Appendix

A Empirical Estimates

Lemma 1. *As $|\mathcal{D}| \to \infty$, if $\mathcal{W}_1(p_S, p_{S_{\boldsymbol{a}}}) < \infty$ for all $\boldsymbol{a}$, the empirical barycenter satisfies $\lim \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) \to \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}})$ almost surely*[7].

Proof. By triangle inequality:

$$\sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, p_{S_{\boldsymbol{a}}}) \leq \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) + \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \,, \tag{4}$$

$$\sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) \leq \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) + p_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \,. \tag{5}$$

Since $p_{\bar{S}}$ and $\hat{p}_{\bar{S}}$ are the weighted barycenters of $\{p_{S_{\boldsymbol{a}}}\}$ and $\{\hat{p}_{S_{\boldsymbol{a}}}\}$ respectively:

$$\sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) \leq \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, p_{S_{\boldsymbol{a}}}) \,, \tag{6}$$

$$\sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) \leq \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) \,. \tag{7}$$

Combining Eqs. (4) and (6), and (5) and (7):

$$\begin{aligned}
\sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) &\leq \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) + p_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \\
&\leq \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) + |\hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) - p_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}})| + p_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \\
&\leq \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) + |\hat{p}_{\boldsymbol{a}} - p_{\boldsymbol{a}}| \cdot |\mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}})| + p_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \\
\sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) &\leq \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) + \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \\
&\leq \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) + |p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) - \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}})| + \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \\
&\leq \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) + |p_{\boldsymbol{a}} - \hat{p}_{\boldsymbol{a}}| \cdot |\mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}})| + \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \,.
\end{aligned}$$

Therefore the following inequality holds almost surely:

$$\begin{aligned}
\Big| \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) - \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) \Big| &\leq \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) + |p_{\boldsymbol{a}} - \hat{p}_{\boldsymbol{a}}| \cdot \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) \\
&\leq \sum_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) + |p_{\boldsymbol{a}} - \hat{p}_{\boldsymbol{a}}| \cdot \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) \\
&\leq \sum_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) + |p_{\boldsymbol{a}} - \hat{p}_{\boldsymbol{a}}| \cdot \mathcal{W}_1(p_S, p_{S_{\boldsymbol{a}}}) \,.
\end{aligned}$$

Since $\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{S_{\boldsymbol{a}}}) \to 0$ almost surely for all $\boldsymbol{a}$ (see Weed and Bach (2017)), and $\hat{p}_{\boldsymbol{a}} \to p_{\boldsymbol{a}}$ almost surely (by the strong law of large numbers) and $\mathcal{W}_1(p_S, p_{S_{\boldsymbol{a}}}) < \infty$ for all $\boldsymbol{a}$, the result follows:

$$\lim \sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, \hat{p}_{S_{\boldsymbol{a}}}) \to \sum_{\boldsymbol{a}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{\bar{S}}, p_{S_{\boldsymbol{a}}}) \,,$$

almost surely. □

[7] See Klenke (2013) for a formal definition of almost sure convergence of random variables.

B Generalization

The following lemma addresses generalization of the Wasserstein-1 objective. Assume $\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, p_{\bar{S}}) \leq L$ for all $\boldsymbol{a} \in \mathcal{A}$. Let $P_S, P_{S_{\boldsymbol{a}}}$ and $P_{\bar{S}}$ be the cumulative density functions of S, $S_{\boldsymbol{a}}$ and $\bar{S}$. If $\int \sqrt{P(t)(1-P(t))} < \infty$ for $P \in \{P_S, P_{\bar{S}}\} \cup \{P_{S_{\boldsymbol{a}}}\}_{\boldsymbol{a}\in\mathcal{A}}$ then:

Lemma 5. *Let $\epsilon, \delta > 0$. If $\min\left[\bar{N}, \min_{\boldsymbol{a}}\left[N_{\boldsymbol{a}}\right]\right] \geq 4\max\left[\frac{1}{\epsilon^{3.1}}, \frac{8\log(2|\mathcal{A}|/\delta)|\mathcal{A}|^2\max[1,L]^2}{\epsilon^2}, 1\right]$, then with probability $1-\delta$:*

$$\sum_{\boldsymbol{a}\in\mathcal{A}} p_{\boldsymbol{a}}\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, p_{\bar{S}}) \leq \sum_{\boldsymbol{a}\in\mathcal{A}} \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) + \epsilon\,.$$

In other words, provided access to sufficient samples, a low value of $\sum_{\boldsymbol{a}} \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}})$ implies a low value for $\sum_{\boldsymbol{a}} p_{\boldsymbol{a}}\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, p_{\bar{S}})$ with high probability and therefore good performance at test time.

Proof. We start with the case when $p_{\bar{S}} = p_S$. By the triangle inequality for Wasserstein-1 distances, for all $\boldsymbol{a} \in \mathcal{A}$:

$$\hat{p}_{\boldsymbol{a}}\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, p_{\bar{S}}) \leq \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) + \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{\bar{S}}, p_{\bar{S}}) + \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, p_{S_{\boldsymbol{a}}})\,. \tag{8}$$

Since $\int \sqrt{P(t)(1-P(t))} < 0$ for $P \in \{P_S, P_{\bar{S}}\} \cup \{P_{S_{\boldsymbol{a}}}\}_{\boldsymbol{a}\in\mathcal{A}}$, as a consequence of Theorem 1.1 in Bolley et al. (2007), and a union bound, with probability $\geq 1 - \frac{\delta}{2}$ the following inequalities hold simultaneously for all $\boldsymbol{a} \in \mathcal{A}$:

$$\hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{\bar{S}}, p_{\bar{S}}) \leq \frac{\hat{p}_{\boldsymbol{a}}\epsilon}{4}, \quad \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, p_{S_{\boldsymbol{a}}}) \leq \frac{\hat{p}_{\boldsymbol{a}}\epsilon}{4}\,.$$

Summing Eq. (8) over $\boldsymbol{a}$ and applying the last observation yields

$$\sum_{\boldsymbol{a}\in\mathcal{A}} \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, p_{\bar{S}}) \leq \sum_{\boldsymbol{a}\in\mathcal{A}} \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) + \frac{\epsilon}{2}\,.$$

Recall that we assume $\forall \boldsymbol{a} \in \mathcal{A}$,

$$\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, p_{\bar{S}}) \leq L\,.$$

By concentration of measure of Bernoulli random variables, with probability $\geq 1 - \frac{\delta}{2}$ the following inequality holds simultaneously for all $\boldsymbol{a} \in \mathcal{A}$:

$$|p_{\boldsymbol{a}} - \hat{p}_{\boldsymbol{a}}| \leq \frac{\epsilon}{4|\mathcal{A}|\max[L,1]}\,.$$

Consequently the desired result holds:

$$\sum_{\boldsymbol{a}\in\mathcal{A}} p_{\boldsymbol{a}}\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, p_{\bar{S}}) \leq \sum_{\boldsymbol{a}\in\mathcal{A}} \hat{p}_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) + \epsilon\,.$$

If $p_{\bar{S}}$ equals the weighted barycenter of the population level distributions $\{p_{S_a}\}$, then

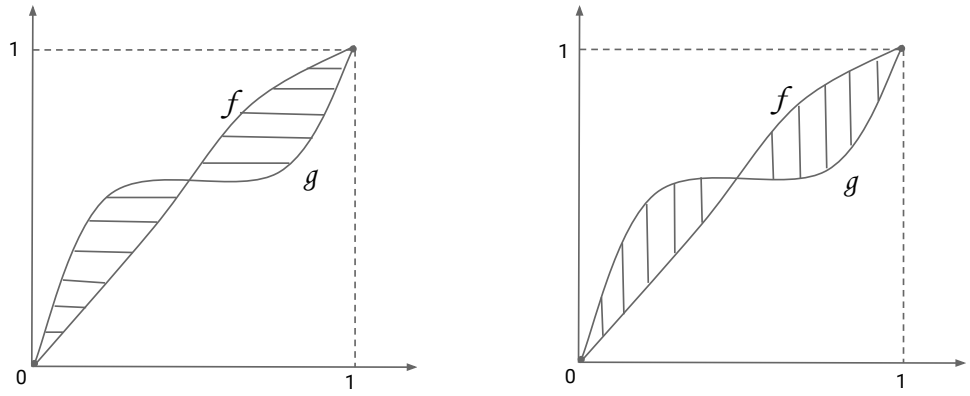
$$\sum_{\boldsymbol{a}\in\mathcal{A}} p_{\boldsymbol{a}}\mathcal{W}_1(p_{S_a}, p_{\bar{S}}) \leq \sum_{\boldsymbol{a}\in\mathcal{A}} p_{\boldsymbol{a}}\mathcal{W}_1(p_{S_a}, \hat{p}_{\bar{S}})\,.$$

Since $p_{\boldsymbol{a}}\mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) \leq p_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) + p_{\boldsymbol{a}}\mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, p_{S_a})$ a similar argument as above yields the desired result. □

C Inverse CDFs

Lemma 6. *Given two differentiable and invertible cumulative distribution functions f, g over the probability space $\Omega = [0,1]$, thus $f, g : [0,1] \to [0,1]$, we have*

$$\int_{s=0}^{1} |f^{-1}(s) - g^{-1}(s)|ds = \int_{\tau=0}^{1} |f(\tau) - g(\tau)|d\tau. \tag{9}$$



(a) Left side of Eq. (9) (b) Right side of Eq. (9)

Figure 3: Integrating $|f^{-1} - g^{-1}|$ along the x axis (left) and integrating $|f - g|$ along the y axis (right) both compute the area of the same shaded region, thus the equality in Eq. (9).

Intuitively, we see that the left and right side of Eq. (9) correspond to two ways of computing the same shaded area in Figure 3. Here is a complete proof.

Proof. Invertible CDFs f, g are strictly increasing functions due to being bijective and non-decreasing. Furthermore, we have $f(0) = 0, f(1) = 1$ by definition of CDFs and $\Omega = [0, 1]$, since $P(X \leq 0) = 0, P(X \leq 1) = 1$ where X is the corresponding random variable. The same holds for the function g. Given an interval $(x_1, x_2) \subset [0, 1]$, let $y_1 = f(x_1), y_2 = f(x_2)$. Since f is differentiable, we have

$$\int_{x=x_1}^{x_2} f(x)dx + \int_{y=y_1}^{y_2} f^{-1}(y)dy = x_2y_2 - x_1y_1. \tag{10}$$

The proof of Eq. (10) is the following (see also Laisant (1905)).

$$\begin{aligned}
& f^{-1}(f(x)) = x \\
\implies & f'(x)f^{-1}(f(x)) = f'(x)x && \text{(multiply both sides by } f'(x)\text{)} \\
\implies & \int_{x=x_1}^{x_2} f'(x)f^{-1}(f(x))dx = \int_{x=x_1}^{x_2} f'(x)xdx && \text{(integrate both sides)} \\
\implies & \int_{y=y_1}^{y_2} f^{-1}(y)dy = \int_{x=x_1}^{x_2} f'(x)xdx && \text{(apply change of variable } y = f(x) \text{ on the left side)} \\
\implies & \int_{y=y_1}^{y_2} f^{-1}(y)dy = xf(x)\Big|_{x=x_1}^{x_2} - \int_{x=x_1}^{x_2} f(x)dx && \text{(integrate by parts on the right side)} \\
\implies & \int_{y=y_1}^{y_2} f^{-1}(y)dy + \int_{x=x_1}^{x_2} f(x)dx = x_2y_2 - x_1y_1.
\end{aligned}$$

Define a function $h := f - g$ on $[0, 1]$. Then h is differentiable and thus continuous. Define the set of roots $A := \{x \in [0, 1] \mid h(x) = 0\}$. Define the set of open intervals on which either $h > 0$ or $h < 0$ by $B := \{(a, b) \mid b = \inf\{s \in A \mid a < s\}, 0 \leq a < b \leq 1, a \in A\}$. By continuity of h, for any $(a, b) \in B$, we have $b \in A$, *i.e.* b is also a root of h. Since there are no other roots of h in (a, b), by continuity of h, we must have either $h > 0$ or $h < 0$ on (a, b). For any two elements $(a, b), (c, d) \in B$, we argue that they must be disjoint intervals. Without loss of generality, we assume $a < c$. Since $b = \inf\{s \in A \mid a < s\} \leq c$, *i.e.* $b \leq c$, then $(a, b) \cap (c, d) = \emptyset$. For any open interval $(a, b) \in B$, there exists a rational number $q \in \mathbb{Q}$ such that $a < q < b$. We pick such a rational number and call it $q_{(a,b)}$. Since all elements of B are disjoint, for any two intervals $(a_0, b_0), (a_1, b_1)$ containing $q_{(a_0,b_0)}, q_{(a_1,b_1)} \in \mathbb{Q}$ respectively, we must have $q_{(a_0,b_0)} \neq q_{(a_1,b_1)}$. We define the set $Q_B := \{q_{(a,b)} \in \mathbb{Q} \mid (a, b) \in B\}$. Then $Q_B \subset \mathbb{Q}$ and $|Q_B| = |B|$. Since the set of rational numbers $\mathbb{Q}$ is countable, the set B must also be countable. Let $B = \{(a_i, b_i)\}_{i=0}^{N}$ where $N \in \mathbb{N}$ or $N = \infty$. Recall that $h = f - g$ on $[0, 1]$, $h(a_i) = 0, h(b_i) = 0$ and either $h < 0$ or $h > 0$ on (a_i, b_i) for $\forall i > 0$.

Consider the interval (a_i, b_i) for some $i > 0$, by Eq.10 we have

$$\int_{\tau=a_i}^{b_i} f(\tau)d\tau + \int_{s=f(a_i)}^{f(b_i)} f^{-1}(s)ds = b_i f(b_i) - a_i f(a_i)$$
$$= b_i g(b_i) - a_i g(a_i) = \int_{\tau=a_i}^{b_i} g(\tau)d\tau + \int_{s=g(a_i)}^{g(b_i)} g^{-1}(s)ds.$$

Thus

$$\int_{\tau=a_i}^{b_i} f(\tau) - g(\tau)d\tau = \int_{s=f(a_i)}^{f(b_i)} g^{-1}(s) - f^{-1}(s)ds.$$

Notice that if $f > g$ on $[a_i, b_i]$, then $f^{-1} < g^{-1}$ on $[f(a_i), f(b_i)]$. This is due to the following. Given any $y \in [f(a_i), f(b_i)] = [g(a_i), g(b_i)]$, we have $g^{-1}(y) \in [a_i, b_i]$ and $f(g^{-1}(y)) > g(g^{-1}(y)) = y = f(f^{-1}(y))$. Thus $g^{-1} > f^{-1}$ since f is strictly increasing. The contrary holds by the same reasoning, *i.e.* if $f < g$ on $[a_i, b_i]$, then $f^{-1} > g^{-1}$ on $[f(a_i), f(b_i)]$. Therefore,

$$\int_{\tau=a_i}^{b_i} |f(\tau) - g(\tau)|d\tau = \int_{s=f(a_i)}^{f(b_i)} |g^{-1}(s) - f^{-1}(s)|ds,$$

which holds for all intervals (a_i, b_i). Summing over i on both sides, we have

$$\sum_{i=0}^{N} \int_{\tau=a_i}^{b_i} |f(\tau) - g(\tau)|d\tau = \sum_{i=0}^{N} \int_{s=f(a_i)}^{f(b_i)} |g^{-1}(s) - f^{-1}(s)|ds,$$

or equivalently,

$$\int_{s=0}^{1} |f^{-1}(s) - g^{-1}(s)|ds = \int_{\tau=0}^{1} |f(\tau) - g(\tau)|d\tau.$$

□