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. $\square$

[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 $\min\left[\bar{N}, \min_{\boldsymbol{a}}\left[N_{\boldsymbol{a}}\right]\right] \geq 4M_0 \max\left[\frac{1}{\epsilon^{3.1}}, \frac{8\log(2|\mathcal{A}|/\delta)|\mathcal{A}|^2\max[1,L]^2}{\epsilon^2}, 1\right]$ for some constant M_0 depending solely on the moments of $\{P_S, P_{\bar{S}}\} \cup \{P_{S_{\boldsymbol{a}}}\}_{\boldsymbol{a}\in\mathcal{A}}$, 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 $\boldsymbol{a} \in \mathcal{A}$:

$$\hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{\bar{S}}, p_{\bar{S}}) \leq \frac{\hat{p}_{\boldsymbol{a}}\epsilon}{4}, \quad \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, p_{S_{\boldsymbol{a}}}) \leq \frac{\hat{p}_{\boldsymbol{a}}\epsilon}{4}\,. \tag{9}$$

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 $\boldsymbol{a} \in \mathcal{A}$:

$$|p_{\boldsymbol{a}} - \hat{p}_{\boldsymbol{a}}| \leq \frac{\epsilon}{4|\mathcal{A}|\max[L,1]}\,. \tag{10}$$

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

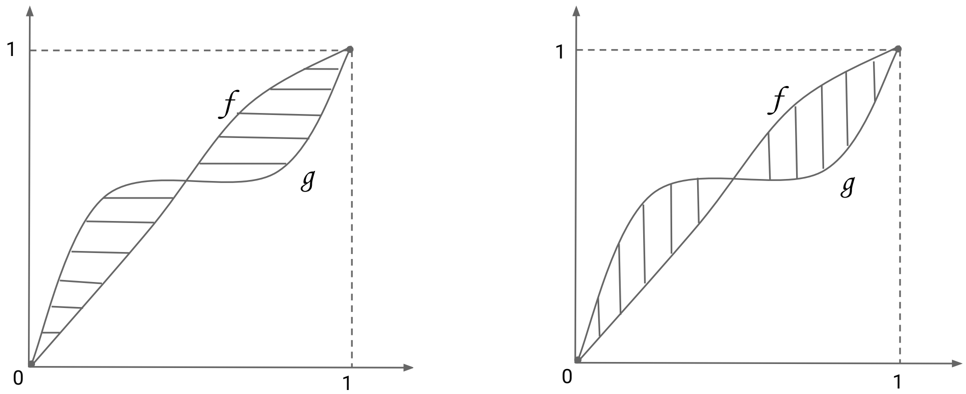
$$\sum_{\boldsymbol{a}\in\mathcal{A}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{S_a}, p_{\bar{S}}) \leq \sum_{\boldsymbol{a}\in\mathcal{A}} p_{\boldsymbol{a}} \mathcal{W}_1(p_{S_a}, \hat{p}_{\bar{S}})\,.$$

Since $\hat{p}_{\boldsymbol{a}} \mathcal{W}_1(p_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) \leq \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, \hat{p}_{\bar{S}}) + \hat{p}_{\boldsymbol{a}} \mathcal{W}_1(\hat{p}_{S_{\boldsymbol{a}}}, p_{S_a})$, with probability $1-\delta$:

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

The first inequality follows from Eq. (10), and the third one by Eq. (9). The result follows.

$\square$



(a) Left side of Eq. (11) (b) Right side of Eq. (11)

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. (11).

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*

$$\int_{s=0}^{1} |f^{-1}(s) - g^{-1}(s)| ds = \int_{\tau=0}^{1} |f(\tau) - g(\tau)| d\tau. \tag{11}$$

Intuitively, we see that the left and right side of Eq. (11) 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

$$\int_{x=x_1}^{x_2} f(x)dx + \int_{y=y_1}^{y_2} f^{-1}(y)dy = x_2 y_2 - x_1 y_1. \tag{12}$$

The proof of Eq. (12) is the following (see also Laisant (1905)).

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

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.12 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,

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

$\square$