
Distributional Counterfactual Explanations With Optimal Transport

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Abstract

Counterfactual explanations (CE) are the de facto method for providing insights into black-box decision-making models by identifying alternative inputs that lead to different outcomes. However, existing CE approaches, including group and global methods, focus predominantly on specific input modifications, lacking the ability to capture nuanced distributional characteristics that influence model outcomes across the entire input-output spectrum. This paper proposes distributional counterfactual explanation (DCE), shifting focus to the distributional properties of observed and counterfactual data, thus providing broader insights. DCE is particularly beneficial for stakeholders making strategic decisions based on statistical data analysis, as it makes the statistical distribution of the counterfactual resembles the one of the factual when aligning model outputs with a target distribution—something that the existing CE methods cannot fully achieve. We leverage optimal transport (OT) to formulate a chance-constrained optimization problem, deriving a counterfactual distribution aligned with its factual counterpart, supported by statistical confidence. The efficacy of this approach is demonstrated through experiments, highlighting its potential to provide deeper insights into decision-making models.

1 Background

In the field of explainable artificial intelligence (XAI), counterfactual explanations (CE) has become the quintessential method for providing insight and explainability in complex decision-making models. This prominence is particularly marked in domains where understanding the causal impact of variables is pivotal for informed decision-making (Verma et al., 2020). The utility of CEs is grounded in their ability to answer “*what-if*” scenarios, offering tangible insights into how slight alterations in input can lead to different model outputs. This not only aids in demystifying the decision process of black-box models but also helps in identifying potential biases and areas for model improvement.

Motivation and Challenges Traditional CE focuses on individual data points, analyzing how changes in specific features influence the model’s output. While this approach is useful, it overlooks scenarios where the statistical distribution of counterfactuals should resemble with that of the original instances (Carrizosa et al., 2024). See Figure 1 for an example. It is important to note that group CE does not bridge this gap because they neglect the statistical properties’ alignment between the factual and the counterfactual. Whereas DCE operates at the distributional level, where the entire input and output of a model are treated as distributions. Since strategical business decisions are made based on trends and patterns rather than single instance, this approach could practically benefit more for the stakeholders making strategic decisions based on statistical data analysis. Related work of this paper is detailed in Appendix A.

Despite the need for DCE, several challenges arise in it. Metrics exist to quantify differences between distributions, but practical interpretation of these differences is often unclear. Unlike traditional CE or group CE, which adjust individual feature values, DCE must extend its mechanism from modifying “quantities” to

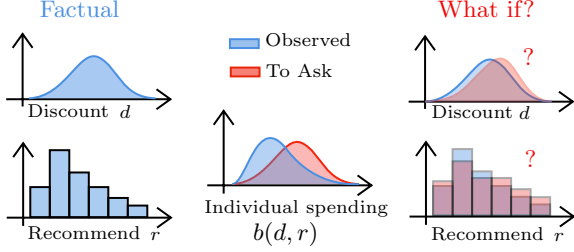


Figure 1: Consider a retail business aiming to understand how a machine learning model b predicts individual customer spending for revenue forecasting, based on discount rates d and product recommendations r . Based on any **observed model outputs**, the business asks to understand how adjusting the entire distributions of discounts and recommendations would impact the prediction **towards another pattern**. Such insights are crucial for 1) making strategic operational decisions and 2) verifying whether the model behavior aligns with the real-world causal relationships. This calls for distributional counterfactual explanations (DCE), which allows the business to find explanations to the model at the distribution level—not just individual instances. To answer the “what-if” question, the **counterfactual d and r** that the business seeks should resemble the **observed factual d and r** . This is because drastic deviations from current practices may be impractical, and similarity ensures actionable recourse. Traditional CE, including group or global method, fail in this aspect.

adapting “quantiles,” fitting naturally within the data science paradigm of using quantile plots and histograms. Furthermore, determining differences between distributions involves sampling, introducing challenges like sampling error, increased sample complexity, and the curse of dimensionality—all of which must be addressed to ensure accurate and computationally feasible counterfactual generation.

Main Contribution We propose a novel approach to DCE using optimal transport (OT), commonly known as Wasserstein distance, along with its sliced version to quantify divergence between distributions. By formulating DCE as a chance-constrained optimization problem, we derive distributional counterfactuals that not only remain close to the original data but also ensure alignment with a predefined target distribution. Our method incorporates statistically rigorous confidence intervals within the optimization process, providing guarantees on the validity and proximity of counterfactuals. The proposed optimization algorithm effectively balances the trade-off between maintaining input similarity and fulfilling counterfactual requirements, with proven convergence rates. This approach establishes a statistically sound link between OT theory and CE, advancing the capability to understand model behavior at a distributional level, and is demonstrated to be highly effective in practical applications.

2 Preliminaries and Problem Setup

We first give a brief introduction of OT and its sliced version. Then we formulate the DCE problem as a chance constrained optimization problem based on OT.

OT and the Wasserstein Distance Denote by $\mathcal{P}(\mathbb{R})$ the set of probability measures with finite second moments. Let $\gamma_1, \gamma_2 \in \mathbb{R}$, and let $\Pi(\gamma_1, \gamma_2)$ denote the set of all joint probability measures on $\mathbb{R} \times \mathbb{R}$ with marginals γ_1 and γ_2 . We refer to $\Pi(\gamma_1, \gamma_2)$ as the set of transport plans between γ_1 and γ_2 . The one-dimensional (1D) squared 2-Wasserstein distance is defined as

$$\mathcal{W}^2(\gamma_1, \gamma_2) \triangleq \inf_{\pi \in \Pi} \int_{\mathbb{R} \times \mathbb{R}} \|a_1 - a_2\|^2 d\pi(a_1, a_2), \quad (1)$$

which represents the OT cost between γ_1 and γ_2 with respect to the squared Euclidean distance $\|a_1 - a_2\|^2$ under the optimized OT plan π .

Sliced Wasserstein Distance Different from its original version, the sliced Wasserstein distance performs 1D linear projections of two high-dimensional measures γ_1 and γ_2 , then it computes the Wasserstein distance between the projected measures. Formally, let $\mathbb{S}^{d-1} \subset \mathbb{R}^d$ stand for the d -dimensional unit sphere:

$$\mathcal{SW}^2(\gamma_1, \gamma_2) \triangleq \int_{\mathbb{S}^{d-1}} \mathcal{W}^2(\theta \# \gamma_1, \theta \# \gamma_2) d\sigma(\theta), \quad (2)$$

where σ is the uniform distribution on \mathbb{S}^{d-1} and $\#$ is the push-forward operator, which projects (high-dimensional) measures γ_1 and γ_2 onto a 1D space.

We choose \mathcal{SW}^2 over other approximations of \mathcal{W}^2 because it retains the same sample complexity as \mathcal{W}^2 , enables the derivation of confidence intervals crucial for the DCE framework, and provides an intuitive, quantile-based interpretation for comparing distributions, as shown by the next section.

DCE Problem Formulation Denote $b : \mathbb{R}^d \rightarrow \mathbb{R}$ a black-box model. Given any data distribution \mathbf{x}' ($\mathbf{x}' \in \mathbb{R}^d$) as a factual (i.e. an observed distribution) input, denote by $y' = b(\mathbf{x}')$ the factual model output distribution¹. Denote by y^* ($y^* \in \mathbb{R}$) a target distribution, and $y^* \neq y'$. The goal is to find a counterfactual \mathbf{x} that closely matches \mathbf{x}' , so that the resulting model output distribution $b(\mathbf{x})$ closely approximates the target distribution y^* . In practical applications, closed-form expressions for these distributions are rarely available, so empirical distributions are used instead. However empirical distributions may contain outliers, we hereby

¹We use the bold \mathbf{y} to represent its empirical distribution version $[y_1, \dots, y_n]$ ($\forall y_i \in \mathbb{R}$).

align \mathbf{x} with \mathbf{x}' and $b(\mathbf{x})$ with y^* probabilistically and hence DCE is formulated as a chance-constrained optimization problem, shown in (3).

$$[\text{DCE Problem}] \quad \max_{\mathbf{x}, P} P \quad (3a)$$

$$\text{s.t.} \quad P \leq \mathbb{P} [SW^2(\mathbf{x}, \mathbf{x}') < U_x] \quad (3b)$$

$$P \leq \mathbb{P} [W^2(b(\mathbf{x}), y^*) < U_y] \quad (3c)$$

$$P \geq 1 - \frac{\alpha}{2} \quad (3d)$$

The inequality (3b) imposes that the sliced Wasserstein distance between the multi-dimensional \mathbf{x}' and its counterfactual distribution \mathbf{x} is subject to a chance constraint such that the distance is smaller than a threshold U_x with a probability no lower than P . The inequality (3c) is for the same goal but for the model output². We set a confidence level $\alpha/2$, such that a feasible solution needs to make both chance constraints hold beyond the level probabilistically.

Revisiting the example in Figure 1, (3b) guarantees that the counterfactual joint distribution of discount rates and product recommendations ensemble the factual one. And (3c) makes sure the counterfactual achieves the ‘‘To Ask’’ model output y^* . Maximizing P ensures that the probability of both the input and output distributions meeting their respective constraints is as high as possible, with a confidence level for at least $1 - \frac{\alpha}{2}$.

3 Theoretical Foundations of DCE

This section shows useful properties of the formulation (3). First, DCE extends CE from quantity comparison to quantile comparison. Second, the slicing approximation in dealing with high-dimensional data does not sacrifice sample complexity. Third, statistical confidence intervals are derived for the chance constraints (3b) and (3c). Otto (Otto, 2001) showed that the space metrized by the 2-Wasserstein distance admits the structure of a formal Riemannian metric. The properties enable solving the DCE problem via Riemannian block coordinated descent (BCD).

Quantile-Based Expression The Wasserstein distance in (3c) can alternatively be written as follows (with $y = b(\mathbf{x})$).

$$W^2(y, y^*) = \int_0^1 \|F_y^{-1}(q) - F_{y^*}^{-1}(q)\|^2 dq \quad (4)$$

In the equation above, $F_y^{-1}(q)$ and $F_{y^*}^{-1}(q)$ are the inverse cumulative distribution functions (i.e. quantile

²This formulation generalizes to multi-dimensional output by using sliced Wasserstein distance in (3c). The method and conclusions proposed in this paper still hold.

functions) of y and y^* . The equation holds due to both y and y^* being 1D distributions, providing an alternative explanation of the Wasserstein distance: It is the integral of the square of the difference between the corresponding quantiles in the interval $[0, 1]$. Essentially, this aligns the model output distribution y ($y = b(\mathbf{x})$) and the target distribution y^* in a way that we are comparing the location of equivalent ‘‘percentiles’’ of mass in each distribution. In fact, it accounts for the full range of variability in the outputs, not just their central tendency (e.g. in contrast to comparing $\mathbb{E}(y)$ and $\mathbb{E}(y^*)$ only), which is crucial for many practical applications where distributional characteristics are important.

Sample Complexity of Slicing Approximation

In (3), the dissimilarity between \mathbf{x} and \mathbf{x}' is evaluated using the sliced Wasserstein distance, which serves as an approximation of their true Wasserstein distance. In real-world applications, we typically have finite samples drawn from the underlying distributions of \mathbf{x} and \mathbf{x}' . The effectiveness of this approximation hinges on its ability to provide accurate distance estimates using a limited number of samples, a property known as ‘‘good sample complexity.’’ A natural question arises: Does the slicing approximation possess the same sample complexity as its original counterpart? We state Nadjahi et al. (2020, Theorem 4) below as Proposition 3.1.

Proposition 3.1. *Consider any measure $z \in \mathcal{P}(\mathbb{R})$ with an empirical measure $\hat{z} = \{z_i\}_{i=1}^n$, and a measure $z' \in \mathcal{P}(\mathbb{R})$ with an empirical measure $\hat{z}' = \{z'_j\}_{j=1}^n$. Let $\xi(n)$ be any function of the sample size n . Suppose that the squared Wasserstein distance W^2 satisfies the following sample complexity:*

$$\mathbb{E} |W^2(z, z') - W^2(\hat{z}, \hat{z}')| \leq \xi(n).$$

Then, for any measures $\mathbf{x}, \mathbf{x}' \in \mathcal{P}(\mathbb{R}^d)$ with corresponding empirical measures $\hat{\mathbf{x}} = \{\mathbf{x}_i\}_{i=1}^n$ and $\hat{\mathbf{x}}' = \{\mathbf{x}'_i\}_{i=1}^n$, the sliced Wasserstein distance SW^2 satisfies

$$\mathbb{E} |SW^2(\mathbf{x}, \mathbf{x}') - SW^2(\hat{\mathbf{x}}, \hat{\mathbf{x}}')| \leq \xi(n).$$

Proposition 3.1 asserts that the sample complexity of the slicing approximation is directly proportional to that of the original Wasserstein distance. Notably, the sample complexity is independent of the dimensionality d . Consequently, formulation (3) scales effectively to high-dimensional inputs.

Upper Confidence Limit (UCL) Let F^{-1} denote the quantile function of a distribution, and F_n^{-1} its empirical counterpart based on n samples. When specifying the distribution for a specific variable, the letter of the variable is put as subscript of them. We define some sequences functions that can be used for

any quantile function, which are used construct confidence intervals (and hence UCL). That is, a confidence interval is represented below

$$\begin{aligned} \mathbb{P} \left(F_n^{-1} \left(\underline{q}_{\alpha,n}(u) \right) \leq F^{-1}(u) \leq F_n^{-1} \left(\bar{q}_{\alpha,n}(u) \right) \right) \\ \geq 1 - \frac{\alpha}{2}, \end{aligned} \quad (5)$$

for some sequences of functions $\underline{q}_{\alpha,n} : (0, 1) \rightarrow \mathbb{R}$ and $\bar{q}_{\alpha,n} : (0, 1) \rightarrow \mathbb{R}$. We use the variable u to refer to the quantile level, and the sequences $\underline{q}_{\alpha,n}$ and $\bar{q}_{\alpha,n}$ serve to transform this quantile level u into a real number. Theorem 3.2 below follows (Manole et al., 2022, Propositions 5 and 6) (proof sketched in Appendix B) providing uniform confidence levels for $\mathcal{SW}^2(\mathbf{x}, \mathbf{x}')$ and $\mathcal{W}^2(b(\mathbf{x}), y^*)$.

Theorem 3.2. *Let $\delta \in (0, 1/2)$ be a trimming constant, the following inequalities hold:*

1. For $\mathcal{W}^2(b(\mathbf{x}), y^*)$ in (3c), we have

$$\mathbb{P} \left[\mathcal{W}^2(b(\mathbf{x}), y^*) \leq \frac{1}{1-2\delta} \int_{\delta}^{1-\delta} D(u) du \right] \geq 1 - \frac{\alpha}{2}, \quad (6)$$

$$\text{where } D(u) \triangleq \max \left\{ F_{y,n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{y^*,n}^{-1}(\underline{q}_{\alpha,n}(u)), F_{y^*,n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{y,n}^{-1}(\underline{q}_{\alpha,n}(u)) \right\}. \quad (7)$$

2. For $\mathcal{SW}^2(\mathbf{x}, \mathbf{x}')$ in (3b), let the projection vectors $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N$ be independent and identically distributed samples from a distribution σ on the unit sphere \mathbb{S}^{d-1} . Let σ_N denote the empirical measure associated with these samples. Then,

$$\begin{aligned} \mathbb{P} \left[\mathcal{SW}^2(\mathbf{x}, \mathbf{x}') \leq \right. \\ \left. \frac{1}{1-2\delta} \int_{\mathbb{S}^{d-1}} \int_{\delta}^{1-\delta} D_{\boldsymbol{\theta},N}(u) du d\sigma_N(\boldsymbol{\theta}) \right] \geq 1 - \frac{\alpha}{2} \end{aligned} \quad (8)$$

where

$$\begin{aligned} D_{\boldsymbol{\theta},N}(u) \triangleq \max \left\{ F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{\boldsymbol{\theta}^\top \mathbf{x}',n}^{-1}(\underline{q}_{\alpha,n}(u)), \right. \\ \left. F_{\boldsymbol{\theta}^\top \mathbf{x}',n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}(\underline{q}_{\alpha,n}(u)) \right\}. \end{aligned} \quad (9)$$

Here, $F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}$ denotes the empirical quantile function of $\boldsymbol{\theta}^\top \mathbf{x}_i$ for $i = 1, \dots, n$, and similarly for $F_{\boldsymbol{\theta}^\top \mathbf{x}',n}^{-1}$.

The inequalities (6) and (8) provide methods to validate and substantiate the chance constraints (3c) and (3b), respectively. The right-hand-side of (3c) is no less than $1 - \alpha/2$ if and only if we have its corresponding UCL, denoted by $\overline{\mathcal{W}}^2$, no larger than U_y , i.e.

$$\overline{\mathcal{W}}^2 \triangleq \frac{1}{1-2\delta} \int_{\delta}^{1-\delta} D(u) du \leq U_y. \quad (10)$$

The computation of (10) lies on $D(u)$, defined in (7), which quantifies the disparity between the quantile functions of $y = b(\mathbf{x})$ and y^* by utilizing pre-specified function sequences $\underline{q}_{\alpha,n}(u)$ and $\bar{q}_{\alpha,n}(u)$. Practically, the quantile level u can be uniformly sampled within $(0, 1)$ and the remaining critical task is to formulate suitable $\underline{q}_{\alpha,n}$ and $\bar{q}_{\alpha,n}$ functions that are grounded in statistical theory³.

Similarly, the right-hand-side of (3b) is no less than $1 - \alpha/2$ if and only if we have its corresponding UCL, denoted by \mathcal{SW}^2 , follows

$$\overline{\mathcal{SW}}^2 \triangleq \frac{1}{1-2\delta} \int_{\mathbb{S}^{d-1}} \int_{\delta}^{1-\delta} D_{\boldsymbol{\theta},N}(u) du d\sigma_N(\boldsymbol{\theta}) \leq U_x, \quad (11)$$

with $D_{\boldsymbol{\theta},N}$ defined in (9). Compared to $\overline{\mathcal{W}}^2$, $\overline{\mathcal{SW}}^2$ aggregates the integral result on $D_{\boldsymbol{\theta},N}(u)$ further on $\boldsymbol{\theta}$ that is distributed on the d -dimensional unit sphere⁴.

Alternatively, the central limit theorem (CLT) is applicable to both OT and its sliced counterpart, allowing $\overline{\mathcal{SW}}^2$ and $\overline{\mathcal{W}}^2$ to be estimated via the bootstrap method. For further information, refer to the theorems presented in (Del Barrio and Loubes, 2019, Theorem 4.1) and (Manole et al., 2022, Theorem 4). Regardless of the approaches, both chance constraints in the DCE formulation (3) are rigorously respected.

4 Optimization for Problem Solving

Revisit the DCE Problem We re-write the DCE problem in (3) in a form for empirical distribution. Let $\mathbf{x} = \{\mathbf{x}_i\}_{i=1}^n$ and $\mathbf{y}^* = \{y_j^*\}_{j=1}^n$ be empirical distributions. Denote the set of projection vectors generated from a uniform distribution on a unit sphere by $\Theta = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_N\}$. Define

$$Q_x(\mathbf{x}, \boldsymbol{\mu}) \triangleq \sum_k \sum_{i=1}^n \sum_{j=1}^n |\boldsymbol{\theta}^\top \mathbf{x}_i - \boldsymbol{\theta}^\top \mathbf{x}'_j|^2 \mu_{ij}^{(k)}, \quad (12)$$

$$Q_y(\mathbf{x}, \boldsymbol{\nu}) \triangleq \sum_{i=1}^n \sum_{j=1}^n |b(\mathbf{x}_i) - y_j^*|^2 \nu_{ij}. \quad (13)$$

³One classic example is $\underline{q}_{\alpha,n} = u - \beta_n$, $\bar{q}_{\alpha,n} = u + \beta_n$, and $\beta_n = \sqrt{\log(4/\alpha)/2n}$. Then (10) holds by Dvoretzky-Kiefer-Wolfowitz (DKW) inequalities (Dvoretzky et al., 1956). One could refer to (Manole et al., 2022, Section 4) for more examples. This transformation adheres to the principles of uniform quantile bounds, a topic extensively discussed in the work of (Shorack and Wellner, 2009).

⁴Remark $\overline{\mathcal{W}}^2$ is finite sample inference whereas $\overline{\mathcal{SW}}^2$ is not. One needs to enlarge $\overline{\mathcal{SW}}^2$ with a factor that is inversely proportional to N to obtain the finite version (Manole et al., 2022).

Both Q_x and Q_y are smooth in \mathbf{x} , $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$. The empirical version of (3) reads:

$$\max_{\mathbf{x} \in \mathcal{M}, P \geq 0} P \quad (14a)$$

$$\text{s.t. } P \leq \mathbb{P}_n \left[\inf_{\boldsymbol{\mu} \in \Pi} Q_x(\mathbf{x}, \boldsymbol{\mu}) \leq U_x \right] \quad (14b)$$

$$P \leq \mathbb{P}_n \left[\inf_{\boldsymbol{\nu} \in \Pi} Q_y(\mathbf{x}, \boldsymbol{\nu}) \leq U_y \right] \quad (14c)$$

$$P \geq 1 - \alpha/2 \quad (14d)$$

Note that Q_x and Q_y are the empirical versions of (1) and (2) (without inf), respectively. That is, for any given \mathbf{x} , optimizing the OT plan $\mu_{ij}^{(k)}$ towards minimizing Q_x , i.e. $\inf_{\boldsymbol{\mu} \in \Pi} Q_x(\mathbf{x}, \boldsymbol{\mu})$, yields $\mathcal{SW}^2(\mathbf{x}, \mathbf{x}')$. Similarly, $\inf_{\boldsymbol{\nu} \in \Pi} Q_y(\mathbf{x}, \boldsymbol{\nu})$ computes $\mathcal{W}^2(b(\mathbf{x}), \mathbf{y}^*)$.

Riemannian BCD Optimization Initially, we established Theorem 3.2 to manage the chance constraints (14b) and (14c). Secondly, we demonstrate below a partial optimality condition for resolving (14), uncovering that achieving the optimum (or local optima) is contingent upon identifying an appropriate balance between Q_x and Q_y . Thirdly, we introduce our algorithm *Discount*, which follows essentially a BCD framework (Peng and Vidal, 2023; Huang et al., 2021; Gutman and Ho-Nguyen, 2023) and supports both discrete and continuous strategies for this balancing. The discrete approach, termed *Set Shrinking*, optimizes the weights by selecting from a finite set of candidate values. In contrast, the continuous method *Interval Narrowing*, utilizes a bisection strategy applied to a progressively narrowing domain of variables. Finally, we remark that the proposed *Discount* comes with a guarantee of convergence regardless of which method is chosen, elaborated in Section 5.

Let \mathcal{M} be a compact smooth Riemannian manifold. Let $\mathbf{x} \in \mathcal{M}_1, \boldsymbol{\mu} \in \mathcal{M}_2, \boldsymbol{\nu} \in \mathcal{M}_3$ ($\mathcal{M} = \mathcal{M}_1 \times \mathcal{M}_2 \times \mathcal{M}_3$), where \mathcal{M}_i ($i = 1, 2, 3$) are bounded submanifolds. Our optimization is around a function $Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}, \eta)$:

$$Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}, \eta) \triangleq (1 - \eta) \cdot Q_x(\mathbf{x}, \boldsymbol{\mu}) + \eta \cdot Q_y(\mathbf{x}, \boldsymbol{\nu}), \quad (15)$$

and the theorem below establishes the partial optimality condition for optimization.

Theorem 4.1. *Assume that the optimization problem in (14) is feasible, i.e. (14b) and (14d) can be achieved simultaneously with at least $1 - \alpha/2$. Then, there exists a value $\eta^* \in [0, 1]$ such that the solution \mathbf{x}^* obtained by optimizing $Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu} \mid \eta^*)$, defined as*

$$\mathbf{x}^* \triangleq \arg \min_{\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}} Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}, \eta^*), \quad (16)$$

is also the optimal solution to the original problem (14), that is,

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} \varphi \quad \text{s.t. (14b) - (14d)}.$$

Algorithm 1 Distributional counterfactual

Require: \mathbf{x}, \mathbf{y}^* , model b , projections Θ , bounds U_x, U_y and significance level α .

Ensure: Counterfactual \mathbf{x} or \emptyset .

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1:  $\mathbf{x}^0 \leftarrow \mathbf{x}' + \sigma; t \leftarrow 0$ 
2: repeat
3:    $\boldsymbol{\mu}^t \leftarrow \arg \min_{\boldsymbol{\mu}} Q_x(\mathbf{x}^t, \boldsymbol{\mu})$ 
4:    $\boldsymbol{\nu}^t \leftarrow \arg \min_{\boldsymbol{\nu}} Q_y(\mathbf{x}^t, \boldsymbol{\nu})$ 
5:    $\overline{\mathcal{W}}^2 \leftarrow \text{Eq. (10)}$ 
6:    $\overline{\mathcal{SW}}^2 \leftarrow \text{Eq. (11)}$ 
7:    $\eta^t \leftarrow \text{Algorithm 2 (or 3 in Appendix D)}$ 
8:    $\tilde{\nabla} Q \leftarrow \tilde{\nabla}_{\mathbf{x}} Q(\mathbf{x}, \boldsymbol{\mu}^t, \boldsymbol{\nu}^t, \eta^t)$ 
9:    $\mathbf{x}^{t+1} \leftarrow \text{Retr}(-\tau \tilde{\nabla} Q)$ 
10:   $t \leftarrow t + 1$ 
11: until  $\|\mathbf{x}^{t+1} - \mathbf{x}^t\| \leq \epsilon$ 
12: if  $\overline{\mathcal{SW}}^2 \leq U_x$  and  $\overline{\mathcal{W}}^2 \leq U_y$  then
13:   return  $\mathbf{x}^{t+1}$ 
14: end if
15: return  $\emptyset$ 
    
```

The proof of Theorem 4.1 is in Appendix C. The theorem demonstrates addressing (14) (and hence the DCE problem in (3)) necessitates finding a proper η .

Algorithm 1 is designed following the framework of BCD, which performs alternating optimization, where one side focuses on optimizing the counterfactual \mathbf{x} , and the OT plans $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$, and the other side searches for a good performed η . First, Lines 3 and 4 compute the OT distances defined in (12) and (13) and obtain the OT plans $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$, respectively. Second, in lines 5 and 6, we compute the two corresponding UCLs $\overline{\mathcal{W}}^2$ and $\overline{\mathcal{SW}}^2$ that are defined in (10) and (11). Because \mathbf{x}^t is updated in every iteration, both UCLs are re-computed per iteration. Third, we use the two UCLs to compute an η as shown in line 7. The computed η influences the optimization direction of the counterfactual distribution $\{\mathbf{x}_i\}_{i=1}^n$ (shown by line 8) to balance the satisfaction of the two chance constraints (14b) and (14c), ensuring that both are adequately addressed in the solution. Fourth, line 8 computes the Riemannian gradient with respect to \mathbf{x} , denoted by $\tilde{\nabla}_{\mathbf{x}} Q$. Line 9 makes a descent step with step size τ using the retraction denoted by Retr (which is a mapping from the tangent space at any point on the manifold back onto the manifold itself (Absil et al., 2008)) and the Riemannian gradient $\tilde{\nabla}_{\mathbf{x}} Q$.

Algorithm 2 optimizes η within a pre-defined interval $[l, r]$, shown by line 1. See Appendix D for how the balance is achieved. In each run, the interval gets narrowed by a small proportion of κ , following a bi-section

Algorithm 2 Interval Narrowing

Require: $\overline{SW^2}$, $\overline{W^2}$, U_x, U_y , $[l, r]$, and κ ($0 < \kappa < 1$)
Ensure: η

- 1: $\eta \leftarrow$ Balance the gaps $U_x - \overline{SW^2}$ and $U_y - \overline{W^2}$
- 2: **if** $\eta > (l + r)/2$ **then**
- 3: $l \leftarrow l + \kappa(r - l)$
- 4: **else**
- 5: $r \leftarrow r - \kappa(r - l)$
- 6: **end if**
- 7: Save $[l, r]$ and κ as the input for the next run
- 8: **return** η

strategy, shown by lines 2–7. The parameter η can also be optimized in a discrete manner, see Algorithm 3 in Appendix D.

5 Convergence Rate Analysis

To ease the presentation, we let $\mathbf{v} = [\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}]$, and perform analysis for the optimization of \mathbf{v} and η . Recall that $\mathbf{v} \in \mathcal{M}$ where \mathcal{M} is a Riemannian manifold. Assume b is continuously differentiable and Lipschitz smooth with respect to \mathbf{x} and constant L . Following (Peng and Vidal, 2023, Lemma 1), we have that 1) there exists $\rho > 0$ such that $\|\text{Retr}_{\mathbf{x}}(\mathbf{s}) - \mathbf{x}\| \leq \rho\|\mathbf{s}\|$ where \mathbf{s} belongs to the tangent space associated with \mathbf{x} ($\mathbf{x} \in \mathcal{M}_1$), and 2) there exists a constant \tilde{L} (dependent on L , \mathcal{M}_1 , and Retr) such that the difference between $Q(\text{Retr}_{\mathbf{x}}(\mathbf{s}), \boldsymbol{\mu}, \boldsymbol{\nu}, \eta)$ and $Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}, \eta)$ is bounded by the Riemannian gradient of $\tilde{\nabla}_{\mathbf{x}}Q$ and \tilde{L} . Using the two constants ρ and \tilde{L} , the convergence rate of *Discount* is derived in Theorem 5.1 below.

Theorem 5.1. Let $\{\mathbf{v}^t\}_{t=0}^T$ denote the iterates of Algorithm 1 combined with either Algorithm 3 or Algorithm 2, using a stepsize $\tau = \frac{1}{L}$. Define

$$C \triangleq \sqrt{2\tilde{L}} + \rho L \cdot \sqrt{\frac{2}{\tilde{L}}} \text{ and } B \triangleq \sup_{\mathbf{v}} \{Q_x(\mathbf{v}), Q_y(\mathbf{v})\},$$

where B is ascertained finite with finite b . Then, the following convergence guarantees hold:

$$\begin{aligned} & \min_{t=0,1,\dots,T} \|\tilde{\nabla}Q(\mathbf{v}^t, \eta^t)\| \\ & \leq C \left[\frac{1}{T+1} (Q_x(\mathbf{v}^0) + Q_y(\mathbf{v}^0) + \Delta) \right]^{\frac{1}{2}}, \end{aligned}$$

where

$$\Delta = \begin{cases} 0, & \text{if Algorithm 3 is used,} \\ \frac{r-l}{\kappa} B, & \text{if Algorithm 2 is used.} \end{cases}$$

Briefly, the theorem states that the magnitude of the Riemannian gradient goes towards zero with the number of iterations. For Set Shrinking, the gradient is

bounded by the values of Q_x and Q_y at the starting point. For Interval Narrowing, the upper bound of Q_x and Q_y matters on top of the size and narrowing rate of the interval. The proof is derived in Appendix E.

6 Numerical Results

We validate the concept of DCE with four datasets, HELOC (FICO, 2018), COMPAS (Jeff Larson et al., 2016), German Credit (Hofmann, 1994), and Cardiovascular Disease (Halder, 2020). Three models are considered: deep neural network (DNN), radial basis function network (RBFNet), and support vector machine (SVM). Throughout our experiments⁵, α is set to 0.1. This setting implies that the significance level for testing the distinctness of two distributions is 5% as $\alpha/2$ corresponds to the one-tailed significance threshold. Quantitative experiments are performed in HELOC and COMPAS, justifying the advantage of DCE (solved by *Discount*) over existing CE methods: diverse counterfactual explanations (DiCE) (Mothilal et al., 2020), actionable resource summaries (ARes) (Rawal and Lakkaraju, 2020), and global & efficient counterfactual explanations (GLOBE) (Ley et al., 2023). DiCE finds counterfactuals for each factual instance and is hence an instance-based CE method. Both ARes and GLOBE are group-based CE. The main experiments focus on the validity and proximity of DCE in the distributional setup, as well as algorithm runtime and convergence. Extended numerical results are shown in Appendix F, focus on data diversity and counterfactual reasoning.

The effectiveness of *Discount* is demonstrated via five major metrics: *coverage*, *cost*, *proximity*, *runtime*, and *diversity*. The comparison of the first four metrics is shown in Table 1. Diversity is shown in Appendix F. Specifically, coverage evaluates how well the counterfactual output distribution approximates the target output distribution. Cost evaluates the payoff on changing the factual input to the counterfactual for higher coverage. Proximity measures how well the counterfactual distribution resembles the factual one. Essentially, any CE method plays trade-offs among coverage, cost, and proximity.

***Discount* achieves the best coverage-cost balance with moderate runtime** The experiments in Table 1 are performed on the HELOC dataset (FICO, 2018) (top table) and COMPAS dataset (Jeff Larson et al., 2016) (bottom table). The setup of the experiments are as follows. We train models for binary clas-


⁵The code is available on  <https://github.com/youlei202/distributional-counterfactual-explanation>

Table 1: [*HELOC (top table) and COMPAS (bottom table)*] The rows with considerably low coverage scores (≤ 0.8) are marked gray. In each column, we use bold text to highlight the row with the best performance, ignoring all gray ones, as one can always gain good performance in cost and proximity by sacrificing coverage, losing comparability. The model test accuracy is stated. The experiments are averaged over 10 runs.

Model	Algo.	Cover.	Cost							Proximity		Time (s)
			AReS Cost	% Difference at Percentiles					OT	MMD		
				0-15	15-30	30-70	70-85	85-100				
DNN (74.9%)	AReS	0.019	0.038	0.000	0.187	43.83	0.321	0.000	0.000	0.000	12	
	Globe	0.962	3.346	101.6	45.08	515.8	95.56	230.5	8.521	0.039	5.3	
	DiCE	0.796	18.41	100.0	100.0	326.0	12.04	30.68	0.324	0.107	7235	
	Discount	0.981	22.87	7.801	8.183	265.0	9.422	6.325	0.202	0.036	632	
RBFNet (73.6%)	AReS	0.058	0.049	0.000	1.002	6.000	0.418	0.000	0.002	0.001	11	
	Globe	0.038	3.302	41.93	28.28	87.70	57.29	117.8	2.899	0.039	4.9	
	DiCE	0.174	10.54	100.0	100.0	95.28	4.257	32.39	0.330	0.148	2735	
	Discount	0.962	16.22	8.461	21.65	185.5	36.89	19.55	0.563	0.039	621	
SVM (75.0%)	AReS	0.038	0.577	0.000	0.000	0.794	0.935	0.000	0.001	0.000	14	
	Globe	1.000	3.600	155.1	95.49	152.2	34.98	178.6	13.72	0.039	4.8	
	DiCE	1.000	13.01	100.0	100.0	636.7	44.13	30.36	0.514	0.130	5767	
	Discount	1.000	4.357	5.591	14.07	256.6	16.63	9.811	0.342	0.036	244	

Model	Algo.	Cover.	Cost						Proximity		Time (s)
			AReS Cost	Cat. Diff.	Num. Distribution Shift %				OT	MMD	
					Priors Count		Time Served				
					Mean	Std	Mean	Std			
DNN (67.1%)	AReS	0.103	6.162	0.241	79.20	87.61	82.49	89.06	0.130	0.169	10
	Globe	1.000	0.785	-	-	-	1729	-	8.007	0.220	4.4
	DiCE	0.939	7.678	0.485	78.78	70.11	64.07	80.59	0.406	0.369	503
	Discount	0.976	4.716	0.156	59.69	8.999	85.29	20.88	0.130	0.116	125
RBFNet (66.9%)	AReS	0.143	2.345	0.040	0.000	0.000	0.000	0.000	0.020	0.025	9.3
	Globe	0.690	2.827	0.000	162.2	0.000	226.3	0.000	0.333	0.133	4.1
	DiCE	0.001	6.653	0.297	46.99	67.96	49.47	78.10	0.269	0.270	544
	Discount	0.912	6.158	0.200	163.88	11.71	54.26	0.118	0.441	0.207	433
SVM (64.7%)	AReS	0.184	2.000	0.324	0.000	0.000	0.000	0.000	0.015	0.019	9.2
	Globe	1.000	1.464	0.000	-	-	3704	-	30.75	0.226	4.2
	DiCE	0.974	5.004	0.172	49.48	68.79	51.85	79.28	0.230	0.228	693
	Discount	0.983	4.758	0.172	53.80	1.649	53.36	1.344	0.141	0.106	138

sifications on the two datasets. Then for each model, we sample an observed distribution \mathbf{x}' from the test set and keep the data points with $\mathbf{y}' = b(\mathbf{x}')$ being **0**. Every explainer is expected to find a counterfactual distribution \mathbf{x} such that $\mathbf{y} = b(\mathbf{x})$ is as close as possible as a distribution to $\mathbf{y}^* = \mathbf{1}$. The metric coverage is defined to be the proportion of the 1 values in \mathbf{y} . The AReS cost metric (Rawal and Lakkaraju, 2020) bins continuous features and it is used to evaluate the cost of moving between two adjacent bins, while its counterpart columns evaluate feature changes in specific percentiles. Namely, the smaller changes, the fewer cost caused by the counterfactual. The distributional proximity between factual and counterfactual is measured by two different metrics that are commonly used for divergence between distributions: OT and maximum mean discrepancy (MMD). AReS (rule-based)

and GLOBE (Ley et al., 2023) (translation-based) are used to benchmark the AReS cost performance, as both algorithms are specifically designed for optimizing this cost metric. DiCE (Mothilal et al., 2020) is used as a gradient-based baseline approach for our proposed *Discount*. Neither DiCE nor *Discount* has any knowledge to the AReS cost information. Gray rows in Table 1 are not considered for comparison due to low (≤ 0.8) coverage, because it is trivial for any algorithm to sacrifice coverage for better performance in any other metric.

In Table 1 (top), GLOBE outperforms the others in terms of AReS cost with reasonable coverage, as expected. The columns under “% Difference at Percentiles” evaluates the percentage change in the value of the feature in the counterfactual compared to the factual in a specific percentile, being averaged across all

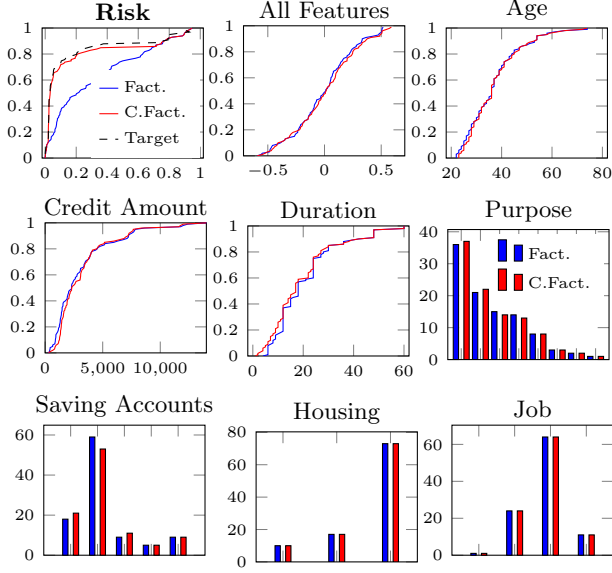


Figure 2: [German-Credit, DNN] The x-axis is feature/target value and the y-axis is quantile/quantities. The first plot “Risk” shows the model’s output distribution. The second plot “All Features” shows the quantiles of the 1D projected (by Θ) factual and counterfactual distributions. The other plots show marginal distributions for each feature, where numerical ones are shown by quantile and categorical by histogram. Factual risk (average) is 31.3% and counterfactual 17.5%.

features. With similar coverage, an algorithm achieving smaller values in these columns is more desirable. Compared to the AReS cost column that simply assumes uniform cost for the whole distribution spectrum of a feature, these columns may serve as an arguably better metric in practice—moving a value around the median should be easier than doing so at the distribution tails (i.e. extreme values), hence being with lower cost. *Discount* remains stable under different models in terms of counterfactual coverage.

Table 1 (bottom) shows similar results, but for *COMPAS*, where most of the features are categorical (one-hot encoded as binary columns). We separately evaluate the action costs of categorical features (abbreviated as Cat.) and the two numerical features, “Priors Count” and “Time Served”. The categorical difference (Cat. Diff) is defined as the average absolute difference (ranging from 0 to 1) between factual and counterfactual data points for all categorical features. *Discount* significantly outperforms the others in both categorical and numerical feature action costs and exceeds DiCE in AReS cost. It is worth noting that *Discount* results in significantly better coverage stability and generally outperforms DiCE in other cost metrics, as well as proximity.

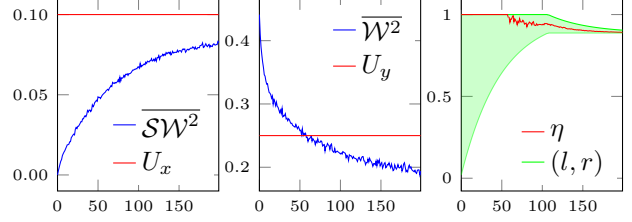


Figure 3: [Cardiovascular Disease, DNN] Convergence of *Discount* with Interval Narrowing. The optimization starts from a point that is near to the factual \mathbf{x}' . At the beginning η stays at $r = 1$ due to the violation of the chance constraint of y , such that the optimization leans entirely towards bringing y to y^* closer gradually. When \overline{W}^2 is below U_2 at iteration 57, a feasible solution is found. Then η is optimized within $[l, r]$ to balance the gaps $U_x - \overline{SW}^2$ and $U_y - \overline{W}^2$, until the algorithm converges.

Discount achieves the best distributional proximity In Table 1, the two columns OT and MMD suggest that *Discount* results in better proximity than the others, with moderate runtime. Figure 2 does visualization for distributional counterfactual proximity and the corresponding counterfactual effect by *Discount*. The figure is obtained by training a DNN on the *German-Credit* dataset with all features. We sample 100 data points from the test data set as the factual distribution, then apply the proposed *Discount* on all training features to obtain the corresponding counterfactual distribution for explanation. Our target \mathbf{y}^* is generated by a Beta distribution that represents a group of customers with very low risk, shown as the dashed black curve. *Discount* achieves this target while having the feature distribution of the counterfactual resembles the one of the factual.

Discount convergence visualization Figure 3 demonstrates the convergence behavior of *Discount*, where η is computed by Interval Narrowing in Algorithm 2. We argue that the convergence behavior of Set Shrinking in Algorithm 3 is similar (guaranteed by Theorem 5.1). Since the interval $[l, r]$ is straightforward to visualize, the convergence behavior of Interval Narrowing is therefore selected to be shown here.

7 Conclusions

We have broadened the scope of CE by introducing it in a distributional context, termed DCE, under a statistically rigorous framework. The numerical results demonstrate the effectiveness of this method. Some explorations on geometric interpretations as well as unresolved challenges are discussed in Appendix G.

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Checklist

- For all models and algorithms presented, check if you include:
 - A clear description of the mathematical setting, assumptions, algorithm, and/or model. [Yes]
 - An analysis of the properties and complexity (time, space, sample size) of any algorithm. [Yes]
 - (Optional) Anonymized source code, with specification of all dependencies, including external libraries. [Yes]
- For any theoretical claim, check if you include:
 - Statements of the full set of assumptions of all theoretical results. [Yes]
 - Complete proofs of all theoretical results. [Yes]
 - Clear explanations of any assumptions. [Yes]
- For all figures and tables that present empirical results, check if you include:
 - The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL). [Yes]
 - All the training details (e.g., data splits, hyperparameters, how they were chosen). [Yes]
 - A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times). [Not Applicable]
Explanations: This question relates to Table 1 and Table 2. The rationale is that the significance is evident, as the substantial differences between the values across methods are clear.
 - A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider). [Yes]
- If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
 - Citations of the creator If your work uses existing assets. [Yes]
 - The license information of the assets, if applicable. [Not Applicable]
 - New assets either in the supplemental material or as a URL, if applicable. [Not Applicable]
 - Information about consent from data providers/curators. [Not Applicable]
 - Discussion of sensible content if applicable, e.g., personally identifiable information or offensive content. [Not Applicable]
- If you used crowdsourcing or conducted research with human subjects, check if you include:
 - The full text of instructions given to participants and screenshots. [Not Applicable]
 - Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable. [Not Applicable]

- (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation. [Not Applicable]

Distributional Counterfactual Explanations With Optimal Transport: Supplementary Materials

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A Related Work

The pioneering study by (Wachter et al., 2017) is a seminal work in the field of CE and has gained notable recognition. This study approaches CE through a minimization problem, laying the foundation for subsequent explorations in the field. A comprehensive overview of the CE literature is presented in the works of (Guidotti, 2022) and (Bodria et al., 2023). Our focus aligns with the model-agnostic optimization approach for generating counterfactuals as proposed by (Wachter et al., 2017). Several studies have explored the generation of multiple counterfactuals in one shot (Ustun et al., 2019; Karimi et al., 2020; Mothilal et al., 2020; Pawelczyk et al., 2020; Brughmans et al., 2023), providing insight into the explanation of individual factual instances.

Recent developments in the field have seen a growing interest in group-based CE. (Rawal and Lakkaraju, 2020) introduced a framework for generating CE for sub-populations within datasets. (Plumb et al., 2020) proposed a counterfactual-summary method for explaining subgroup data points. Furthermore, (Warren et al., 2023) developed a novel approach for creating group-based counterfactual explanations (GCE), focusing on common feature differences among similar individuals. (Carrizosa et al., 2024) takes a stakeholder’s point of view to explain the necessity of considering GCE.

In (Kulinski and Inouye, 2023; Koebler et al., 2023), the authors target interpreting the distribution shift phenomenon and monitoring that. We remark that leveraging methods like Kulinski and Inouye (2023); Koebler et al. (2023) post hoc to interpret the distributions and transportation maps produced by our proposed DCE could provide qualitative insights, which is further discussed in Appendix G.

To our knowledge, no prior work has established a theoretical framework to ensure that the generated group of counterfactual data points is in provable proximity to the factual distribution. Our work addresses this critical gap by embedding statistical rigor into the CE framework, providing guarantees for distributional similarity.

B Proof of Theorem 3.2: UCL for Problem Solving

Theorem B.1 (Theorem 3.2 in the main text). *Let $\delta \in (0, 1/2)$ be a trimming constant, the following inequalities hold:*

1. For $\mathcal{W}^2(b(\mathbf{x}), y^*)$ in (3c), we have

$$\mathbb{P} \left[\mathcal{W}^2(b(\mathbf{x}), y^*) \leq \frac{1}{1 - 2\delta} \int_{\delta}^{1-\delta} D(u) du \right] \geq 1 - \frac{\alpha}{2}, \quad (17)$$

$$\text{where } D(u) \triangleq \max \left\{ F_{y,n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{y^*,n}^{-1}(q_{\alpha,n}(u)), F_{y^*,n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{y,n}^{-1}(q_{\alpha,n}(u)) \right\}. \quad (18)$$

2. For $\mathcal{SW}^2(\mathbf{x}, \mathbf{x}')$ in (3b), let the projection vectors $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N$ be independent and identically distributed samples from a distribution σ on the unit sphere \mathbb{S}^{d-1} . Let σ_N denote the empirical measure associated with these samples. Then,

$$\mathbb{P} \left[\mathcal{SW}^2(\mathbf{x}, \mathbf{x}') \leq \frac{1}{1-2\delta} \int_{\mathbb{S}^{d-1}} \int_{\delta}^{1-\delta} D_{\boldsymbol{\theta},N}(u) du d\sigma_N(\boldsymbol{\theta}) \right] \geq 1 - \frac{\alpha}{2} \quad (19)$$

$$\text{where } D_{\boldsymbol{\theta},N}(u) \triangleq \max \left\{ F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{\boldsymbol{\theta}^\top \mathbf{x}',n}^{-1}(q_{\alpha,n}(u)), F_{\boldsymbol{\theta}^\top \mathbf{x}',n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}(q_{\alpha,n}(u)) \right\}. \quad (20)$$

Here, $F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}$ denotes the empirical quantile function of $\boldsymbol{\theta}^\top \mathbf{x}_i$ for $i = 1, \dots, n$, and similarly for $F_{\boldsymbol{\theta}^\top \mathbf{x}',n}^{-1}$.

Proof. The proof is a sketch of the key results of (Manole et al., 2022, Section 4), with necessary modifications in details to suit the need of this paper. The proof applies for δ -trimmed ($\delta \in (0, 1/2)$) empirical distributions, without assumptions on the knowledge of the distributions. The trimming is necessary, such that certain amount of data points are left out for capturing the tail behavior of the distributions. Note that (5) reads

$$\inf \mathbb{P}_n(F_n^{-1}(q_{\alpha,n}(u)) \leq F^{-1}(u) \leq F_n^{-1}(\bar{q}_{\alpha,n}(u)), \forall u \in (0, 1)) \geq 1 - \frac{\alpha}{2}, \quad (21)$$

which indeed establishes a confidence band for the two sequences of functions, $q_{\alpha,n}$ and $\bar{q}_{\alpha,n}$. The proof then pivots on the assertion that the 1D 2-Wasserstein distance can be characterized as the L^2 -norm of the quantile functions of y ($y = b(\mathbf{x})$) and \mathbf{x}' ($y' = b(\mathbf{x}')$), namely⁶,

$$\mathcal{W}^2(\gamma_1, \gamma_2) = \int_0^1 |F_{\gamma_1,n}^{-1}(u) - F_{\gamma_2,n}^{-1}(u)|^2 du. \quad (22)$$

holds for any 1D empirical distribution γ_1 and γ_2 . Then, the uniform quantile bounds can be used to construct the two sequences functions $q_{\alpha,n}$ and $\bar{q}_{\alpha,n}$ (Shorack and Wellner, 2009), such that the above inequality (21) gets hold. Straightforwardly, this yields a UCL on $F_{\gamma_1,n}^{-1}(u)$ and $F_{\gamma_2,n}^{-1}(u)$, and therefore a UCL on the absolute difference between them, i.e. $|F_{y,n}^{-1}(u) - F_{y^*,n}^{-1}(u)|$. That is

$$|F_{y,n}^{-1}(u) - F_{y^*,n}^{-1}(u)| \leq \max \left\{ F_{y,n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{y^*,n}^{-1}(q_{\alpha,n}(u)), F_{y^*,n}^{-1}(\bar{q}_{\alpha,n}(u)) - F_{y,n}^{-1}(q_{\alpha,n}(u)) \right\} = D(u)$$

This inequality holds probabilistically with confidence level $1 - \alpha/2$ ⁷. Consequently, by (22), the UCL on $\mathcal{W}^2(b(\mathbf{x}), y^*)$ is hence derived by taking the square of the UCL on $|F_{y,n}^{-1}(u) - F_{y^*,n}^{-1}(u)|$ then taking integral over u . Hence, given $y = b(\mathbf{x})$.

$$\mathcal{W}^2(b(\mathbf{x}), y^*) = \int_0^1 |F_{b(\mathbf{x}),n}^{-1}(u) - F_{y^*,n}^{-1}(u)|^2 du \leq \frac{1}{1-2\delta} \int_{\delta}^{1-\delta} D(u) du, \quad (23)$$

where the correction factor $1/(1-2\delta)$ on the right-hand side makes it a trimmed estimator, such that a certain percentage (determined by δ) of the tail values of the distributions can be disregarded in the computation. Hence

⁶This equation is exactly discussed in (4) in Section 3.

⁷To explain this, notice that

$$\inf \mathbb{P}_n(F_y^{-1}(u) \leq F_{y,n}^{-1}(\bar{q}_{\alpha,n}(u)), \forall u \in (0, 1)) \geq 1 - \frac{\alpha}{4}, \text{ and}$$

$$\inf \mathbb{P}_n(F_{y^*}^{-1}(u) \leq F_{y^*,n}^{-1}(\bar{q}_{\alpha,n}(u)), \forall u \in (0, 1)) \geq 1 - \frac{\alpha}{4}.$$

Hence the probability of $|F_y^{-1}(u) - F_{y^*}^{-1}(u)|$ being no larger than the maximum of the two possible differences between $F_{y,n}^{-1}(\bar{q}_{\alpha,n}(u))$ and $F_{y^*,n}^{-1}(\bar{q}_{\alpha,n}(u))$, is $1 - \frac{\alpha}{2}$.

we obtain the UCL in (17), i.e.

$$\mathbb{P} \left[\mathcal{W}^2(b(\mathbf{x}), y^*) \leq \frac{1}{1-2\delta} \int_{\delta}^{1-\delta} D(u) du \right] \geq 1 - \frac{\alpha}{2}. \quad (24)$$

Next, we derive the UCL in (19). Consider using Monte Carlo for computing the Sliced Wasserstein distance:

$$\mathcal{SW}^2(\mathbf{x}, \mathbf{x}') = \frac{1}{N} \sum_{k=1}^N \mathcal{W}^2(\boldsymbol{\theta}^\top \mathbf{x}, \boldsymbol{\theta}^\top \mathbf{x}')$$

We construct $\underline{q}_{\alpha,n}$ and $\bar{q}_{\alpha,n}$ independently for each $\boldsymbol{\theta}$ ($\boldsymbol{\theta} \in \Theta$) projected 1D distributions $\boldsymbol{\theta}^\top \mathbf{x}$ and $\boldsymbol{\theta}^\top \mathbf{x}'$ based on the confidence band below

$$\inf \mathbb{P}_n(F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}(\underline{q}_{\alpha,n}(u)) \leq F_{\boldsymbol{\theta}^\top \mathbf{x}}^{-1}(u) \leq F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}(\bar{q}_{\alpha,n}(u)), \forall u \in (0, 1)) \geq 1 - \frac{\alpha}{2N}.$$

where $F_{\boldsymbol{\theta},n}^{-1}$ is the (empirical) quantile function for the $\boldsymbol{\theta}$ -projected distribution and $N = |\Theta|$. Then, for any $\boldsymbol{\theta}$,

$$\mathcal{W}^2(\boldsymbol{\theta}^\top \mathbf{x}, \boldsymbol{\theta}^\top \mathbf{x}') = \int_0^1 |F_{\boldsymbol{\theta}^\top \mathbf{x},n}^{-1}(u) - F_{\boldsymbol{\theta}^\top \mathbf{x}',n}^{-1}(u)|^2 du \leq \underbrace{\frac{1}{1-2\delta} \int_{\delta}^{1-\delta} D_{\boldsymbol{\theta},N}(u) du}_{\text{The UCL of } \mathcal{W}^2(\boldsymbol{\theta}^\top \mathbf{x}, \boldsymbol{\theta}^\top \mathbf{x}')} du$$

holds with probability $1 - \alpha/2N$. By applying the Bonferroni correction across the N projection directions $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N$, we adjust the significance level for each individual test to $\frac{\alpha}{2N}$. This ensures that the combined probability of any of the UCL failing is at most $\frac{\alpha}{2}$. Therefore, with probability at least $1 - \frac{\alpha}{2}$, all individual UCL hold simultaneously. Consequently, conditioned on these fixed projection directions, the inequality below holds almost surely,

$$\inf_{\mathbf{x}, \mathbf{x}'} \mathbb{P} \left[\mathcal{SW}^2(\mathbf{x}, \mathbf{x}') \leq \underbrace{\frac{1}{1-2\delta} \int_{\mathbb{S}^{d-1}} \int_{\delta}^{1-\delta} D_{\boldsymbol{\theta},N}(u) du d\sigma_N(\boldsymbol{\theta})}_{\text{The UCL of } \mathcal{SW}^2(\mathbf{x}, \mathbf{x}')} \mid \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N \right] \geq 1 - \frac{\alpha}{2}.$$

Hence the conclusion. \square

C Proof of Theorem 4.1: Partial Optimality Condition

Theorem C.1 (Theorem 4.1 in the main text). *Assume that the optimization problem in (14) is feasible, i.e. (14b) and (14d) can be achieved simultaneously with at least $1 - \alpha/2$. Then, there exists a value $\eta^* \in [0, 1]$ such that the solution \mathbf{x}^* obtained by optimizing $Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu} \mid \eta^*)$, defined as*

$$\mathbf{x}^* \triangleq \arg \min_{\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}} Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}, \eta^*),$$

is also the optimal solution to the original problem (14), that is,

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} \varphi \quad \text{s.t. (14b) - (14d)}.$$

Proof. Remark that the minimization of $Q(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\nu}, \eta)$ is equivalent to the optimization below with respect to \mathbf{x} :

$$\min_{\mathbf{x}} Q(\mathbf{x}, \eta) = (1 - \eta) \cdot \inf_{\boldsymbol{\mu}} Q_x(\mathbf{x}, \boldsymbol{\mu}) + \eta \cdot \inf_{\boldsymbol{\nu}} Q_y(\mathbf{x}, \boldsymbol{\nu}).$$

Since the problem (14) is feasible, there exists at least one pair (\mathbf{x}, P) that satisfies the constraints (14b)-(14d) for any η in the interval $[0, 1]$. Given that Q_x and Q_y are continuous in their respective variables, the above definition ensures that $Q(\mathbf{x}, \eta)$ is continuous in \mathbf{x} for any fixed η .

Algorithm 3 Set Shrinking

Require: $\overline{\mathcal{SW}^2}$, $\overline{\mathcal{W}^2}$, U_x, U_y , $\mathcal{K} = \{\eta_k\}_{k=1}^K$
Ensure: η

- 1: $\eta \leftarrow$ Balance the gaps $U_x - \overline{\mathcal{SW}^2}$ and $U_y - \overline{\mathcal{W}^2}$
 - 2: **if** $K > 1$ **then**
 - 3: $\mathcal{K} \leftarrow \mathcal{K} \setminus \{\eta\}$
 - 4: **end if**
 - 5: Save \mathcal{K} as the input of the next run
 - 6: **return** η
-

Let us consider the set S of all η such that the corresponding $\mathbf{x}_\eta = \arg \min_x Q(\mathbf{x}, \eta)$ is feasible for (14). Since the constraints (14b)-(14d) are continuous in x , and x_η is continuous in η , the set S is nonempty and compact. Thus, there exists a minimum and maximum η in S , denoted as η_{\min} and η_{\max} respectively.

We now show that at least for one $\eta^* \in [\eta_{\min}, \eta_{\max}]$, the \mathbf{x}_{η^*} is optimal for (14). Note that η is a parameter that interpolates between $Q_x(\mathbf{x}, \boldsymbol{\mu})$ and $Q_y(\mathbf{x}, \boldsymbol{\nu})$. Since $Q(\mathbf{x}, \eta)$ is continuous in \mathbf{x} and η , and the feasible region is closed and bounded, by the Extreme Value Theorem, $Q(\mathbf{x}, \eta)$ achieves its minimum for some \mathbf{x}^* in the feasible region of (14).

Hence, there exists an $\eta^* \in [\eta_{\min}, \eta_{\max}]$ such that $\mathbf{x}^* = \arg \min_x Q(\mathbf{x}, \eta^*)$ satisfies all the constraints (14b)-(14d) and thus is optimal for (14). This concludes the proof. \square

D Optimization of η

We explore the optimization strategy for η , as outlined in line 1 of both Algorithm 3 and Algorithm 2. The parameter η , as defined in (15), plays a crucial role in determining the descent direction during the optimization process, as seen in line 8 of Algorithm 1. The optimization aims to adjust this direction to fulfill the dual chance constraints (3b) and (3c), effectively maximizing the probability of meeting both constraints.

We first consider the Interval Narrowing in Algorithm 2. The general strategy involves the following steps:

1. When either $U_x - \overline{\mathcal{SW}^2}$ or $U_y - \overline{\mathcal{W}^2}$ is negative (indicating constraint violation), while the other is non-negative, priority is given to addressing the constraint that is violated (i.e., the one with the negative value). In this case, optimizing the non-violated constraint is less urgent.
2. If both $U_x - \overline{\mathcal{SW}^2}$ and $U_y - \overline{\mathcal{W}^2}$ are negative or positive, η is assigned a value based on these gaps. Let $a = U_x - \overline{\mathcal{SW}^2}$ and $b = U_y - \overline{\mathcal{W}^2}$. The value of η is then determined as follows:

$$\eta = \begin{cases} \frac{b}{a+b} & \text{if } a \text{ and } b \text{ are both negative} \\ \frac{a}{a+b} & \text{if } a \text{ and } b \text{ are both non-negative (but not both zero)} \\ 0.5 & \text{if both } a \text{ and } b \text{ are exactly zero (unlikely to happen numerically in computation)} \end{cases} \quad (25)$$

In the case where both a and b are negative, the term with the larger absolute value (hence, more significantly violating its constraint) receives a greater weight in the optimization of (15). Conversely, if both are non-negative (and not both zero), it indicates that both constraints are satisfied, but the one with the smaller absolute value is closer to its limit, and thus receives more attention in the optimization.

Then, we consider the Set Shrinking in Algorithm 3.

Algorithm 3 provides a way to select η from a pre-defined set \mathcal{K} consisting of multiple candidate values of η . If one value is expected to be selected more than once, then it is duplicated with corresponding copies in \mathcal{K} . Line 1 optimizes η towards balancing the satisfactory of UCLs (10) and (11), see Appendix D for how the balance is achieved, in details. The set \mathcal{K} shrinks in every run as the selected η gets removed from it, until $K = 1$ and the last η is used until convergence. The main different is that η must be selected from \mathcal{K} . One could perform sorting on \mathcal{K} first to obtain a $\mathcal{K}_{\text{sorted}}$, and then use bisection search to find the element in $\mathcal{K}_{\text{sorted}}$ that is close to η in (25).

E Proof of Theorem 5.1: Convergence Rate

Theorem E.1 (Theorem 5.1 in the main text). *Let $\{\mathbf{v}^t\}_{t=0}^T$ denote the iterates of Algorithm 1 combined with either Algorithm 3 or Algorithm 2, using a stepsize $\tau = \frac{1}{L}$. Define*

$$C \triangleq \sqrt{2L} + \rho L \cdot \sqrt{\frac{2}{L}} \text{ and } B \triangleq \sup_{\mathbf{v}} \{Q_x(\mathbf{v}), Q_y(\mathbf{v})\}. \quad (26)$$

where B is ascertained finite with finite b . Then, the following convergence guarantees hold:

$$\min_{t=0,1,\dots,T} \left\| \tilde{\nabla} Q(\mathbf{v}^t, \eta^t) \right\| \leq C \left[\frac{1}{T+1} (Q_x(\mathbf{v}^0) + Q_y(\mathbf{v}^0) + \Delta) \right]^{\frac{1}{2}}, \quad (27)$$

where

$$\Delta = \begin{cases} 0, & \text{if Algorithm 3 is used,} \\ \frac{r-l}{\kappa} B, & \text{if Algorithm 2 is used.} \end{cases}$$

Proof. Consider the iteration process of *Discount* where η sequentially gets to be $\eta_{(1)}, \eta_{(2)}, \dots, \eta_{(K)}$, with $\mathcal{K} = \{\eta_{(1)}, \eta_{(2)}, \dots, \eta_{(K)}\}$. Correspondingly, the function Q defined in (15) given each of these η values are denoted by $Q_{(1)}, Q_{(2)}, \dots, Q_{(K)}$. Given that each value of η may remain constant for several iterations before transitioning to the next, we denote T_1, T_2, \dots, T_K as the respective number of iterations for which it persists.

Consider $Q_{(1)}$ under $\eta_{(1)}$. It is shown in (Peng and Vidal, 2023, Proof of Theorem 4) that the sum of the square of the Riemannian gradient of $Q_{(1)}$ on \mathbf{v} is bounded by $(b-1) \cdot C_{b-1}^2 \cdot [Q_{(1)}(\mathbf{v}^0) - Q_{(1)}(\mathbf{v}^{T_1})]$, where b is the number of blocks of which the variables are subject to optimization. We have two blocks in *Discount*, \mathbf{x} and $[\boldsymbol{\mu}, \boldsymbol{\nu}]$, where the former is subject to Riemannian gradient descent (i.e. lines 8 and 9) and the latter Exact Minimization (i.e. solving the OT problem to the exact minimum in lines 3 and 4). Hence $b = 2$, and we can use C without index $b-1$ to represent the bound, and the value of this C equals exactly the one defined in (26) (Peng and Vidal, 2023, Proof of Theorem 4). This gives the first inequality below.

$$\begin{aligned} \sum_{t=0}^{T_1-1} \left\| \tilde{\nabla} Q_{(1)}(\mathbf{v}^t) \right\|^2 &\leq C^2 [Q_{(1)}(\mathbf{v}^0) - Q_{(1)}(\mathbf{v}^{T_1})] \\ &\stackrel{(i)}{=} C^2 \left\{ [(1 - \eta_{(1)})Q_x(\mathbf{v}^0) + \eta_{(1)}Q_y(\mathbf{v}^0)] - [(1 - \eta_{(1)})Q_x(\mathbf{v}^{T_1}) + \eta_{(1)}Q_y(\mathbf{v}^{T_1})] \right\} \\ &\stackrel{(ii)}{\leq} C^2 \{ [Q_x(\mathbf{v}^0) - Q_x(\mathbf{v}^{T_1})] + [Q_y(\mathbf{v}^0) - Q_y(\mathbf{v}^{T_1})] \} \end{aligned} \quad (28)$$

Note that (i) holds by the definition of Q in (15), and (ii) by $0 \leq \eta \leq 1$, as well as the non-negativity of $Q_x(\mathbf{v}^0) - Q_x(\mathbf{v}^{T_1})$ and $Q_y(\mathbf{v}^0) - Q_y(\mathbf{v}^{T_1})$. This non-negativity is due to the fact that the Riemannian gradient descent yields a decreasing objective.

Similarly, we can apply the same conclusions to $Q_{(2)}, Q_{(3)} \dots Q_{(K)}$ and obtain

$$\begin{aligned} \sum_{t=T_1}^{T_2-1} \left\| \tilde{\nabla} Q_{(2)}(\mathbf{v}^t) \right\|^2 &\leq C^2 [Q_{(2)}(\mathbf{v}^{T_1}) - Q_{(2)}(\mathbf{v}^{T_2})] \\ &\leq C^2 \{ [Q_x(\mathbf{v}^{T_1}) - Q_x(\mathbf{v}^{T_2})] + [Q_y(\mathbf{v}^{T_1}) - Q_y(\mathbf{v}^{T_2})] \}, \\ &\vdots \\ \sum_{t=T_{K-1}}^{T_K-1} \left\| \tilde{\nabla} Q_{(K)}(\mathbf{v}^t) \right\|^2 &\leq C^2 [Q_{(K)}(\mathbf{v}^{T_{K-1}}) - Q_{(K)}(\mathbf{v}^{T_K})] \\ &\leq C^2 \{ [Q_x(\mathbf{v}^{T_{K-1}}) - Q_x(\mathbf{v}^{T_K})] + [Q_y(\mathbf{v}^{T_{K-1}}) - Q_y(\mathbf{v}^{T_K})] \}. \end{aligned} \quad (29)$$

Denote $T = T_K - 1$. For any $t = 0, 1, \dots, T$, let ϱ_t be the corresponding index of η at the iteration t . Summing up the inequalities above, we obtain

$$\begin{aligned}
 & \sum_{t=0}^T \left\| \tilde{\nabla} Q_{(\varrho_t)} \right\|^2 \\
 & \leq C^2 \left\{ \left[Q_x(\mathbf{v}^0) - Q_x(\mathbf{v}^{T_1}) + Q_x(\mathbf{v}^{T_1}) - Q_x(\mathbf{v}^{T_2}) + \dots + Q_x(\mathbf{v}^{T_{K-1}}) - Q_x(\mathbf{v}^{T_K}) \right] \right. \\
 & \quad \left. + \left[Q_y(\mathbf{v}^0) - Q_y(\mathbf{v}^{T_1}) + Q_y(\mathbf{v}^{T_1}) - Q_y(\mathbf{v}^{T_2}) + \dots + Q_y(\mathbf{v}^{T_{K-1}}) - Q_y(\mathbf{v}^{T_K}) \right] \right\} \\
 & = C^2 \left\{ \left[Q_x(\mathbf{v}^0) - Q_x(\mathbf{v}^{T_K}) \right] + \left[Q_y(\mathbf{v}^0) - Q_y(\mathbf{v}^{T_K}) \right] \right\} \\
 & \stackrel{(i)}{\leq} C^2 \left[Q_x(\mathbf{v}^0) + Q_y(\mathbf{v}^0) \right]
 \end{aligned} \tag{30}$$

The inequality (i) holds due to the non-negativity of Q_x and Q_y , as defined in (12) and (13) respectively. Notice that the minimum of $\tilde{\nabla} Q_{\varrho_t}$ is bounded by this summation. Therefore,

$$\min_{t=0,1,\dots,T} \left\| \tilde{\nabla} Q_{(\varrho_t)} \right\|^2 \leq \frac{1}{T+1} \sum_{t=1}^T \left\| \tilde{\nabla} Q_{(\varrho_t)} \right\|^2 \leq \frac{C^2}{T+1} \left[Q_x(\mathbf{v}^0) + Q_y(\mathbf{v}^0) \right]$$

Taking root square of both side yields the convergence rate (27) with $\delta = 0$.

We use the same notations as for the proof of the convergence for Algorithm 2. Suppose η sequentially gets to be $\eta_{(1)}, \eta_{(2)}, \dots$, corresponding to functions $Q_{(1)}, Q_{(2)}, \dots$. Let the initial interval in Interval Narrowing be $[l, r]$. At each iteration of the algorithm, the interval is reduced by a fixed proportion κ where $0 < \kappa < 1$. After t iterations, the length of the interval will be $(1 - \kappa)^t(r - l)$.

Consider two arbitrary iteration steps corresponding to η_k and $\eta_{(h)}$, where $h > k$ in the sequence of η . By the definition of Q in (15), we have

$$Q_{(k)}(\mathbf{v}) = (1 - \eta_k) \cdot Q_x(\mathbf{v}) + \eta_k \cdot Q_y(\mathbf{v}) \text{ and } Q_{(h)}(\mathbf{v}) = (1 - \eta_{(h)}) \cdot Q_x(\mathbf{v}) + \eta_{(h)} \cdot Q_y(\mathbf{v})$$

Next, we show that the gap between $Q_{(k)}(\mathbf{v})$ and $Q_{(h)}(\mathbf{v})$ is bounded by the interval length and B . Let T_k be the number of elapsed iterations by the moment of η_k .

$$\begin{aligned}
 \left| Q_{(k)}(\mathbf{v}) - Q_{(h)}(\mathbf{v}) \right| &= \left| (1 - \eta_k) \cdot Q_x(\mathbf{v}) + \eta_k \cdot Q_y(\mathbf{v}) - (1 - \eta_{(h)}) \cdot Q_x(\mathbf{v}) - \eta_{(h)} \cdot Q_y(\mathbf{v}) \right| \\
 &= \left| (\eta_{(h)} - \eta_k) Q_x(\mathbf{v}) + (\eta_k - \eta_{(h)}) Q_y(\mathbf{v}) \right| \\
 &\stackrel{(i)}{\leq} |\eta_{(h)} - \eta_k| \cdot \left| Q_x(\mathbf{v}) - Q_y(\mathbf{v}) \right| \stackrel{(ii)}{\leq} (1 - \kappa)^{T_k}(r - l) \left| Q_x(\mathbf{v}) - Q_y(\mathbf{v}) \right| \stackrel{(iii)}{\leq} (1 - \kappa)^{T_k}(r - l) B
 \end{aligned} \tag{31}$$

The step (i) comes from the triangle inequality. The step (ii) holds due to the interval narrowing mechanism. Namely, the interval narrows down to $(1 - \kappa)^{T_k}(r - l)$ when we encounter η_k . Note that $\eta_{(h)}$ is encountered later than η_k , hence the interval at the moment of $\eta_{(h)}$ is a subset of that of η_k . Therefore, the gap between η_k and $\eta_{(h)}$ is no larger than $(1 - \kappa)^{T_k}(r - l)$. The step (iii) holds because of the definition of B ($B \triangleq \sup_{\mathbf{v} \in \mathcal{M}} \{Q_x(\mathbf{v}), Q_y(\mathbf{v})\}$), as well as the fact that Q_x and Q_y are non-negative.

Consider the iteration process in *Discount*. For any $t = 0, 1, \dots, T$, let ϱ_t be the corresponding index of η at the iteration t . We obtain the same inequalities as (28)–(29). The difference is that there are infinite number of such inequalities in Interval Narrowing, rather than the fixed number K as for Set Shrinking. Consider an arbitrary K

in the η sequence $\eta_{(1)}, \eta_{(2)} \dots \eta_{(K)} \dots$ then let $T = T_K - 1$ and sum up all these inequalities:

$$\begin{aligned}
 \sum_{t=0}^T \left\| \tilde{\nabla} Q_{(\varrho_t)}(\mathbf{v}^t) \right\| &\leq C^2 \left\{ \left[Q_{(1)}(\mathbf{v}^0) - Q_{(1)}(\mathbf{v}^{T_1}) \right] + \left[Q_{(2)}(\mathbf{v}^{T_1}) - Q_{(2)}(\mathbf{v}^{T_2}) \right] \right. \\
 &\quad \left. + \dots + \left[Q_{(K)}(\mathbf{v}^{T_{K-1}}) - Q_{(K)}(\mathbf{v}^{T_K}) \right] \right\} \\
 &\leq C^2 \left\{ Q_{(1)}(\mathbf{v}^0) + \left[Q_{(2)}(\mathbf{v}^{T_1}) - Q_{(1)}(\mathbf{v}^{T_1}) \right] + \left[Q_{(3)}(\mathbf{v}^{T_2}) - Q_{(2)}(\mathbf{v}^{T_2}) \right] \right. \\
 &\quad \left. + \dots + \left[Q_{(K)}(\mathbf{v}^{T_{K-1}}) - Q_{(K-1)}(\mathbf{v}^{T_{K-1}}) \right] - Q_{(K)}(\mathbf{v}^{T_K}) \right\} \\
 &\leq C^2 \left\{ Q_{(1)}(\mathbf{v}^0) + \left| Q_{(1)}(\mathbf{v}^{T_1}) - Q_{(2)}(\mathbf{v}^{T_1}) \right| + \left| Q_{(2)}(\mathbf{v}^{T_2}) - Q_{(3)}(\mathbf{v}^{T_2}) \right| \right. \\
 &\quad \left. + \dots + \left| Q_{(K-1)}(\mathbf{v}^{T_{K-1}}) - Q_{(K)}(\mathbf{v}^{T_{K-1}}) \right| - Q_{(K)}(\mathbf{v}^{T_K}) \right\} \\
 &\stackrel{(i)}{\leq} C^2 \left\{ Q_{(1)}(\mathbf{v}^0) + (1 - \kappa)^{T_1}(r - l)B + (1 - \kappa)^{T_2}(r - l)B \right. \\
 &\quad \left. + \dots + (1 - \kappa)^{T_{K-1}}(r - l)B - Q_{(K)}(\mathbf{v}^{T_K}) \right\} \\
 &\stackrel{(ii)}{\leq} C^2 \left\{ Q_{(1)}(\mathbf{v}^0) + (r - l)B \left[1 + (1 - \kappa) + (1 - \kappa)^2 + \dots \right] - Q_{(K)}(\mathbf{v}^{T_K}) \right\} \\
 &\stackrel{(iii)}{\leq} C^2 \left[Q_{(1)}(\mathbf{v}^0) - Q_{(K)}(\mathbf{v}^{T_K}) + \frac{1}{\kappa}(r - l)B \right] \\
 &\stackrel{(iv)}{\leq} C^2 \left[Q_{(1)}(\mathbf{v}^0) + \frac{1}{\kappa}(r - l)B \right] \\
 &\stackrel{(v)}{=} C^2 \left\{ [(1 - \eta_{(1)})Q_x(\mathbf{v}^0) + \eta_{(1)}Q_y(\mathbf{v}^0)] + \frac{1}{\kappa}(r - l)B \right\} \\
 &\stackrel{(vi)}{\leq} C^2 \left[Q_x(\mathbf{v}^0) + Q_y(\mathbf{v}^0) + \frac{1}{\kappa}(r - l)B \right]
 \end{aligned}$$

The step (i) holds because of the inequality (31) for arbitrary two values η_k and $\eta_{(h)}$ ($h > k$), following which we obtain the summation of the geometric series in (ii) ($0 < \kappa < 1$). In step (iii) we take the summation of the series. Step (iv) is because the non-negativity of $Q_{(K)}$. Step (v) is by the definition of Q in (15). Finally, step (vi) is because of $0 < \eta < 1$ as well as the non-negativity of Q_x and Q_y .

Notice that the minimum of $\tilde{\nabla} Q_{\varrho_t}$ is bounded by this summation $\sum_{t=0}^T \left\| \tilde{\nabla} Q_{(\varrho_t)}(\mathbf{v}^t) \right\|$. Therefore, we have

$$\min_{t=0,1,\dots,T} \left\| \tilde{\nabla} Q_{(\varrho_t)} \right\|^2 \leq \frac{1}{T+1} \sum_{t=0}^T \left\| \tilde{\nabla} Q_{(\varrho_t)}(\mathbf{v}^t) \right\| \leq \frac{C^2}{T+1} \left[Q_x(\mathbf{v}^0) + Q_y(\mathbf{v}^0) + \frac{1}{\kappa}(r - l)B \right]$$

We remark that B is finite because of its definition in (26). Note that Q_x and Q_y are continuous on the bounded and compact manifold \mathcal{M}_1 with respect to \mathbf{x} . Since $\boldsymbol{\mu}, \boldsymbol{\nu} \in \Pi$ (namely, each being non-negative and with elements summed up to 1) during the optimization, the two functions $Q_x(\mathbf{v})$ and $Q_y(\mathbf{v})$ are therefore bounded.

Hence the conclusion. \square

F Numerical Results Extended

This subsection extends our nemurical results by quantitative experiments, performed on German Credit (Hofmann, 1994), and Cardiovascular Disease (Halder, 2020).

Clarification of the Metrics in Numerical Results Recall that DCE demonstrates a significant advantage over the baseline methods (AReS, Globe, and DiCE) in Table 1. While these baseline methods were developed to solve different explanation problems, the metrics in Table 1 were chosen to fairly reflect the goals of all methods, rather than being tailored specifically for DCE. Below, we explain the metrics in detail and their relevance:

- *Coverage* is a widely used metric for CE algorithms. It is defined to be the ratio of the number of valid counterfactual data points over the total data points found by a CE algorithm.
- *AReS Cost* was proposed in AReS and is used in both AReS and Globe, defined to be the magnitude of feature changes given known cost on each feature. Both the two algorithms were specifically designed to optimize this metric and have direct knowledge of it. Neither DiCE nor our proposed *Discount* algorithm directly incorporates such knowledge.
- *Percentiles Difference* and *Distribution Shift* These metrics measure the shift in quantile distributions between factual and counterfactual instances. Both *Discount* and DiCE aim to indirectly minimize such shifts:
 - *Discount* does so by minimizing the Optimal Transport (OT) distance between the factual and counterfactual distributions.
 - DiCE minimizes Euclidean distances between factual and counterfactual instances, subject to a soft diversity constraint.
- *OT* and *MMD Proximity*: *Discount* is explicitly designed to optimize OT distance, defined in (1) and (2). MMD is defined as

$$\text{MMD}^2(x, x') = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(x_i, x_j) + \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m k(x'_i, x'_j) - \frac{2}{nm} \sum_{i=1}^n \sum_{j=1}^m k(x_i, x'_j)$$

where k is the gaussian kernel.

While these metrics reflect different aspects of counterfactual explanations, they were not specifically chosen to favor DCE or the *Discount* algorithm. Instead, they were selected to ensure fair evaluation across different CE methods by covering a range of performance goals. Importantly, our results in Table 1 show that even though *Discount* was not specifically designed to optimize metrics like Coverage or AReS Cost, it still performs well on them when OT proximity is optimized. This highlights the versatility and robustness of *Discount* across diverse evaluation criteria. The results demonstrate that DCE and *Discount* not only excel in tasks they were designed for but also perform competitively in tasks aligned with the objectives of the baselines.

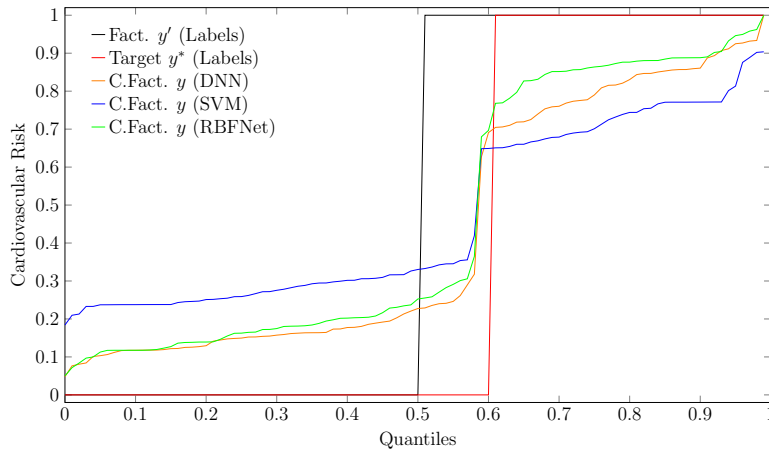


Figure 4: [Cardiovascular Disease] The models are trained on all features whereas the DCE optimization is performed only on age, weight, and height.

Counterfactual Reasoning. Our investigation into the German Credit dataset, depicted in Figure 2 and Figure 5, explores the model’s distinct responses to groups with similar feature distributions. Key observations

include the model’s sensitivity to age and credit amount, where minor variations can result in significant risk alterations, particularly in the 40–50 age group with around 8000 in credit amount. Notably, we identified a counterintuitive behavior where increasing credit amounts paradoxically lowers risk for younger individuals. This suggests a misinterpretation of risk factors by the model, mistaking age-related risk indicators as credit amount related. This is because there are quite many young (age 20–30) people who took a small credit amount for loan in the dataset, and their risk is marked as high because of their age (rather than the fact of taking small credit). Yet the model learns its relation to credit amount, failing to realize this being not causation. Employing DCE, we analyze quantile shifts across features, allowing us to delve into the model’s decision-making process and discern substantial risk profile discrepancies between groups, even with identical distributions in certain features. This approach yields deeper statistical insights into the model’s distributional behavior and its implications.

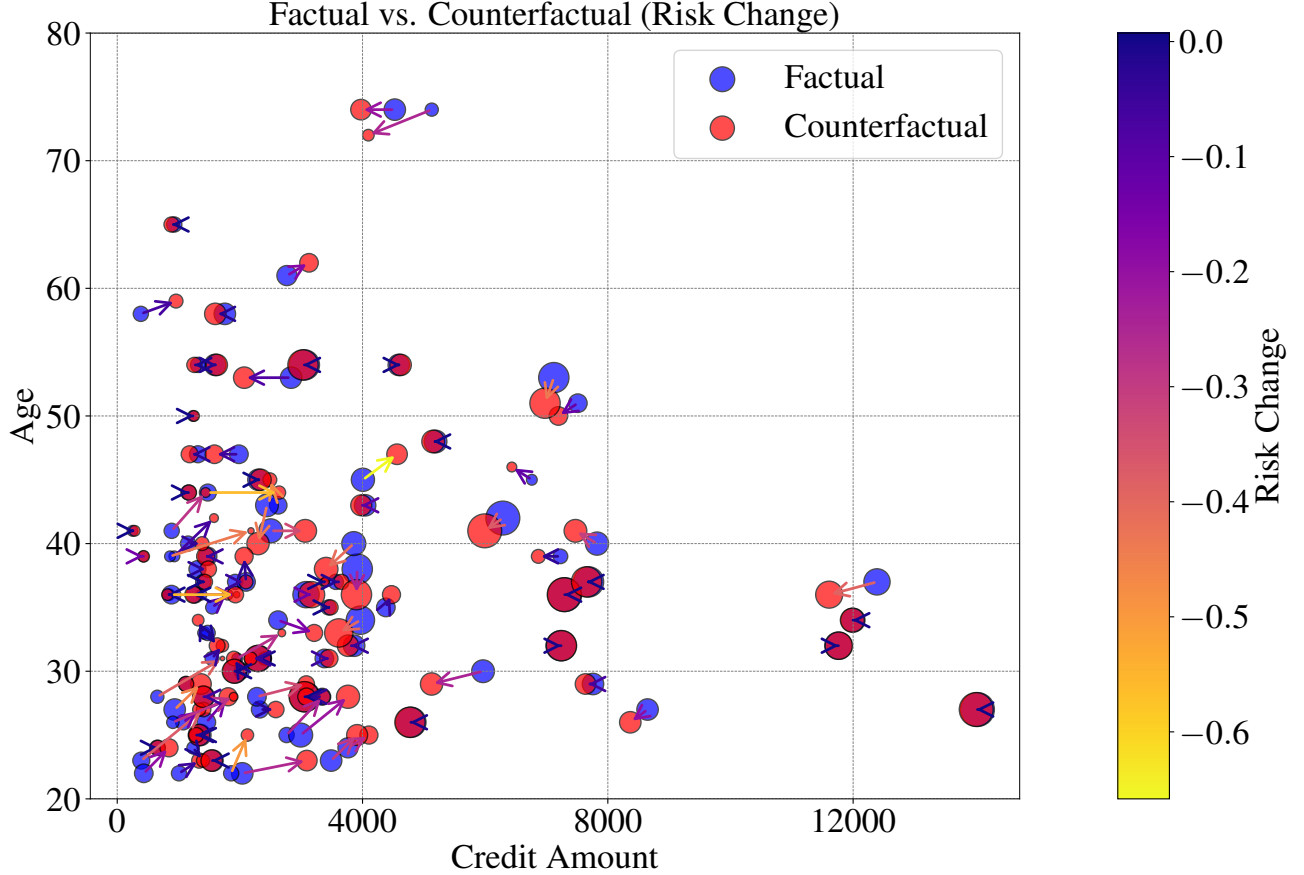


Figure 5: [German-Credit, DNN] Risk with respect to credit amount, age, and duration (indicated by the size of each point). The models are trained on all features whereas the DCE optimization is performed only on credit amount, age, and duration.

In our study with the Cardiovascular Disease dataset, we employed three models: DNN, SVM, and RBFNet, training them on all available features. We then selected a sample of 100 data points from the test set to represent our empirical factual distribution. Specifically, we curated a subset of 100 individuals with low cardiovascular risk to form the target output distribution y^* . The quantile-based comparison of the factual y and target y^* , as shown in Figure 4, underscores the effectiveness of DCE. Notably, the risk profiles of these counterfactual distributions, when converted to binary form, closely align with the target distribution.

We remark such insights for both dataset above are uniquely accessible through a DCE framework, which goes beyond the capabilities of classical or group-based CEs by focusing on distributional shifts and relationships. Additionally, we discussed how the transportation plan μ and ν can be used for reasoning in Appendix G.

Counterfactual Diversity. Additionally, a high diversity score guarantees that the explainer provides a wide range of suggested changes offering users multiple options. In Table 2, the diversity Score is computed as the

Table 2: Performance of counterfactual diversity. For each row, we use bold text to highlight the column with the highest score (hence the best performance). The DPC Score is defined to be the diversity score normalized by OT proximity then multiplied by coverage. The data diversity shows the diversity score computed on the dataset rather than just the counterfactual, for reference. The experiments are averaged over 10 runs.

HELOC (Data Diversity 0.239)									
Metric	DNN			RBF			SVM		
	Globe	DiCE	Discount	Globe	DiCE	Discount	Globe	DiCE	Discount
Diversity Score	0.244	0.003	0.278	0.254	0.295	0.225	0.239	0.001	0.246
DPC Score	0.028	0.007	1.351	0.003	0.156	0.384	0.017	0.001	0.720

COMPAS (Data Diversity 3.266)									
Metric	DNN			RBF			SVM		
	Globe	DiCE	Discount	Globe	DiCE	Discount	Globe	DiCE	Discount
Diversity Score	3.266	1.738	3.861	3.299	1.964	3.339	3.361	2.011	3.448
DPC Score	0.408	4.022	28.50	6.847	0.000	6.668	0.109	8.526	23.78

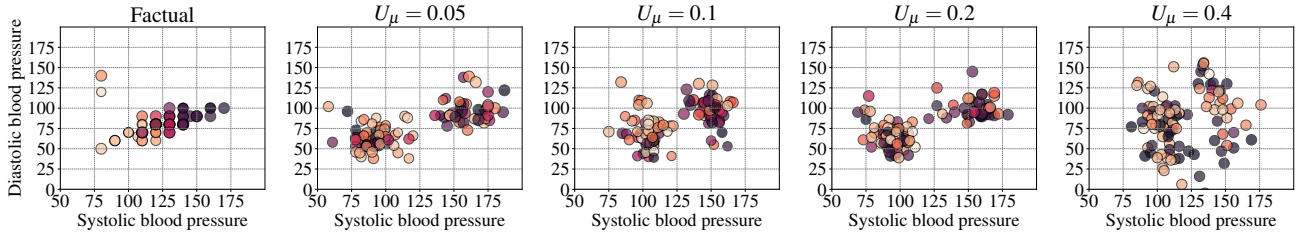


Figure 6: [Cardiovascular Disease, RBFNet] The model is trained on all features, whereas the DCE optimization is performed only on the two features Diastolic/Systolic blood pressure. The four counterfactuals are obtained by optimizing from the same factual (show left). The darker color indicates the higher risk (see the color bar in Figure 5).

average pairwise distance within the empirical counterfactual distributions, following (Mothilal et al., 2020). The diversity-proximity-coverage (DPC) score is defined to be the diversity score divided by the OT proximity then multiplied by coverage. The DPC score is a comprehensive metric to justify the diversity, as it amortizes the payoff of obtaining diversity over the proximity. Practically, we want the counterfactual to score highly in all of coverage, proximity, and diversity. *Discount* achieves the best performance in almost all datasets and all models. One exception is GLOBE with RBF, which trades off its coverage significantly for gaining a higher diversity score.

Besides, Figure 6 shows the capability of *Discount* for generating diverse counterfactual distributions with different setups of U_x given fixed U_y . These counterfactuals differ in their features distributions, yet all yield very close prediction distributions. A small U_x constrains the flexibility of counterfactual optimization but ascertains the generated distribution is close to observations. One could use U_x to control the trade-off between validity and proximity.

G Geometric Explanations and Open Problems Discussions

The 2-Wasserstein distance effectively determines how “far apart” two distributions are in a geometric sense. The confidence interval defined by the Wasserstein ball then represents a geometric region on this manifold, encompassing counterfactual distributions that are within a certain ‘distance’ (as measured by the 2-Wasserstein metric) from the central factual distribution.

In the context of a Riemannian manifold, geodesics are the shortest paths between two points (in this case, between two probability distributions). The 2-Wasserstein distance is a geodesic distance on the manifold (Cédric, 2008, Corollary 7.22). This framework allows for a geometric interpretation of how distributions relate to each other within this space. For any given factual distribution \mathbf{x}' , the region of counterfactual distribution \mathbf{x} defined by the probability constraint can geometrically be visualized as a kind of radius U_x sphere (i.e. Wasserstein Ball) centered at \mathbf{x}' where a significant majority (more than the probability P) strictly adheres to the boundary

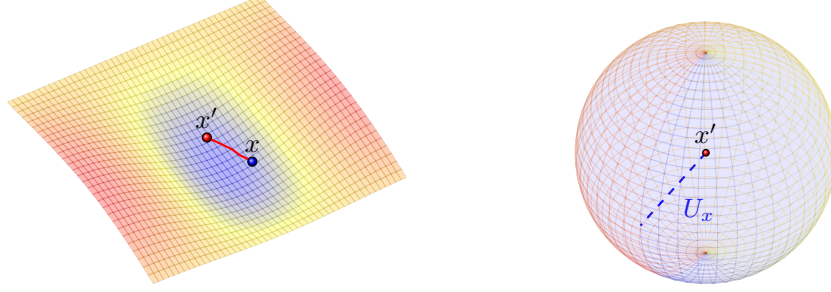


Figure 7: Geometric illustration of geodesic distance between two distributions x and x' and the Wasserstein ball centered at x' .

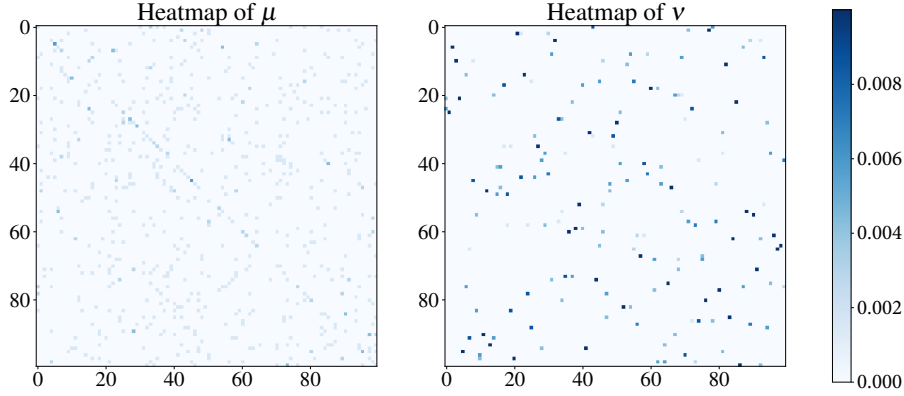


Figure 8: [Cardiovascular Disease, DNN] Visualization of the transportation plan for μ and ν , as computed in lines 3 and 4 of Algorithm 1, respectively. This heatmap depicts the averaged values of μ over $\theta \in \Theta$, normalized to form a distribution with elements summing to one. Factual and counterfactual points are aligned (in their original order) along the x-axis and y-axis, respectively.

constraint of the sphere. See Figure 7 for an illustration.

Transportation Plan. The transportation plan can be conceptualized as a geometric mapping that delineates the optimal transfer of probability mass across the manifold from the factual input distribution \mathbf{x}' to the counterfactual input distribution x . Embedded within the structure of the manifold, the values of μ and ν represent the relative extent of mass reallocation necessary between specific points or regions in the probability space. Large values in Π indicate areas that require substantial mass movement, reflecting significant distributional changes, while smaller values suggest minor adjustments. Zero values denote regions where the existing distribution aligns with the target and requires no modification. This transportation plan, therefore, becomes an integral tool in understanding and visualizing the nature of distributional shifts required in counterfactual scenarios.

Figure 8 demonstrates the use of the transport plans μ and ν in DCE. A key observation from the heatmap of μ is the pronounced diagonal, suggesting that the predominant mass transfer occurs between each factual point and its direct counterpart in the counterfactual data set. This implies that individuals in the factual group are more likely to correspond to their original counterparts in the counterfactual group, rather than to others. This pattern is typical when the distribution distance between \mathbf{x} and \mathbf{x}' is restricted to be very close. In the extreme case of identical distributions, OT would occur strictly along the diagonal (and hence the heatmap ν also looks strictly diagonal).

In contrast, the heat map of ν shows a less distinct diagonal pattern, indicating a notable shift in the risk ranking of individuals from the factual group to the counterfactual group. This suggests that the individual with the highest cardiovascular risk in the factual group might not maintain a comparably high risk in the counterfactual group. Although this is not inherently problematic, it highlights that the model may be highly sensitive to certain features, with minor changes in \mathbf{x} that potentially lead to significant alterations in \mathbf{y} . However, if the diagonal is prominently visible in μ but not in ν , further investigation is warranted to determine whether the model is acting as intended. This discrepancy may suggest that, while the model maintains individual correspondences

between the factual and counterfactual groups (as indicated by μ), the implications or outputs (reflected in ν) do not preserve these correspondences. Such a scenario could reveal potential issues or sensitivities in the model’s learning process that merit closer examination.

Combining DCE with previous work. Once a distributional counterfactual \mathbf{x} has been constructed via the DCE framework, the methods proposed in (Kulinski and Inouye, 2023) and (Koebler et al., 2023) become natural post-hoc complements for enhanced explainability. Specifically, (Kulinski and Inouye, 2023) interprets the shift between two *observed* distributions by constructing an OT-based decomposition of where and how the mass is moved. Although the counterfactual distribution \mathbf{x} in DCE is *not* empirically observed, one can sample from it (or treat it as a reweighted empirical set), thereby enabling (Kulinski and Inouye, 2023) to generate interpretable “transportation maps” showing which subpopulations or feature ranges changed most substantially. Meanwhile, (Koebler et al., 2023) examines how real-world distribution drifts affect model performance and reliability. Applied analogously to \mathbf{x}' (factual) and \mathbf{x} (DCE counterfactual), the approach in (Koebler et al., 2023) can reveal how performance, fairness metrics, or predictive reliability might degrade or improve under the hypothesized distributional shift. Thus, (Kulinski and Inouye, 2023) and (Koebler et al., 2023) effectively extend DCE’s basic capability—beyond simply constructing a new distribution—to provide finer-grained analysis of *why* particular transport plans emerge and *what* their consequence is for the model’s predictive behavior.

Entropic optimal transport (EOT) and Information Geometry There is also a link between OT and information geometry, established by introducing an entropy-regularization term for \mathcal{W}^2 (Cuturi, 2013), i.e.

$$\mathcal{W}_\varepsilon^2(\gamma_1, \gamma_2) = \inf_{\pi \in \Pi(\gamma_1, \gamma_2)} \left\{ \int_{\mathbb{R}^d \times d} \|a_1 - a_2\|^2 d\pi(a_1, a_2) + \varepsilon H(\pi | \gamma_1 \otimes \gamma_2) \right\} \quad (32)$$

where the regularization term $H(\pi | \gamma_1 \otimes \gamma_2)$ denotes the relative entropy with respect to the product measure $\gamma_1 \otimes \gamma_2$, defined as

$$H(\pi | \gamma_1 \otimes \gamma_2) = \int_{\mathbb{R}^d} \log \left(\frac{d\pi}{d\gamma_1 d\gamma_2} \right) d\pi. \quad (33)$$

Using $\mathcal{W}_\varepsilon^2$ as replacement for its counterparts in the objective and the constraint of the formulation (3) reduces the computational effort to obtain the transportation plan π . Furthermore, this regularization term is equivalent to using Kullback-Liebler (KL) divergence as a regularizer and naturally defines certain geometrical structures from the information geometry point of view (Karakida and Amari, 2017; Khan and Zhang, 2022). The role of the product of marginal distributions $\gamma_1 \otimes \gamma_2$ in the divergence term KL is to establish a baseline of independence between the distributions being compared. By measuring the divergence of the transport plan π from this baseline, the entropy term encourages solutions that respect the underlying structure of the individual distributions, rather than overly concentrating the mass transfer in a few specific regions. By increasing the value of ε , one tends to seek a counterfactual \mathbf{x} that is drawn “more independently” from the distribution of the original input \mathbf{x}' , leading to solutions that consider a broader range of possibilities, resulting in more diverse and potentially more insightful counterfactuals that better capture the overall structure of the data.

The integration of the entropic term makes \mathcal{W}^2 a quasi-distance (due to loss of symmetry). The entropic Wasserstein quasi-distance may be regarded as such a metric in scenarios where the expense associated with the transfer of information across distinct nodes is contingent upon the spatial coordinates of these nodes (Oizumi et al., 2014), and the entropic term controls the amount of information integration (Amari et al., 2018), which is measured by the amount of interactions of information among different nodes.

Open Problems of DCE with EOT. The solution of the chance-constrained optimization problem (3) is essentially based on a statistically trustworthy estimation of the upper bounds of \mathcal{W}^2 and \mathcal{SW}^2 . Remark that Theorem 3.2 hinges on the fact that the 1D Wasserstein distance may be expressed as quantile functions, so it does not generalize to entropic regularized \mathcal{W}^2 or \mathcal{SW}^2 (because they are no longer rigorously tied to the quantile expressions). CLT is proved for the EOT cost that is centered at the population cost, and this yields an asymptotically valid confidence interval for EOT (del Barrio et al., 2023, Theorem 3.6). Furthermore, bootstrap is shown to be valid for EOT (Goldfeld et al., 2022, Theorem 7), making asymptotic inference for the interval efficient and straightforward. To our knowledge, it remains open whether the sliced version of EOT accepts an (even asymptotic) inference for the confidence interval. Hence, if one uses EOT in (3b), its theoretical foundation calls for further investigation.

H Reproducibility

To ensure the reproducibility of our experiments for the proposed DCE, we provide detailed information on our computational environment and data preprocessing steps.

The experiments were carried out on a high performance computing (HPC) cluster, utilizing four nodes (one for each dataset) in parallel. Each node is equipped with two Intel Xeon Processor 2660v3 (10 core, 2.60GHz) CPUs and 128 GB of memory. The duration of the experiment is approximately 5 hours per node, depending on the size of the dataset. Although reproducing these experiments on a standard laptop is feasible, it generally requires more computational time compared to using an HPC cluster.

For the four datasets used in our experiments, numerical features are standardized to ensure that each feature has a mean of zero and a standard deviation of one. Categorical features are encoded using either label encoding or one-hot encoding. We did not observe significant differences in the performance of the DCE framework between these two encoding methods. The data sets are divided into training and testing sets with a ratio of 0.8 : 0.2.

The experiments were implemented using Python, with key libraries including NumPy, Pandas, Scikit-learn, and PyTorch. Detailed versions and dependencies are given in the source code to facilitate exact replication of the experiments.

The complete codebase, along with detailed instructions for setting up the environment and running the experiments, is available in a public repository (see the footnote in Section 6). This includes scripts for data preprocessing, model training, evaluation, and the generation of CE.