled "having surgery" points from the $\psi = \text{yes}$ box in the left term to the $\psi = \text{yes}$ box in the right term.

e.g., x is the "weight of the baby" (at birth), in g.

Discrimination, with different perspectives

$$P[\psi = \text{yes} \mid A = \text{white}; X = x] \stackrel{?}{=} P[\psi = \text{yes} \mid A = \text{black}; X = x^?]; 8x$$

Diagram illustrating discrimination with different perspectives:

- The left side shows the probability $P[\psi = \text{yes} \mid A = \text{white}; X = x]$. The event $\psi = \text{yes}$ is highlighted in red, and $A = \text{white}$ is highlighted in green. A green arrow labeled "sensitive" points from the word "sensitive" to the green box.
- The right side shows the probability $P[\psi = \text{yes} \mid A = \text{black}; X = x^?]; 8x$. The event $\psi = \text{yes}$ is highlighted in red, $A = \text{black}$ is highlighted in yellow, and $X = x^?$ is highlighted in blue. A yellow arrow labeled "sensitive" points from the word "sensitive" to the yellow box.
- A red arrow labeled "having surgery" points from the red box on the left to the red box on the right.

e.g., x is the "weight of the baby" (at birth), in g.

Discrimination, with different perspectives

See [Charpentier et al. \(2023a\)](#) or [Fernandes Machado et al. \(2026\)](#)

$$\begin{aligned} & \text{"ceteris paribus difference"} : m(A = 1; X = x) - m(A = 0; X = x) \\ & \text{"mutatis mutandis difference"} : m(A = 1; X = T_{0 \rightarrow 1}^?(x)) - m(A = 0; X = x) \end{aligned}$$

suggested also in [Pöhl and Meinshausen \(2020\)](#), [Pöhl et al. \(2021\)](#) and [De Lara et al. \(2024\)](#). We need to transport $X|A = 0$ to $X|A = 1$ (multivariate transport).

- ok if we assume that $X|A = 1 \sim N(\mu_1; \Sigma_1)$: $x^?(1) = T_{0 \rightarrow 1}^?(x) = \mu_1 + M(x - \mu_0)$; where M is a symmetric positive matrix that satisfies $M^T M = \Sigma_1 - \Sigma_0$
- ok if we consider individual empirical coupling $x_j^? = T_{0 \rightarrow 1}^?(x_i)$ but we cannot get $T_{0 \rightarrow 1}^?(x)$ if x is not an observed individual (in group 0).
- we can consider sequential conditional univariate transport (even if not optimal...)

Transport on a Probabilistic Graphical Model

As explained in Villani (2003); Carlier et al. (2010); Bonnotte (2013), the Knothe-Rosenblatt rearrangement is directly inspired by the Rosenblatt chain rule, from Rosenblatt (1952), and some extensions obtained on general measures by Knothe (1957). The Knothe-Rosenblatt rearrangement is

$$T_{\text{kr}}(x_1; \dots; x_d) = \begin{matrix} 0 & & & & 1 \\ \text{⌈} & T_{\frac{1}{1}}^?(x_1|x_2; \dots; x_d) & & & \text{⌋} \\ & T_{\frac{2}{2}}^?(x_2|x_3; \dots; x_d) & & & \\ & \vdots & & & \\ \text{⌈} & T_{\frac{d-1}{d-1}}^?(x_{d-1}|x_d) & & & \text{⌋} \\ & T_{\frac{d}{d}}^?(x_d) & & & \end{matrix} \quad \text{or} \quad T_{\text{kr}}(x_1; \dots; x_d) = \begin{matrix} 0 & & & & 1 \\ \text{⌈} & & T_{\frac{1}{1}}^?(x_1) & & \text{⌋} \\ & & T_{\frac{2}{2}}^?(x_2|x_1) & & \\ & & \vdots & & \\ \text{⌈} & & T_{\frac{d-1}{d-1}}^?(x_{d-1}|x_1; \dots; x_{d-2}) & & \text{⌋} \\ & & T_{\frac{d}{d}}^?(x_d|x_1; \dots; x_{d-1}) & & \end{matrix}$$

the "monotone lower triangular map", defined in Bogachev et al. (2005).

Transport on a Probabilistic Graphical Model

Transport on a Probabilistic Graphical Model

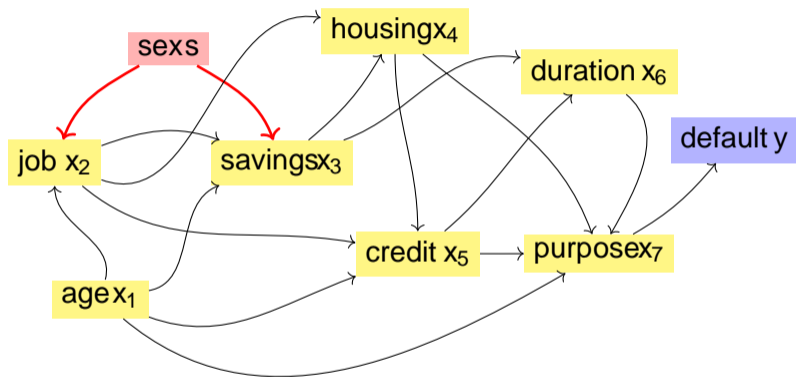
Transport on a Probabilistic Graphical Model

Multivariate observations for individuals in two groups, 0 and 1 (densities).

Transport on a Probabilistic Graphical Model

Sequential transport.

Transport on a Probabilistic Graphical Model



Causal graph in the German Credit dataset from [Watson et al. \(2021\)](#).

Transport on a Probabilistic Graphical Model

The joint distribution of X was written using the **chain rule**, **Rosenblatt (1952)**

$$P[x_1; \dots; x_d] = P[x_1] \prod_{j=2}^d P[x_j | x_1; \dots; x_{j-1}] \text{ or } P[x_d] \prod_{j=1}^{d-1} P[x_j | x_{j+1}; \dots; x_d]$$

The joint distribution of X satisfies the **Markov property**

$$P[x_1; \dots; x_d] = P[x_1] \prod_{j=2}^d P[x_j | x_{j-1}]$$

The joint distribution of X satisfies the **Markov property** w.r.t. PGM:

$$P[x_1; \dots; x_d] = \prod_{j=1}^d P[x_j | \text{parents}(x_j)];$$

where $\text{parents}(x_i)$ are nodes with edges directed towards x_i in PGM.

Transport on a Probabilistic Graphical Model

A classical algorithm for topological sorting is [Kahn \(1962\)](#)'s "Depth First Search" (DFS), and other algorithms are discussed in Section 20.4 in [Cormen et al. \(2022\)](#). For the causal graph on the German Credit dataset, variables are sorted, and

$$T_{\text{PGM}}^?(x_1; \dots; x_7) = \begin{matrix} 0 & & 1 \\ \text{⋮} & T_1^?(x_1) & \text{⋮} \\ & T_2^?(x_2|x_1) & \text{⋮} \\ & T_3^?(x_3|x_1; x_2) & \text{⋮} \\ & T_4^?(x_4|x_2; x_3) & \text{⋮} \\ & T_5^?(x_5|x_1; x_2; x_4) & \text{⋮} \\ \text{⋮} & T_6^?(x_6|x_3; x_5) & \text{⋮} \\ & T_7^?(x_7|x_1; x_4; x_5; x_6) & \text{⋮} \end{matrix} :$$

See [Fernandes Machado et al. \(2025b\)](#), with an applications on two real datasets.

Optimal Transport on the Simplex (for Categorical Variables)

How to transport X_j if X_j is categorical (e.g. $X_j \in \{A, B, C\}$) ? See [Fernandes Machado et al. \(2025a\)](#)

- use a classifier to get **probabilities** associated to $A, B, C \in S_d$,

A	0.69	0.30	0.01
C	0.04	0.31	0.65
A	0.49	0.19	0.32
B	0.01	0.63	0.36
⋮	⋮	⋮	⋮

- transport probabilities (taking into account the geometry of the simplex)

$$S_d = \left\{ x \in (0, 1)^d \mid \sum_{i=1}^d x_i = 1 \right\} \subset \mathbb{R}^d$$

Optimal Transport on the Simplex (for Categorical Variables)

	A	B	C
(0)	43.713%	18.572%	37.715%
(1)	29.831%	48.605%	21.564%
T ()	29.553%	48.517%	21.930%

	A	B	C
(0)	43.713%	18.572%	37.715%
(1)	29.831%	48.605%	21.564%
T ()	43.728%	18.553%	37.719%

Optimal Transport on the Simplex (for Categorical Variables)

First approach, "Dirichlet transport" from Baxendale and Wong (2022).

Let $C: \mathbb{R}_+^d \rightarrow S_d$ denote the "closure operator",

$$C[x_1; x_2; \dots; x_d] = \left(\prod_{i=1}^d \frac{x_i}{x_i} \right); \left(\prod_{i=1}^d \frac{x_2}{x_i} \right); \dots; \left(\prod_{i=1}^d \frac{x_d}{x_i} \right);$$

If we define the binary operator on S_d ,

$$x \cdot y = \left(\prod_{i=1}^d \frac{x_i y_i}{x_i y_i} \right); \dots; \left(\prod_{i=1}^d \frac{x_d y_d}{x_i y_i} \right);$$

then $(S_d; \cdot)$ is a commutative group, with identity $\mathbf{1}$, and the inverse of x is

$$x^{-1} = \left(\prod_{i=1}^d \frac{1=x_1}{1=x_i} \right); \dots; \left(\prod_{i=1}^d \frac{1=x_d}{1=x_i} \right) = C(\mathbf{1}=x):$$

Optimal Transport on the Simplex (for Categorical Variables)

Following [Pal and Wong \(2016, 2018, 2020\)](#), consider the optimal transport problem with the following cost function, on $\mathcal{S}_d \times \mathcal{S}_d$,

$$c(x; y) = \log \frac{1}{d} \sum_{i=1}^d \frac{y_i}{x_i} \frac{1}{d} \sum_{i=1}^d \log \frac{y_i}{x_i} ; \quad (4)$$

[Pal and Wong \(2020\)](#) proved that there exists an exponentially concave function $\tau : \mathcal{S}_d \rightarrow \mathbb{R}$ such that

$$T^\tau(x) = x \otimes \tau(x)^{-1}$$

where $\tau : \mathcal{S}_d \rightarrow \mathcal{S}_d$ satisfies

$$\tau(x) = x_1 (1 + r_{e_1} x) \tau(x) ; \quad ; x_d (1 + r_{e_d} x) \tau(x) ;$$

where e_1, \dots, e_d is the standard orthonormal basis of \mathbb{R}^d .

Optimal Transport on the Simplex (for Categorical Variables)

Second approach, "transport on transformed space"

Define a transport mapping based on some isomorphism $\phi: S_d \rightarrow E$ and then define the inverse mapping $\phi^{-1}: E \rightarrow S_d$, where E is some Euclidean space, classically \mathbb{R}^d . This is the dual transport problem in [Pal and Wong \(2018\)](#). E.g.,

$$\text{alr}(x) = \left[\log \frac{x_1}{x_d}; \dots; \log \frac{x_{d-1}}{x_d} \right]$$

with inverse, for any $z \in \mathbb{R}^{d-1}$,

$$\text{alr}^{-1}(z) = C(\exp(z_1); \dots; \exp(z_{d-1}); 1) = C \exp([z; 0]) :$$

Optimal Transport on the Simplex (for Categorical Variables)

A more popular one is

$$\text{clr}(x) = \left(\log \frac{x_1}{\bar{x}_g}; \dots; \log \frac{x_D}{\bar{x}_g} \right);$$

where \bar{x}_g denotes the geometric mean of x . Its inverse is

$$\text{clr}^{-1}(z) = \text{C}(\exp(z_1); \dots; \exp(z_d)) = \text{C}(\exp(z)); z \in \mathbb{R}^d;$$

that is the softmax function

Optimal Transport on the Simplex (for Categorical Variables)

with two models, random forest (left) and gradient boosting (right)

Optimal Transport on the Simplex (for Categorical Variables)

	random forest			boosting		
	cars	equipmt.	other	cars	equipmt.	other
categorical (M)	30.323%	53.226%	16.452%	30.323%	53.226%	16.452%
categorical (F)	35.217%	44.638%	20.145%	35.217%	44.638%	20.145%
composition (M)	32.055%	49.882%	18.063%	31.843%	50.712%	17.445%
composition (F)	34.977%	45.409%	19.614%	34.714%	45.341%	19.945%
T ()	32.046%	49.883%	18.070%	31.871%	50.675%	17.455%

See [Fernandes Machado et al. \(2025a\)](#) for more details.

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