Robust Hypothesis Testing with Wasserstein Uncertainty Sets

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Abstract

We consider a data-driven robust hypothesis test where the optimal test will minimize the worst-case performance regarding distributions that are close to the empirical distributions with respect to the Wasserstein distance. This leads to a new non-parametric hypothesis testing framework based on distributionally robust optimization, which is more robust when there are limited samples for one or both hypotheses. Such a scenario often arises from applications such as health care, online change-point detection, and anomaly detection. We study the computational and statistical properties of the proposed test by presenting a tractable convex reformulation of the original infinite-dimensional variational problem exploiting Wasserstein’s properties and characterizing the radii selection for the uncertainty sets. We also demonstrate the good performance of our method on synthetic and real data.

1 Introduction

Hypothesis testing is a fundamental problem in statistics and an essential building block for machine learning problems such as classification and anomaly detection. The goal of hypothesis testing is to find a decision rule to discriminate between two hypotheses given new data while achieving a small probability of errors. However, the exact optimal test is difficult to obtain when the underlying distributions are unknown. This issue is particularly challenging when the number of samples is limited, and we cannot obtain accurate estimations of the distributions. The limited sample scenario (for one or both hypotheses) commonly arises in many real-world applications such as medical imaging diagnosis [1], online change-point detection [34], and online anomaly detection [8].
1.1 Why distribution-free minimax test

For hypothesis testing, the well-known Neyman-Pearson Lemma [30] establishes that the likelihood ratio gives the optimal test for two simple hypotheses. This requires to specify a priori two true distribution functions $P_1$ and $P_2$ for the two hypotheses, which, however, are usually unknown in practice. When the assumed distributions deviate from true distributions, the likelihood ratio test may experience a significant performance loss.

Typically there are “training” samples available for both hypotheses. A commonly used approach is the generalized likelihood ratio test (GLRT), which assumes parametric forms for the distributions and estimates parameters using data and plug into the likelihood ratio statistic. Another popular method is the density ratio estimation [45]. However, in many scenarios, the training samples for one or both hypotheses can be small. For instance, we tend to have a small sample size for patients in healthcare applications. In limited-sample scenarios, it can be challenging to estimate parameters for GLRT (especially in the high dimensional case) or to estimate density ratios accurately. Without reliable estimation of the underlying distributions, various forms of robust hypothesis testing [20, 21, 27, 18] have been developed by considering different “uncertainty sets”. Huber’s seminar work [20] sets the uncertainty set as the $\epsilon$-contamination sets that contain distributions close to a nominal distribution defined by total-variation distance. In [21], the optimal tests are characterized under majorization conditions, which, however, are intractable in general. Thus, there remains a computational challenge to find the optimal test, especially when the data is multi-dimensional. This has become a significant obstacle in applying robust hypothesis tests in practice.

We consider a setting where the sample size is small. When there are limited samples, the empirical distribution may have “holes” in the sample space: places where we do not have samples yet, but there is a non-negligible probability for the data to occur, as illustrated in Figure 1. Thus, we may not want to restrict the true distribution to be on the same support of the empirical distribution. However, many commonly used distance divergences for probability distributions, such as Kullback-Leibler divergence, are defined for distributions with common support. Thus, in our setting, it can be restrictive if we were to construct uncertainty sets using the Kullback-Leibler divergence (e.g., [27] and [18]). Similarly, total-variational norm-induced uncertainty sets will have this issue since they encourage distributions with the same support as the nominal distribution. This motivates us to consider an uncertainty set formed by the Wasserstein distance. It measures the distance between distributions using optimal transport metric, which is more suitable for distributions without common support.
1.2 Contributions

In this paper, we present a new non-parametric minimax hypothesis test assuming the distributions under each hypothesis belong to two disjoint “uncertainty sets” constructed using the Wasserstein distance. Specifically, the uncertainty sets contain all distributions close to the empirical distributions formed by the training samples in Wasserstein distance. This approach is more robust in small-sample-size regimes when we cannot estimate the true data-generating distributions accurately.

A notable feature of our approach is the computational tractability and explicit characterization of the optimal test. The optimal test is based on a pair of least favorable distributions (LFD) from the uncertainty sets, which is a reminiscence of Huber’s robust test. However, here the optimal test form is different, and our LFDs are computationally tractable in general. An outstanding challenge in finding the minimax test is that we face an infinite-dimensional optimization problem (finding the saddle point for optimal test and LFDs), which is hard to solve in general. To tackle the challenge, we make a connection to recent advances in distributionally robust optimization. In particular, we decouple the original minimax problem into two sub-problems using strong duality, which enable us first to find the optimal test for a given pair of distribution $P_1$ and $P_2$, and then find the LFDs $P_1^*$ and $P_2^*$ by solving a finite-dimensional convex optimization problem. We further characterize the robust optimal test and extend the test to the “batch” setting containing multiple test samples.

We also characterize the radii choice of the uncertainty sets, which is an important question that affects the optimal test’s generalization property. We prove a theoretical upper bound for the sufficient radii based on the so-called profile function that is defined.
as the minimum Wasserstein distance between the empirical distributions and distributions that yields the same test as the oracle one. Compared with the commonly used approach in distributionally robust optimization – the uncertainty set must contain the true distribution, our results shows a matching order that can be attained in worst-case. On the other hand, our results show the advantage of providing the explicit constant term that depends on the densities of the underlying true data-generating distributions.

Finally, we show our method’s good performance using simulated and real data, and demonstrate its applicability for sequential human activity detection.

1.3 Related work

Robust hypothesis testing has been developed under the minimax framework by considering various forms of “uncertainty sets”. Seminal work by Huber [20] considers the \( \epsilon \)-contamination sets that contain distributions close to a nominal distribution defined by total-variation distance. Huber and Strassen later generalized the results in [21] based on the observation that the \( \epsilon \)-contamination sets can be described using the so-called alternating capacities. It is claimed that under this capacity assumption, there is a representative pair (namely the LFDs) such that the Neyman-Pearson test between this pair is minimax optimal. Although Huber provides an explicit characterization of the robust hypothesis test in the form of a truncated likelihood ratio, the “capacities” condition is required to obtain the optimality result; the LFDs are difficult to obtain in general. Our result is consistent with [20] in that our robust test also depends on the least favorable distributions, but we find the LFDs from data by solving a tractable optimization problem.

More recently, [27] and [18] consider uncertainty sets induced by Kullback-Leibler (KL) divergence in the one-dimensional setting without specifying parametric forms; the optimal test is obtained using the strong duality of problem induced by the KL divergence. Aiming to develop a computationally efficient procedure, [17, 6] consider a convex optimization framework for hypothesis testing, assuming parametric forms for the distributions and the parameters under the null and the alternative hypothesis belong to convex sets. We consider a new way to construct uncertainty sets using Wasserstein metrics and empirical distributions to achieve distributional robustness. Using Wasserstein metric to achieve robustness is a popular technique and has been applied to many areas, including computer vision [38, 26, 36], generative adversarial networks [2, 19], and two-sample test [37].

Our work is also closely related to the Wasserstein distributionally robust optimization (DRO) [10, 4, 15, 43, 39]. However, existing DRO problems typically involve only one class of empirical samples, but our problem involves two classes. Hence we cannot rely
on existing strong duality results in DRO [4, 10, 15] to obtain our results. Besides, we provide new insights regarding our solution’s structural properties that are different from those that occurred in other DRO problems. Similarly, the line of work in DRO which aims to characterize the size of uncertainty set focuses on a single uncertainty set, including asymptotic results in the finite-dimensional parametric case [3] and infinite-dimensional case [42], as well as non-asymptotic bound [10, 40, 14]. We adopt a similar principle as in [3, 42] but develop different analysis for the case of two uncertainty sets.

1.4 Organization
The remainder of the paper is organized as follows. Section 2 sets up the problem. Section 3 presents the optimal test. Section 4 characterizes the selection of the radii of the uncertainty sets. Section 5 demonstrates our robust tests’ good performance using both synthetic and real data. Finally, Section 6 concludes the paper with some discussions. We delegate all proofs to the appendix.

2 Wasserstein Minimax Test
Let $\Omega \subset \mathbb{R}^d$ be the sample space, where $d$ is the data dimension. Denote $\mathcal{P}(\Omega)$ as the set of Borel probability measures on $\Omega$. Given $P_1, P_2 \in \mathcal{P}(\Omega)$, the simple hypothesis test decides whether a given test sample $\omega$ is from $P_1$ or $P_2$. In many practical situations, $P_1, P_2$ are not exactly known, but instead we have access to $n_1$ and $n_2$ i.i.d. training samples following distributions $P_1$ and $P_2$, respectively. Denote the two sets of training samples as $\hat{\Omega}_k = \{\hat{\omega}_1, \ldots, \hat{\omega}_{n_k}\}, k = 1, 2$, and define empirical distributions constructed using training data sets as

$$Q_k = \frac{1}{n_k} \sum_{i=1}^{n_k} \delta_{\hat{\omega}_i}, \ k = 1, 2.$$

Here $\delta_\omega$ denotes the Dirac point mass concentrated on $\omega \in \Omega$.

To capture the distributional uncertainty, we consider composite hypothesis test of the form:

$$H_0 : \ \omega \sim P_1, \ P_1 \in \mathcal{P}_1;$$

$$H_1 : \ \omega \sim P_2, \ P_2 \in \mathcal{P}_2,$$

where $\mathcal{P}_1, \mathcal{P}_2$ are collections of relevant probability distributions. In particular, we will consider them to be Wasserstein uncertainty sets. Below we describe our problem setup.
2.1 Randomized test

We consider the set of all randomized tests defined as follows [22].

**Definition 1 (Randomized test).** Given hypotheses $H_0, H_1$, a randomized test is any Borel measurable function $\pi : \Omega \to [0, 1]$ which, for any observation $\omega \in \Omega$, accepts the hypothesis $H_0$ with probability $\pi(\omega)$ and $H_1$ with probability $1 - \pi(\omega)$.

In the randomized test, the decision to accept a hypothesis can be a random selection based on the function $\pi(\omega)$. Thus, the usual deterministic test (e.g., considered in [16]) is a special case by setting $\pi(\omega) \in \{0, 1\}$ and the randomized test is more general.

For a simple hypothesis test with hypotheses $P_1$ and $P_2$, we define the risk of a randomized test $\pi$ as the summation of Type-I and Type-II errors:

$$\Phi(\pi; P_1, P_2) := \mathbb{E}_{P_1}[1 - \pi(\omega)] + \mathbb{E}_{P_2}[\pi(\omega)].$$

(1)

Here we consider equal weights on the Type-I and Type-II errors; other weighted combinations can be addressed similarly.

2.2 Wasserstein minimax formulation

The minimax hypothesis test finds the optimal test that minimizes the worst-case risk over all possible distributions in the composite hypotheses:

$$\inf_{\pi} \sup_{P_1 \in \mathcal{P}_1, P_2 \in \mathcal{P}_2} \Phi(\pi; P_1, P_2).$$

The resulting worst-case solution $P_1^*, P_2^*$ are called the least favorable distributions (LFDs) in the classical robust hypothesis test literature [20, 21].

In this paper, we consider uncertainty sets based on the Wasserstein metric, defined as:

$$\mathcal{W}(P, Q) := \min_{\gamma \in \Gamma(P, Q)} \left\{ \mathbb{E}_{(\omega, \omega')} \left[ c(\omega, \omega') \right] \right\},$$

where $c(\cdot, \cdot) : \Omega \times \Omega \to \mathbb{R}_+$ is a metric on $\Omega$, and $\Gamma(P, Q)$ is the collection of all Borel probability measures on $\Omega \times \Omega$ with marginal distributions $P$ and $Q$. Define the Wasserstein uncertainty sets $\mathcal{P}_1, \mathcal{P}_2$ as Wasserstein balls centering at two empirical distributions:

$$\mathcal{P}_k := \{ P_k \in \mathcal{P}(\Omega) : \mathcal{W}(P_k, Q_k) \leq \theta_k \}, \quad k = 1, 2,$$

(2)

where $\theta_1, \theta_2 > 0$ specify the radii of the uncertainty sets.
2.3 Comparison with Huber’s censored likelihood ratio test

Huber’s seminal work [20] considered a deterministic minimax test with uncertainty sets referred to as \( \epsilon \)-contamination sets:

\[
P_k = \{ (1 - \epsilon_k)p_k + \epsilon_k f_k, \ f_k \in \mathcal{P}(\Omega) \},
\]

where \( \epsilon_k \in (0, 1) \), \( p_k \) is the nominal density function, and \( f_k \) is the density that can be viewed as the perturbation, \( k = 1, 2 \). Huber proved that the optimal test in this setting is a censored version of the likelihood ratio test, with censoring thresholds \( c', c'' \), and the LFDs are given by:

\[
q_1(x) = \begin{cases} 
(1 - \epsilon_1)p_1(x) & p_2(x)/p_1(x) < c'' \\
\frac{1}{ca}(1 - \epsilon_1)p_2(x) & p_2(x)/p_1(x) \geq c''
\end{cases}
\]

\[
q_2(x) = \begin{cases} 
(1 - \epsilon_2)p_2(x) & p_2(x)/p_1(x) > c' \\
c'(1 - \epsilon_2)p_1(x) & p_2(x)/p_1(x) \leq c'
\end{cases}
\]

Huber assumed the exact knowledge of the nominal distributions \( p_1 \) and \( p_2 \). This is different from our setting, where we only have limited samples from each hypothesis. A simple observation is that if we set \( p_k \) to be the empirical distribution, then the ratio \( p_2(x)/p_1(x) \) will be \( \infty \) on \( \hat{\Omega}_2 \setminus \hat{\Omega}_1 \) and 0 on \( \hat{\Omega}_1 \setminus \hat{\Omega}_2 \). In such a case, the LFDs proposed by Huber are degenerate

\[
q_1(x) = \begin{cases} 
(1 - \epsilon_1)/n_1 & x \in \hat{\Omega}_1 \\
\epsilon_1/n_2 & x \in \hat{\Omega}_2
\end{cases} \quad q_2(x) = \begin{cases} 
(1 - \epsilon_2)/n_2 & x \in \hat{\Omega}_2 \\
\epsilon_2/n_1 & x \in \hat{\Omega}_1
\end{cases}
\]

which do not lead to any meaningful test.

3 Tractable Convex Reformulation and Optimal Test

The saddle point problem (2.2) for the Wasserstein minimax test is an infinite-dimensional variational problem, which in the original form does not amend to any tractable solution. In this section, we derive a finite-dimensional convex reformulation for finding the optimal test.

We will show the following strong duality result, which means we can exchange the order of infimum and supremum in our problem:

\[
\inf_{\pi} \sup_{P_1 \in \mathcal{P}_1, P_2 \in \mathcal{P}_2} \Phi(\pi; P_1, P_2) = \sup_{P_1 \in \mathcal{P}_1, P_2 \in \mathcal{P}_2} \inf_{\pi} \Phi(\pi; P_1, P_2). \tag{3}
\]
This is essential in leading to closed-form expression for the optimal test and convex reformulation in solving the LFDs. Our proof strategy is as follows. First, in Section 3.1, we derive a closed-form expression of the optimal test for the simple hypothesis problem \( \inf_\pi \Phi(\pi; P_1, P_2) \). Next in Section 3.2, we develop a convex reformulation of the sup inf problem on the right-hand side of (3), whose optimal solution gives the LFDs that are supported on the empirical data points. A byproduct of our analysis specifies the optimal test on empirical data points. Finally, in Section 3.3, we construct the optimal minimax test for the original formulation (left-hand side of (3)). At the core of our analysis is proving that the optimal test can be found by extending the optimal test on the empirical data points to the entire space.

Note that here we cannot directly rely on existing tools such as Sion’s minimax theorem [44], because (i) the space of all randomized tests is not endowed with a linear topological structure and, (ii) Wasserstein ball is not compact in the space \( \mathcal{P}(\Omega) \) since \( \Omega \) may not be compact.

### 3.1 Optimal test for simple hypothesis test

Let us start by considering the simple hypothesis test for given \( P_1, P_2 \in \mathcal{P}(\Omega) \), the inner minimization in the right-hand side of (3):

\[
\inf_\pi \Phi(\pi; P_1, P_2). 
\]

Define the total variation distance between two distributions \( P_1 \) and \( P_2 \) as \( \text{TV}(P_1, P_2) := (1/2) \int_\Omega |dP_1(\omega) - dP_2(\omega)| \). The following Lemma gives a closed-form expression for the optimal test, which resembles a randomized version of the Neyman-Pearson Lemma. The proof is provided in Appendix A.1.

**Lemma 1.** Let \( p_1(\omega) := \frac{dP_1}{d(P_1 + P_2)}(\omega) \). The test

\[
\pi(\omega) = \begin{cases} 
1, & \text{if } p_1(\omega) > 1/2, \\
0, & \text{if } p_1(\omega) < 1/2, \\
\text{any real number in } [0,1], & \text{otherwise,}
\end{cases}
\]

is optimal for (4) with the risk:

\[
\psi(P_1, P_2) := \int_\Omega \min\{p_1(\omega), 1-p_1(\omega)\} d(P_1 + P_2)(\omega) = 1 - \text{TV}(P_1, P_2). 
\]
Lemma 1 shows that the optimal test for the simple hypothesis takes a similar form as the likelihood ratio test that accepts the hypothesis with a higher likelihood and breaks the tie arbitrarily. An important observation from the lemma is that the risk only depends on the common support of the two distributions, defined as $\Omega_0(P_1, P_2) := \{ \omega \in \Omega : 0 < p_1(\omega) < 1 \}$, on which $P_1$ and $P_2$ are absolutely continuous with respect to each other. In particular, if the supports of $P_1, P_2$ have measure-zero overlap, then $\inf_{\pi} \Phi(\pi; P_1, P_2)$ equals to zero — the optimal test for two non-overlapping distributions $P_1, P_2$ has zero risk.

### 3.2 Least favorable distributions

Now we continue with finding the LFDs given the form of the optimal test in Lemma 1, which corresponds to the remaining supermum part of the right-hand side of (3):

$$\sup_{P_1 \in \mathcal{P}_1, P_2 \in \mathcal{P}_2} \psi(P_1, P_2).$$

Note that from the definition of $\psi$ in (5), the risk associated with the optimal test, the problem of finding LFDs admits a clear statistical interpretation: the LFDs correspond to a pair of distributions in the uncertainty sets that are closest to each other in the total variation distance.

To tackle the infinite-dimensional variational problem (6), let us first discuss some structural properties of the LFDs that will lead to a finite-dimensional convex reformulation. Consider a toy example where $Q_1 = \delta_{\hat{\omega}_1}, Q_2 = \delta_{\hat{\omega}_2}$, i.e., there is only one sample in each training data set. The goal of solving LFDs can be understood as moving part of the probability mass on $\hat{\omega}_1$ and $\hat{\omega}_2$ to other places such that the objective function $\psi(P_1, P_2)$ is maximized. Note that, to find the LFDs, we need to (i) move the probability mass such that $P_1$ and $P_2$ overlap as much as possible, since the objective value $\psi(P_1, P_2)$ depends only on the common support; (ii) then if we were to move $p_k$ from $\hat{\omega}_k$ to a common point $\omega \in \Omega$, $k = 1, 2$, in the least favorable way, then we solve $\min_{\omega \in \Omega} [p_1 c(\omega, \hat{\omega}_1) + p_2 c(\omega, \hat{\omega}_2)]$ by the definition of the Wasserstein metric. From the triangle inequality satisfied by the metric $c(\cdot, \cdot)$, we need $\omega$ to be on the linear segment connecting $\hat{\omega}_1$ and $\hat{\omega}_2$ and in fact, it has to be one of the endpoints $\hat{\omega}_1$ or $\hat{\omega}_2$. More generally, one can generalize this argument, and there exist LFDs supported on the empirical observations.

The following lemma shows that the LFDs can be solved via a finite-dimensional convex optimization problem. The proof is provided in Appendix A.2. For simplicity, define the total number of observations $n := n_1 + n_2$ and the union of observations from both hypotheses

$$\hat{\Omega} := \hat{\Omega}_1 \cup \hat{\Omega}_2.$$
Without causing confusions, we re-label the samples in $\hat{\Omega}$ as $\{\hat{\omega}^1, \ldots, \hat{\omega}^n\}$.

**Lemma 2 (LFDs).** The LFD problem in (6) can be reformulated as the following finite-dimensional convex program

$$\max_{p_1, p_2 \in \mathbb{R}_+^n} \sum_{l=1}^n \min \{p_{1,l}^l, p_{2,l}^l\}$$

subject to

$$\sum_{l=1}^n \sum_{m=1}^n \gamma_{k,l,m} c(\hat{\omega}^l, \hat{\omega}^m) \leq \theta_k, \ k = 1, 2;$$

$$\sum_{m=1}^n \gamma_{k,l,m} = Q_{l,k}, \ 1 \leq l \leq n, k = 1, 2;$$

$$\sum_{l=1}^n \gamma_{k,l,m} = p_{m,k}, \ 1 \leq m \leq n, k = 1, 2.$$ (7)

Above, the decision variables $\gamma_k$ are square matrices that can be viewed as a joint distribution on $\hat{\Omega} \times \hat{\Omega}$ with marginals specified by $Q_k$ and candidate LFDs $p_k$. The $lm$-th entry of $\gamma_k$ is specified by $\gamma_{k,l,m}$ and the $l$-th entry of $p_k$ (respectively, $Q_k$) is specified by $p_{l,k}^l$ (respectively, $Q_{l,k}^l$). In the following, we will denote $(P_1^*, P_2^*)$ as the LFDs solved from (7). Note that Lemma 2 simplifies the LFD problem (6) from infinite-dimensional to finite-dimensional, using the fact that there exist LFDs supported on a finite set $\hat{\Omega} \subset \Omega$ due to our analysis. We also comment that the complexity of solving the LFDs in (7) is independent of the dimension of the data, once the pairwise distances $c(\hat{\omega}^l, \hat{\omega}^m)$ are calculated and given as input parameters of the convex program.

### 3.3 Robust optimal test: extension from test on training samples

Thus far, we have found one of the LFDs defined on the discrete set of training samples $\hat{\Omega}$ by solving the right-hand side of (3), which in turn, defines the optimal test on training samples. However, it may be common in practice that the given test sample is different from all training samples. In this case, the current optimal test in Lemma 1 associated with the LFDs is not well-defined on test samples. Besides, this optimal test is not uniquely defined when there is a tie between the likelihood of samples under two hypotheses. In this subsection, we will establish an optimal test that is well-defined anywhere in the observation space $\Omega$.

Our main result is the following theorem which specifies the general form of the robust optimal test $\pi^*$ and LFDs $(P_1^*, P_2^*)$ to the saddle point problem (2.2), whose proof is given in Appendix A.3.
Theorem 1 (Robust optimal test). Let \((P_1^*, P_2^*)\) be the LFDs solved from (7). The robust optimal test \(\pi^* : \Omega \rightarrow [0, 1]\) to problem (2) is given by

(i) On the support of training samples \(\omega \in \hat{\Omega}, \pi^*(\omega) = \hat{\pi}_m^*, \) for \(\omega = \hat{\omega}^m, \) where \(\hat{\pi}_m^* \in [0, 1], m = 1, \ldots, n,\) is the solution to the following system of linear equations

\[
\sum_{m=1}^{n} (1 - \hat{\pi}_m) P_1^*(\hat{\omega}^m) = \min_{\lambda_1 \geq 0} \left\{ \lambda_1 \theta_1 + \frac{1}{n_1} \sum_{l=1}^{n} \max_{1 \leq m \leq n} \{ 1 - \hat{\pi}_m - \lambda_1 c(\hat{\omega}^l, \hat{\omega}^m) \} \right\}, \tag{8}
\]

\[
\sum_{m=1}^{n} \hat{\pi}_m P_2^*(\hat{\omega}^m) = \min_{\lambda_2 \geq 0} \left\{ \lambda_2 \theta_2 + \frac{1}{n_2} \sum_{l=1}^{n} \max_{1 \leq m \leq n} \{ \hat{\pi}_m - \lambda_2 c(\hat{\omega}^l, \hat{\omega}^m) \} \right\};
\]

the solution is guaranteed to exist.

(ii) Off the support of training samples \(\omega \in \Omega \setminus \hat{\Omega}, \pi^*(\omega) \in [\ell(\omega), u(\omega)],\) where

\[
\ell(\omega) = \max \left\{ \max_{i=1, \ldots, n_1} \min_{\hat{\omega} \in \hat{\Omega}} \{ \pi^*(\hat{\omega}) + \lambda_1^* c(\hat{\omega}, \hat{\omega}_1^i) - \lambda_1^* c(\omega, \hat{\omega}_1^i) \}, 0 \right\},
\]

\[
u(\omega) = \min \left\{ \min_{j=1, \ldots, n_2} \max_{\hat{\omega} \in \hat{\Omega}} \{ \pi^*(\hat{\omega}_2^j) - \lambda_2^* c(\hat{\omega}_2^j, \hat{\omega}_2^j) + \lambda_2^* c(\omega, \hat{\omega}_2^j) \}, 1 \right\}, \tag{9}
\]

\(\lambda_k^*, k = 1, 2\) are the minimizers to the inf problems on the right hand side of (8), and it is guaranteed that \(u(\omega) \geq \ell(\omega), \forall \omega \in \Omega \setminus \hat{\Omega}.

The first part of the theorem defines the optimal test on training samples, resulting from the finite-dimensional saddle point problem

\[
\sup_{P_1 \in \mathcal{P}_1 \cap \mathcal{P}_{\hat{\Omega}}} \inf_{P_2 \in \mathcal{P}_2} \Phi(\pi; P_1, P_2),
\]

where \(\mathcal{P}_k := \mathcal{P}_k \cap \mathcal{P}(\hat{\Omega}), k = 1, 2.\) By Lemma 2, this is equivalent to the right-hand side of (3). The second part extends the optimal test on training samples to the whole space. This is a non-trivial results that build on the properties of Wasserstein metric and the duality result.

To illustrate Theorem 1, let us consider a toy example as shown in Figure 2. Suppose the training samples for hypothesis \(H_0\) is \(\hat{\omega}_1 = -2\) and for hypothesis \(H_1\) are \(\hat{\omega}_2 = 1\) and \(\hat{\omega}_3 = 3.\) Then, the two empirical distributions \(Q_1\) is a point mass on \(\hat{\omega}_1 = -2\) and \(Q_2\) is a discrete distribution that \(\hat{\omega}_2 = 1\) and \(\hat{\omega}_3 = 3\) occur with equal probability \(1/2.\) By setting the radii of the uncertainty sets \(\theta_1 = \theta_2 = 1,\) the LFDs solution to (7) becomes \(P_1^*(\hat{\omega}_1) = 0.69, P_1^*(\hat{\omega}_2) = 0.28, P_1^*(\hat{\omega}_3) = 0.03,\) and \(P_2^*(\hat{\omega}_1) = 0.29, P_2^*(\hat{\omega}_2) = 0.28, P_2^*(\hat{\omega}_3) = 0.43.\) Notice
that there is a tie at the point $\hat{\omega}_2$. Now we will invoke Theorem 1 to break this tie. According to (8), the robust optimal test $\pi^*(\hat{\omega}_i)$, $i = 1, 2, 3$ needs to satisfy

$$1 - \pi^*(\hat{\omega}_1) - \lambda_i^* c(\hat{\omega}_1, \hat{\omega}_1) = 1 - \pi^*(\hat{\omega}_2) - \lambda_i^* c(\hat{\omega}_1, \hat{\omega}_2) = 1 - \pi^*(\hat{\omega}_3) - \lambda_i^* c(\hat{\omega}_1, \hat{\omega}_3).$$

Therefore, we can set $\pi^*(\hat{\omega}_2) = 1 - c(\hat{\omega}_1, \hat{\omega}_2)/c(\hat{\omega}_1, \hat{\omega}_3) = 0.4$. This means that the optimal test at $\hat{\omega}_2$ should accept the hypothesis $H_0$ with probability 0.4 (note that the tie is not broken arbitrarily). As a comparison, consider a different case where $\hat{\omega}_2 = 2$ while everything else is kept the same. It can be verified that there is still a tie at $\hat{\omega}_2$. However, this time we have $\pi^*(\hat{\omega}_2) = 1 - c(\hat{\omega}_1, \hat{\omega}_2)/c(\hat{\omega}_1, \hat{\omega}_3) = 0.2$, meaning that the optimal test at $\hat{\omega}_2$ should accept the hypothesis $H_0$ with probability 0.2. We note that in this simple experiment, the chance of accepting $H_0$ decreases if we move $\hat{\omega}_2$ away from $\hat{\omega}_1$, which is consistent with our intuition as illustrated in Figure 2. Moreover, we also plot the upper and lower bounds $u(\omega)$ and $\ell(\omega)$, as defined in (9), showing the range of the optimal test off the support of training samples. This example also demonstrates the advantage of using Wasserstein metrics in defining the uncertainty sets: the optimal test will directly reflect the data geometry.

Figure 2: A toy example illustrating the optimal test depends on the training data configuration. In these two cases, there are three samples, and only $\hat{\omega}_2$ is different, which takes values 1 and 2, respectively. Note that the optimal test $\pi^*(\hat{\omega}_2)$ will change when the gap between empirical samples are different. We also illustrate the upper and lower bounds $u(\omega)$ and $\ell(\omega)$ from (9).

3.4 Extension to whole space via kernel smoothing

We observe that for samples $\omega$ off the empirical support, it is possible to have $u(\omega)$ strictly larger than $\ell(\omega)$ with $u(\cdot)$, $\ell(\cdot)$ given in Equation (9). In such cases, there are infinite choices for $\pi^*(\omega)$ according to Theorem 1. In this subsection, we describe a specific choice for $\pi^*(\omega)$
under such situation by kernel smoothing. As a natural strategy, we may use kernel smoothing to extend LFDs solved from (7) to the whole space. This can be done by convolving the discrete LFDs with a kernel function $G_h : \mathbb{R}^d \rightarrow \mathbb{R}$ parameterized by a (bandwidth) parameter $h$:

$$P_k^h(\omega) := \sum_{l=1}^{n} P^*_l(\hat{\omega}) G_h(\omega - \hat{\omega}), \; k = 1, 2, \; \forall \omega \in \Omega.$$ (10)

There can be various choices of kernel functions. For instance, given normalized data, we can use the product of one-dimensional kernel function $g : \mathbb{R} \rightarrow \mathbb{R}$ with bandwidth $h > 0$:

$$G_h(x) = \frac{1}{h^d} \prod_{i=1}^{d} g\left(\frac{x_i}{h}\right), \; x \in \mathbb{R}^d.$$ An example of the kernel-smoothed LFDs is shown in Figure 1. Through convolution, we can obtain the kernel-smoothed LFDs and the corresponding test $\pi^*_h$ that is defined as the optimal test for the simple hypothesis under $(P^*_1, P^*_2)$ as specified in Lemma 1. To ensure the risk after kernel-smoothing is comparable to that of the robust optimal test $\pi^*$, we truncate the resulted $\pi^*_h$ such that (9) is satisfied after truncation. After such a procedure, the test based on the kernel-smoothed LFDs will achieve a good performance as validated by the numerical experiments in Section 5.

### 3.5 Test with batch samples

Testing using a batch of samples is important in practice, as one test sample may not achieve sufficient power. We can construct a test for a batch of samples by assembling the optimal test for each individual sample. Assume $m$ i.i.d. test samples $\omega_1, \omega_2, \ldots, \omega_m$. Consider a batch test based on the “majority rule” with the acceptance region for $H_0$ defined as $A := \{ (\omega_1, \omega_2, \ldots, \omega_m) : \pi^m(\omega_1, \omega_2, \ldots, \omega_m) \geq 1/2 \}$, where

$$\pi^m(\omega_1, \omega_2, \ldots, \omega_m) = \frac{1}{m} \sum_{i=1}^{m} \pi^*(\omega_i),$$

can be viewed as the fraction of votes in favor of hypothesis $H_0$ (due to Lemma 1). We can bound the risk of such a majority rule batch test:

**Proposition 1** (Risk for batch test). The risk of the test $\pi^m(\omega_1, \ldots, \omega_m)$ is be upper bounded by

$$\max \left\{ \sup_{P_1 \in \mathcal{P}_1} \mathbb{P}_{P_1}[A^c], \sup_{P_2 \in \mathcal{P}_2} \mathbb{P}_{P_2}[A] \right\} \leq \sum_{m/2 \leq i \leq m} \binom{m}{i} (\epsilon^*)^i (1 - \epsilon^*)^{m-i},$$
where
\[
\epsilon^* = \sup_{P_1 \in P_1, P_2 \in P_2} \Phi(\pi^*; P_1, P_2),
\]
is the worst-case risk of the optimal randomized test and \( \mathbb{A} \) is the acceptance region for \( H_0 \).
Thus, when \( \epsilon^* < 1/2 \), the above probability tends to 0 exponentially fast as the batch size \( m \to \infty \).

## 4 Radii Selection

In this section, we discuss how to select the radii \( \theta_1, \theta_2 \), which is critical to the performance of the robust optimal test. There is clearly a trade-off: when the radius is too small, the optimal test is not robust and does not generalize well to new test data; while the radius is too large, the solution may be too conservative, causing performance degradation. We expect sample sizes \( n_1 \) and \( n_2 \) to play a major role in determining the radii, and thus in the following we emphasize by denoting the radii as \( \theta_{k,n_k} \) and the empirical distributions as \( Q_{k,n_k} \). It should also be remembered that the uncertainty sets \( P_k(\theta_{k,n_k}), k = 1, 2 \), also depend on the sample sizes.

To characterize the radii selection, we adopt the profile-based inference proposed by [3], which extends the empirical likelihood method for divergence-based distributionally robust optimization [24, 9] by replacing likelihood with transport cost. It selects the radii based on the principle that the distributional uncertainty set should contain a pair of distributions whose resulting optimal test (for the corresponding simple hypothesis test) coincides with the optimal test for the underlying true distributions. More precisely, let \( P_1^0, P_2^0 \) be the underlying true distributions of the hypotheses \( H_0 \) and \( H_1 \) respectively. Define the oracle test \( \pi^0 \) as the optimal test of the simple hypothesis test associated with \( P_1^0, P_2^0 \), which is specified by Lemma 1. Also define the set of optimal tests for resolving simple hypothesis test associated with each pair of distributions in our uncertainty sets (using Lemma 1) as

\[
\Pi(\theta_{1,n_1}, \theta_{2,n_2}) := \left\{ \pi : \exists P_1 \in P_1(\theta_{1,n_1}), P_2 \in P_2(\theta_{2,n_2}) \text{ such that } \pi \in \arg\min_{\pi'} \Phi(\pi'; P_1, P_2) \right\}.
\]

We are interested in finding the radii such that the set is likely to include the oracle test, i.e., \( \pi^0 \in \Pi(\theta_{1,n_1}, \theta_{2,n_2}) \). To achieve this goal, we introduce a set \( \mathcal{S} \) that contains all possible pairs of distributions giving rise to the oracle test \( \pi^0 \):

\[
\mathcal{S} := \left\{ (P_1, P_2) \in \mathcal{P}(\Omega) \times \mathcal{P}(\Omega) : \pi^0 \in \arg\min_{\pi, \Omega \to [0,1]} \Phi(\pi; P_1, P_2) \right\}.
\]
Note that $\mathcal{S}$ is guaranteed to be non-empty since it contains at least the true distribution \( \{P_1^0, P_2^0\} \). Then consider within $\mathcal{S}$, the distributions that are closest to the empirical distributions $Q_{k,n_k}$ and define the so-called profile function to capture the notion of “distance to the empirical distributions” within the set:

$$
F_{n_1,n_2} := \inf_{\{P_1,P_2\} \in \mathcal{S}} \max_{k=1,2} \mathcal{W}(P_k,Q_{k,n_k}),
$$

(11)

here the subscript indicates its dependence on the sample sizes $n_1$ and $n_2$. Clearly if the radii $\theta_{1,n_1}, \theta_{2,n_2} \geq F_{n_1,n_2}$, then the intersection \( \mathcal{P}_1(\theta_{1,n_1}) \times \mathcal{P}_2(\theta_{2,n_2})) \cap \mathcal{S} \) is nonempty, and thus $\pi^0 \in \Pi(\theta_{1,n_1}, \theta_{2,n_2})$, as illustrated in Figure 3.

Our goal is to find an asymptotic upper bound of such distance and use it as the radii; such a choice will be such that the robust optimal test lies in the confidence region of $\pi^0$. Indeed, if we can provide a theoretical upper bound for the asymptotic value of the right-hand side of (11), then by setting the radii accordingly, the intersection \( \mathcal{P}_1(\theta_{1,n_1}) \times \mathcal{P}_2(\theta_{2,n_2})) \cap \mathcal{S} \) is nonempty and thus $\pi^0 \in \Pi(\theta_{1,n_1}, \theta_{2,n_2})$. From the strong duality in (3) which has been proved in the previous section, any optimal solution to the left-hand side of (3) will belong to the set $\Pi(\theta_{1,n_1}, \theta_{2,n_2})$. This ensures that the optimal test we obtained belongs to the confidence region for the oracle test $\pi^0$.

![Figure 3: An illustration of the profile function. The set $\mathcal{S}$ contains all pairs of distributions $\{P_1, P_2\}$ such that the oracle test is optimal; $F_{n_1,n_2}$ denotes the minimal distance from the empirical distribution to the set $\mathcal{S}$.](image)

We first derive an equivalent dual representation of the profile function $F_{n_1,n_2}$. We introduce some additional definitions and notations as follows. We partition the sample space $\Omega$ as

$$
\Omega_1^\circ := \{\omega \in \Omega : dP_1^0(\omega) \geq dP_2^0(\omega)\}, \quad \Omega_2^\circ := \{\omega \in \Omega : dP_1^0(\omega) < dP_2^0(\omega)\}.
$$

Thereby the oracle test $\pi^0$ accepts hypothesis $H_0$ on set $\Omega_1^\circ$ and accept hypothesis $H_1$ on set
The boundary between $\Omega_1^2$ and $\Omega_2^2$ corresponds to the decision boundary of the oracle test $\pi^*$; the boundary is typically of measure zero for continuous distributions. Denote by $\mathcal{B}_+(\Omega)$ (Lip($\Omega$)) the set of bounded and non-negative (respectively, 1-Lipschitz continuous) functions on $\Omega$. Define the function class:

$$
\mathcal{A} := \left\{ \alpha = \alpha_2 \mathbb{I}_{\Omega_2^2} - \alpha_1 \mathbb{I}_{\Omega_1^2} : \alpha_k \in \mathcal{B}_+(\Omega_k^2) \cap \text{Lip}(\Omega_k^2), \alpha(\omega_k^0) = 0, \ k = 1, 2 \right\},
$$

(12)

where $\mathbb{I}$ is the indicator function and $\omega_k^0 \in \Omega_k^2$, $k = 1, 2$. Thus for each function $\alpha \in \mathcal{A}$, the positive part is on $\Omega_2^2$ and the negative part is on $\Omega_1^2$, and all functions in $\mathcal{A}$ coincide on $\omega_1^0, \omega_2^0$. We have the following lemma, whose proof is given in Appendix B.1.

**Lemma 3.** The profile function $F_{n_1,n_2}$ defined in (11) equals

$$
F_{n_1,n_2} = \sup_{\lambda_1, \lambda_2 \geq 0, \lambda_1 + \lambda_2 \leq 1} \left\{ \mathbb{E}_{\omega_1 \sim Q_{1,n_1}} \left[ \inf_{\omega \in \Omega} \{ \lambda_1 c(\omega, \hat{\omega}_1) + \alpha(\omega) \} \right] + \mathbb{E}_{\omega_2 \sim Q_{2,n_2}} \left[ \inf_{\omega \in \Omega} \{ \lambda_2 c(\omega, \hat{\omega}_2) - \alpha(\omega) \} \right] \right\}. 
$$

The objective function, denoted as $F_{n_1,n_2}(\lambda_1, \lambda_2, \alpha)$, of the above supreme problem can be decoupled into two terms: $F_{n_1,n_2}(\lambda_1, \lambda_2, \alpha) = E_{n_1,n_2}(\lambda_1, \lambda_2, \alpha) + G_{n_1,n_2}(\alpha)$, where

$$
E_{n_1,n_2}(\lambda_1, \lambda_2, \alpha) := \frac{1}{n_1} \sum_{i=1}^{n_1} \inf_{\omega \in \Omega} \{ \lambda_1 c(\omega, \hat{\omega}_1^i) + \alpha(\omega) - \alpha(\hat{\omega}_1^i) \}
$$

$$
+ \frac{1}{n_2} \sum_{j=1}^{n_2} \inf_{\omega \in \Omega} \{ \lambda_2 c(\omega, \hat{\omega}_2^j) - (\alpha(\omega) - \alpha(\hat{\omega}_2^j)) \},
$$

$$
G_{n_1,n_2}(\alpha) := \frac{1}{n_1} \sum_{i=1}^{n_1(N)} \alpha(\hat{\omega}_1^i) - \frac{1}{n_2} \sum_{j=1}^{n_2(N)} \alpha(\hat{\omega}_2^j).
$$

It follows that $E_{n_1,n_2}(\lambda_1, \lambda_2, \alpha) \leq 0$ since the inf value is non-positive by taking $\omega = \hat{\omega}_1^i$ and $\omega = \hat{\omega}_2^j$, respectively, whence $F_{n_1,n_2}(\lambda_1, \lambda_2, \alpha) \leq G_{n_1,n_2}(\alpha)$ and

$$
F_{n_1,n_2} \leq \sup_{\alpha \in \mathcal{A}} G_{n_1,n_2}(\alpha).
$$

Based on the definition of $\mathcal{A}$ in (12), we observe a close-form solution for $\sup_{\alpha \in \mathcal{A}} G_{n_1,n_2}(\alpha)$ as follows. By definition of $\mathcal{A}$, $\alpha(\hat{\omega}_1^i) \leq 0$ for $\hat{\omega}_1^i \in \Omega_1^2$ and $\alpha(\hat{\omega}_2^j) \geq 0$ for $\hat{\omega}_2^j \in \Omega_2^2$. Therefore, to maximize $G_{n_1,n_2}(\alpha)$, we can set $\alpha(\hat{\omega}_1^i) = 0$ for $\hat{\omega}_1^i \in \Omega_1^2$ and $\alpha(\hat{\omega}_2^j) = 0$ for $\hat{\omega}_2^j \in \Omega_2^2$. In addition, since $\alpha_1, \alpha_2$ are 1-Lipschitz, we have $\alpha(\hat{\omega}_1^i) \leq \min_{j: \omega_2^j \in \Omega_2^2} c(\hat{\omega}_1^i, \hat{\omega}_2^j)$ for $\hat{\omega}_1^i \in \Omega_2^2$ and
\( \alpha(\hat{\omega}_2^j) \geq -\min_{i} \omega_i^{c}(\hat{\omega}_2^j, \hat{\omega}_1^j) \) for \( \hat{\omega}_2^j \in \Omega_1^c \). Hence we have

\[
\sup_{\alpha \in A} G_{n_1,n_2}(\alpha) = \frac{1}{n_1} \sum_{i : \hat{\omega}_1^i \in \Omega_1^c} \min_{j : \hat{\omega}_2^j \in \Omega_2^c} c(\hat{\omega}_1^i, \hat{\omega}_2^j) + \frac{1}{n_2} \sum_{j : \hat{\omega}_2^j \in \Omega_2^c} \min_{i : \hat{\omega}_1^i \in \Omega_1^c} c(\hat{\omega}_2^j, \hat{\omega}_1^i). \tag{13}
\]

Note that the profile function defined in (11) measures the minimal transport cost from the empirical distributions to some distribution in the set \( S \) that yields the same optimal test as the oracle test. From this perspective, the right-hand side of (13) provides an upper bound on such minimal transport cost. It basically suggests to move those empirical samples \( \hat{\omega}_1^i \) (resp. \( \hat{\omega}_2^j \)) falling into the wrong region \( \Omega_2^c \) (resp. \( \Omega_1^c \)) to the closest empirical samples in a different class \( \arg\min_{j : \hat{\omega}_2^j \in \Omega_2^c} c(\hat{\omega}_1^i, \hat{\omega}_2^j) \) (resp. \( \arg\min_{i : \hat{\omega}_1^i \in \Omega_1^c} c(\hat{\omega}_2^j, \hat{\omega}_1^i) \)). Thereby, this form sheds light on an approximate optimal distributions of (11) that are obtained by moving empirical points to some neighboring points in a different class. The resulting distributions can be different from the true distribution, but yield an optimal test close to the oracle test.

Next, we compute the asymptotic value of \( \sup_{\alpha \in A} G_{n_1,n_2}(\alpha) \) using (13), which only involves the minimum-distance-type statistics of two sets of sample, which are easier to analyze than \( F_{n_1,n_2} \). We consider a balanced sample size regime.

**Theorem 2.** Suppose \( \lim_{n_1,n_2 \to \infty} n_2/n_1 = c > 0 \). Assume that \( f_1 \) and \( f_2 \) are respectively the density functions of \( P_1^c \) and \( P_2^c \) that are absolutely continuous to each other and satisfy

\[
\int_{\Omega_1^c} f_2(x)f_1(x)^{-1/d} dx < \infty, \quad \int_{\Omega_2^c} f_1(x)f_2(x)^{-1/d} dx < \infty,
\]

and for some \( \epsilon > 0 \) it holds that

\[
\sup_{n \in \mathbb{N}} \mathbb{E}_{x \sim f_1|\Omega_2^c, x_1, \ldots, x_n \sim f_2|\Omega_2^c} [(n^{1/d} \min_{1 \leq i \leq n} \|x - x_i\|)^{1+\epsilon}] < \infty,
\]

\[
\sup_{n \in \mathbb{N}} \mathbb{E}_{x \sim f_2|\Omega_1^c, x_1, \ldots, x_n \sim f_1|\Omega_1^c} [(n^{1/d} \min_{1 \leq i \leq n} \|x - x_i\|)^{1+\epsilon}] < \infty,
\]

where \( f|_A \) denotes the density of the restriction of distribution \( f \) on a set \( A \). Then

\[
n_1^{1/d} \sup_{\alpha \in A} G_{n_1,n_2}(\alpha) \to \frac{\Gamma(1 + 1/d)}{V_d} \left( c^{-1/d} \int_{\Omega_1^c} f_1(x) dx + \int_{\Omega_2^c} f_2(x) dx \right), \tag{14}
\]

in \( L^1 \) as \( n_1, n_2 \to \infty \), where \( V_d = \pi^{d/2}/\Gamma(1 + d/2) \) is the volume of the unit ball in \( \mathbb{R}^d \), and \( \Gamma(x) = \int_0^\infty z^{x-1}e^{-z}dz \) is the Gamma function.

The assumptions on the true data-generating densities resemble the assumptions required for computing the nearest neighbor distances in [11, 32, 33]. Under these assumptions,
the weak law of large numbers is applied to the right-hand side of (13). They can be satisfied under several scenarios, which includes but not limited to: (i) the set $\Omega_1^\circ, \Omega_2^\circ$ are both a finite union of convex bounded sets with non-empty interior and the restricted density $f_1|_{\Omega_1^\circ}, f_2|_{\Omega_2^\circ}$ are bounded away from zero, and (ii) the restricted densities satisfy that for some $r > d/(d-1)$, we have $\int_{\Omega_j^\circ} \|x\|_2 f_k|_{\Omega_j^\circ}(x)dx < \infty, k, j = 1, 2$ [32].

The first component on the right-hand side of (14) equals the limit of the expectation of $n_2^{1/d} \min_{1 \leq i \leq n_2} \|x - x_i\|$, where $x \sim f_1|_{\Omega_2^\circ}$ and $x_i \sim f_2|_{\Omega_2^\circ}$; similar for the second component. It is computed by a conditioning argument where we condition on the random variable with respect to which we compute its nearest-neighbor distance, following a same argument as in [33, Lemma 3.2]. Observe that $\int_{\Omega_2^\circ} f_1/f_2^{1/d} dx = \int_{\Omega_2^\circ} (f_1/f_2)^{1/d} f_1^{d-1} dx$. Hence it depends on the true densities and the value will be smaller if the density $f_1$ is relatively smaller on the set $\Omega_2^\circ$, and if the density ratio $f_1/f_2$ is close to 0 (note that it is always less than or equal to 1 on $\Omega_2^\circ$). This indicates that our choice of the radii tends to be smaller for distributions that are more different and thus it would be easier to distinguish between them.

Based on our principle, Theorem 2 shows that our choice of the radii will be of the order $O(n_1^{1/d})$ under a balanced sample size regime. Since our framework yields a non-parametric test, this order is consistent with other non-parametric methods, and represents only the worst-case scenario and may be improved if additional conditions on the true data-generating distributions are imposed. We would like to point out that although the same order can be obtained using the concentration principle that the uncertainty sets contain true distributions with high probability [5, 12, 10], our bound in (14) provides a more informative constant term that involves the density ratio of the two underlying distributions; while the constant term obtained from the concentration principle would not involve any relationship between the two underlying distributions.

Moreover, we remark that if the support $\Omega_1^\circ, \Omega_2^\circ$ are compact convex sets and the restricted densities $f_1|_{\Omega_1^\circ}, f_2|_{\Omega_2^\circ}$ are continuous, bounded away from zero, and has bounded partial derivatives, then the rate of convergence has been provided explicitly in [11]: for all $0 < \rho < 1/d$, we have that as $N \to \infty$, the higher order terms on the right-hand side of (14) would be $O \left( n_1^{-(1/d-\rho)} \right)$.

We also remark that although we adopt a similar principle as used in [3, 42] by considering the profile function $F_{n_1, n_2}$, the proof in our case is much more challenging, because: (1) the uncertainty set here involves the empirical samples from two classes instead of one uncertainty set; (2) the introduced variable $\alpha_1, \alpha_2$ are functions in the continuous samples space instead of a finite-dimensional vector, thus the optimality condition is not a simple first-order condition but involves inequalities yielding from variational principle, resulting in an additional constraints for solving $F_{n_1, n_2}$. Thus, we develop quite different analytical
techniques to obtain the results. Details can be found in Appendix B.2.

5 Numerical Experiments

In this section, we present several numerical experiments to demonstrate the good performance of our method.

5.1 Synthetic data: Testing Gaussian mixtures

Assume the dimension is 100 and the samples under two hypotheses are generated from Gaussian mixture models (GMM) following the distributions $0.5 \mathcal{N}(0.4e, I_{100}) + 0.5 \mathcal{N}(-0.4e, I_{100})$ and $0.5 \mathcal{N}(0.4f, I_{100}) + 0.5 \mathcal{N}(-0.4f, I_{100})$, respectively. Here $e \in \mathbb{R}^{100}$ is a vector with all entries equal to 1, and $f \in \mathbb{R}^{100}$ is a vector with the first 50 entries equal to 1 and remaining 50 entries equal to $-1$. Consider a setting with a small number of training samples $n_1 = n_2 = 10$, and then test on 1000 new samples from each mixture model. The radius of the uncertainty set and the kernel bandwidth are determined by cross-validation.

Table 1: GMM data, 100-dimensional, comparisons averaged over 500 trials.

| # observation (m) | Ours | GMM   | Logistic | Kernel SVM | 3-layer NN |
|-------------------|------|-------|----------|------------|------------|
| 1                 | 0.2145 | 0.2588 | 0.4925   | 0.3564     | 0.4164     |
| 2                 | 0.2157 | 0.2597 | 0.4927   | 0.3581     | 0.4164     |
| 3                 | 0.1331 | 0.1755 | 0.4905   | 0.3122     | 0.3796     |
| 4                 | 0.1329 | 0.1762 | 0.4905   | 0.3129     | 0.3808     |
| 5                 | 0.0937 | 0.1310 | 0.4888   | 0.2877     | 0.3575     |
| 6                 | 0.0938 | 0.1315 | 0.4881   | 0.2893     | 0.3570     |
| 7                 | 0.0715 | 0.1034 | 0.4880   | 0.2727     | 0.3399     |
| 8                 | 0.0715 | 0.1038 | 0.4876   | 0.2745     | 0.3401     |
| 9                 | 0.0579 | 0.0850 | 0.4873   | 0.2634     | 0.3264     |
| 10                | 0.0578 | 0.0851 | 0.4874   | 0.2641     | 0.3267     |

We compare the performance of the proposed approach with several commonly used classifiers. They are comparable since binary classifiers can be used for deciding hypotheses, although they are designed with different targets. The competitors include the Gaussian Mixture Model (GMM), logistic regression, kernel support vector machine (SVM) with radial basis function (RBF) kernel, and a three-layer perceptron [13] to illustrate the performance of neural networks. The results are summarized in Table 1, where the first column corresponds to the single observation scheme, while other columns are results using multiple observations, with the number of observations $m$ varying from 2 to 10. We use the majority rule for
GMM, logistic regression, kernel SVM, and three-layer neural networks (NN) for testing batch samples. Note that there are over 2500 parameters in the neural network model with two hidden layers (50 nodes in each layer), which is challenging to learn when the training data size is small. Moreover, given only ten samples per class, estimating the underlying Gaussian mixture model is unrealistic, so that any parametric methods will suffer. The results demonstrate that when there is a small sample size, our minimax test outperforms other methods.

5.2 Real data: MNIST handwritten digits classification

We also compare the performance using MNIST handwritten digits dataset [25]. The full dataset contains 70,000 images, from which we randomly select five training images from each class. We solve the optimal randomized test from (7) with the radii parameters chosen by cross-validation. For the batch test setting, we divide test images from the same class into batches, each consisting of \( m \) images. The decision for each batch is made using the majority rule for the optimal test in Section 3.5, as well as for logistic regression and SVM. We repeat this process to 500 randomly selected batches, and the average misclassification rates are reported in Table 2. The results show that our method significantly outperforms logistic regression and SVM. Moreover, the performance gain is higher in the batch test setting: the errors decay quickly as \( m \) increases. Note that the neural network-based deep learning model is not appropriate for this setting since the data-size is too small to train the model.

| # observation (\( m \)) | Ours  | Logistic | SVM   |
|--------------------------|-------|----------|-------|
| 1                        | 0.3572| 0.3729   | 0.3674|
| 2                        | 0.3631| 0.3797   | 0.3712|
| 3                        | 0.2772| 0.2897   | 0.2840|
| 4                        | 0.2122| 0.2239   | 0.2169|
| 5                        | 0.1786| 0.1882   | 0.1827|
| 6                        | 0.1540| 0.1643   | 0.1588|
| 7                        | 0.1347| 0.1446   | 0.1391|
| 8                        | 0.1185| 0.1276   | 0.1222|
| 9                        | 0.1063| 0.1160   | 0.1119|
| 10                       | 0.0960| 0.1057   | 0.1010|
5.3 Application: Human activity detection

In this subsection, we apply the optimal test for human activity detection from sequential data, using a dataset released by the Wireless Sensor Data Mining Lab in 2013 [28, 49, 23]. In this dataset, 225 users were asked to perform specific activities, including walking, jogging, stairs, sitting, standing, and lying down; the data were recorded using accelerometers. Our goal is to detect the change of activity in real-time from sequential observations. Since it is difficult to build precise parametric models for distributions of various activities, traditional parametric change-point detection methods do not work well. We compare the proposed method with a standard nonparametric multivariate sequential change-point detection procedure based on the Hotelling’s $T^2$-squared statistic [29]. The raw data consists of sequences of observations for one person; each sequence may contain more than one change-points, and the time duration for each activity is also different. For this experiment, we only consider two types of transitions of activities: walking to jogging and jogging to walking. We extract 360 sequences of length 100 such that each sequence only contains one change-point.

We construct a change-point detection procedure using our optimal test as follows. Denote the data sequence as $\{\omega_t, t = 1, 2, \ldots\}$. At any possible change-point time $t$, we treat samples in time windows $[t-w, t-1]$ and $[t+1, t+w]$ as two groups of training data and find the LFDs $\{P^*_1, P^*_2\}$ by solving the convex problem in Equation (7). Then we calculate the detection statistic as $P^*_2(\omega_t) - P^*_1(\omega_t)$, inspired by the optimal detector in Lemma 1. We couple this test statistic with the CUSUM-type recursion [31], which can accumulate change and detects small deviations quickly. The recursive detection statistic is defined as $S_t = \max\{0, S_{t-1} + P^*_2(\omega_t) - P^*_1(\omega_t)\}$, with $S_0 = 0$. A change is detected when $S_t$ exceeds a pre-specified threshold for the first time. Such scheme is similar to the combination of convex optimization solution and change-point detection procedure [7]. In the experiment, we set the window size $w = 10$ and choose the same radii for uncertainty sets using cross-validation. The Hotelling’s $T^2$-squared procedure is constructed similarly. Using historical samples, we estimate the nominal (pre-change) mean $\hat{\mu}$ and covariance $\hat{\Sigma}$. The Hotelling’s $T^2$-squared statistics at time $t$ is defined as $(\omega_t - \hat{\mu})^T\hat{\Sigma}^{-1}(\omega_t - \hat{\mu})$ and the Hotelling procedure uses a CUSUM-type recursion: $H_t = \max\{0, H_{t-1} + (\omega_t - \hat{\mu})^T\hat{\Sigma}^{-1}(\omega_t - \hat{\mu})\}$.

We compare the expected detection delay (EDD) versus Type-I error. Here EDD is defined as the average number of samples that a procedure needs before detects a change after it has occurred, which is a commonly used metric for sequential change-point detection [50]. The Type-I error corresponds to the probability of detecting a change when there is no change. We consider a range of thresholds such that the corresponding Type-I error is from 0.05 to 0.35. The results in Figure 4 show that our test significantly outperforms Hotelling’s $T^2$-squared procedure in detecting the change quicker under the same Type-I error.
Figure 4: Comparison of the Expected Detection Delay (EDD) of our test with the Hotelling’s $T^2$-squared procedure for detecting two type of activity transitions: jogging to walking (left) and walking to jogging (right).

6 Conclusions and Discussions

In this paper, we present a new approach for robust hypothesis testing when there are limited “training samples” for each hypothesis. We formulate the problem as a minimax hypothesis testing problem to decide between two disjoint sets of distributions centered around empirical distributions in Wasserstein metrics. This formulation, although statistically sound – can be treated as a “data-driven” version of Huber’s robust hypothesis test, is computationally challenging since it involves an infinitely dimensional optimization problem. Thus, we present a computationally efficient framework for solving the minimax test, revealing the optimal test’s statistical meaning. We also prove how to extend the minimax test from empirical support to the whole space and use it for the “batch” test settings. Moreover, we characterize the radius selection by providing an asymptotic upper bound for the sufficient radii and shed light on the optimal test’s generalization property. We demonstrate the good performance of the proposed robust test on simulated and real data.

The method can be kernelized to handle more complex data structures (e.g., the observations are not real-valued). The kernelization can be conveniently done by replacing the metric $c(\cdot, \cdot)$ used in solving the optimal test (7) with other distances metrics between features after kernel transformation. Take the Euclidean norm as an example. Given a kernel function $\mathcal{K}(\cdot, \cdot)$ that measures similarity between any pair of data, the pairwise norm $c(\omega^l, \omega^m) = \|\omega^l - \omega^m\|$ in (7) can be replaced with the kernel version distance $\mathcal{K}(\omega^l, \omega^m)$. Moreover, this means that the proposed framework can be combined with feature selection and neural networks to enhance its performance in practice for complex datasets.
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A Proofs for Section 3

A.1 Proof of Lemma 1

Note that the probability measures $P_1, P_2$ are absolutely continuous with respect to $P_1 + P_2$, hence we have

$$\inf_{\pi} \Phi(\pi; P_1, P_2) = \inf_{\pi} \int_{\Omega} \left[ \left(1 - \pi(\omega)\right) \frac{dP_1}{d(P_1 + P_2)}(\omega) + \pi(\omega) \frac{dP_2}{d(P_1 + P_2)}(\omega) \right] d(P_1 + P_2)(\omega)$$

$$= \inf_{\pi} \int_{\Omega_0} \left[ \left(1 - \pi(\omega)\right) \frac{dP_1}{d(P_1 + P_2)}(\omega) + \pi(\omega) \frac{dP_2}{d(P_1 + P_2)}(\omega) \right] d(P_1 + P_2)(\omega)$$

$$= \int_{\Omega_0} \inf_{0 \leq x \leq 1} \left[ \left(1 - x\right) \frac{dP_1}{d(P_1 + P_2)}(\omega) + x \frac{dP_2}{d(P_1 + P_2)}(\omega) \right] d(P_1 + P_2)(\omega),$$

where the second equality holds because the integral depends only on the subset $\Omega_0 := \{ \omega \in \Omega : 0 < \frac{dP_k}{d(P_1 + P_2)}(\omega) < 1, k = 1, 2 \}$, on which $P_1, P_2$ are absolutely continuous with respect to each other; the third equality is due to Lemma 7, with $\mathcal{M}$ being the set of measurable functions and $f(x, \omega) = \left[ \left(1 - x\right) \frac{dP_1}{d(P_1 + P_2)}(\omega) + x \frac{dP_2}{d(P_1 + P_2)}(\omega) \right] \chi_{[0,1]}(x)$, where $\chi_{[0,1]}(x) = 1$ if $x \in [0,1]$ and $\infty$ otherwise.

For any $\omega$, the infimum $\pi^*(\omega)$ of the inner minimization in (15) is attained at 0 or 1. Therefore, for any $\omega \in \Omega$,

$$\left(1 - \pi^*(\omega)\right) \frac{dP_1}{d(P_1 + P_2)}(\omega) + \pi^*(\omega) \frac{dP_2}{d(P_1 + P_2)}(\omega) = \min \left\{ \frac{dP_1}{d(P_1 + P_2)}(\omega), \frac{dP_2}{d(P_1 + P_2)}(\omega) \right\}.$$

This completes the proof.
A.2 Proof of Lemma 2

Denote by $L^1(\mu)$ the space of all integrable functions with respect to the measure $\mu$. Using Lagrangian and Kantorovich’s duality (Lemma 6), we rewrite the problem as

$$\sup_{P_1, P_2 \in \mathcal{P}(\Omega)} \inf_{\lambda_1, \lambda_2 \geq 0} \left\{ \psi(P_1, P_2) + \sum_{k=1}^{2} \lambda_k \theta_k - \sum_{k=1}^{2} \lambda_k \left( \frac{1}{n_k} \sum_{i=1}^{n_k} u_k^i \right) + \int_{\Omega} v_k dP_k : u_k^i + v_k(\omega) \leq c(\omega, \hat{\omega}_k^i), \ \forall 1 \leq i \leq n_k, \forall \omega \in \Omega \right\}$$

$$= \sup_{P_1, P_2 \in \mathcal{P}(\Omega)} \inf_{\lambda_1, \lambda_2 \geq 0} \left\{ \psi(P_1, P_2) + \sum_{k=1}^{2} \lambda_k \theta_k - \sum_{k=1}^{2} \lambda_k \left( \frac{1}{n_k} \sum_{i=1}^{n_k} u_k^i \right) + \int_{\Omega} v_k dP_k : u_k^i + \min_{\lambda} \left\{ \lambda \leq c(\omega, \hat{\omega}_k^i) \right\}, \ \forall 1 \leq i \leq n_k, \forall \omega \in \Omega \right\}$$

where the second equality holds by combining the innermost supreme problem with the infimum problem; and the third equality holds by replacing $\lambda_k u_k^i$ with $u_k^i$ and $\lambda_k v_k$ with $v_k$ (note that such change of variable is valid even when $\lambda_k = 0$). Furthermore, since the objective function is non-increasing in $v_k$, we can replace $v_k$ with $\min_{1 \leq i \leq n_k} \left\{ \lambda_k c(\omega, \hat{\omega}_k^i) - u_k^i \right\}$ without changing the optimal value. Interchanging sup and inf yields

$$\sup_{P_1, P_2 \in \mathcal{P}(\Omega)} \psi(P_1, P_2) \leq \inf_{\lambda_1, \lambda_2 \geq 0} \left\{ \sum_{k=1}^{2} \lambda_k \theta_k - \sum_{k=1}^{2} \frac{1}{n_k} \sum_{i=1}^{n_k} u_k^i + \sup_{P_1, P_2 \in \mathcal{P}(\Omega)} \left\{ \psi(P_1, P_2) - \int_{\Omega} \sum_{1 \leq i \leq n_k} \left\{ \lambda_k c(\omega, \hat{\omega}_k^i) - u_k^i \right\} dP_k \right\} \right\}.$$ (16)

Now let us study the inner supremum in (16). For a given distribution $(P_1, P_2)$ and any
By definition we have \( \omega \in \text{supp } P_1 \cup \text{supp } P_2 \), let \( i_k(\omega) = \arg \min_i \{ \lambda_k c(\omega, \hat{\omega}_k^i) - u_k^i \} \), \( k = 1, 2 \), set

\[
T(\omega) := \begin{cases} 
\hat{\omega}_1^{i_1(\omega)}, & \text{if } \lambda_1 \frac{dP_1}{d(P_1 + P_2)}(\omega) \geq \lambda_2 \frac{dP_2}{d(P_1 + P_2)}(\omega), \\
\hat{\omega}_2^{i_2(\omega)}, & \text{if } \lambda_1 \frac{dP_1}{d(P_1 + P_2)}(\omega) < \lambda_2 \frac{dP_2}{d(P_1 + P_2)}(\omega), 
\end{cases}
\]

whence

\[
T(\omega) \in \arg \min_{\omega' \in \Omega} \left\{ \sum_{k=1}^{2} \left[ \lambda_k c(\omega', \hat{\omega}_k^{i_k(\omega)}) - u_k^{i_k(\omega)} \right] \frac{dP_k}{d(P_1 + P_2)}(\omega) \right\}.
\]

By definition we have \( T(\omega) \in \hat{\Omega} \). Define another solution \((P'_1, P'_2)\) such that \( P'_k(B) = P_k\{ \omega \in \Omega : T(\omega) \in B \} \) for any Borel set \( B \subset \hat{\Omega} \). It follows that

\[
\sum_{k=1}^{2} \int_{\hat{\Omega}} \min_{1 \leq i \leq n_k} \left\{ \lambda_k c(\omega, \hat{\omega}_k^i) - u_k^i \right\} dP'_k(\omega) \\
= \sum_{k=1}^{2} \int_{\Omega} \min_{1 \leq i \leq n_k} \left\{ \lambda_k c(T(\omega), \hat{\omega}_k^i) - u_k^i \right\} dP_k(\omega) \\
\leq \sum_{k=1}^{2} \int_{\Omega} \left( \lambda_k c(T(\omega), \hat{\omega}_k^{i_k(\omega)}) - u_k^{i_k(\omega)} \right) dP_k(\omega) \\
\leq \sum_{k=1}^{2} \int_{\Omega} \left( \lambda_k c(\omega, \hat{\omega}_k^{i_k(\omega)}) - u_k^{i_k(\omega)} \right) dP_k(\omega).
\]

In addition, by a simple fact that \( \sum_{i} \min\{x_i, y_i\} \leq \min\{\sum_{i} x_i, \sum_{i} y_i\} \) for any series \( \{x_i, y_i\} \), we have

\[
\psi(P_1, P_2) = \int_{\Omega} \min \left\{ \frac{dP_1}{d(P_1 + P_2)}(\omega), \frac{dP_2}{d(P_1 + P_2)}(\omega) \right\} d(P_1 + P_2)(\omega) \\
\leq \sum_{\hat{\omega} \in \hat{\Omega}} \min\{P_1\{\omega \in \Omega : T(\omega) = \hat{\omega}\}, P_2\{\omega \in \Omega : T(\omega) = \hat{\omega}\}\} \\
= \sum_{\hat{\omega} \in \hat{\Omega}} \min\{P'_1(\hat{\omega}), P'_2(\hat{\omega})\} \\
= \psi(P'_1, P'_2).
\]

Hence \((P'_1, P'_2)\) yields an objective value no worse than \((P_1, P_2)\) for the inner supremum in (16). This suggests that in order to solve the inner supremum of (16), it suffices to only consider \((P_1, P_2)\) with \( \text{supp } P_1 \subset \hat{\Omega} \) and \( \text{supp } P_2 \subset \hat{\Omega} \).

For \( l = 1, \ldots, n \), set \( P'_k = P_k(\hat{\omega}_l) \), and note that \( \gamma_k \in \Gamma(P_k, Q_{k,n}) \) can be identified with a non-negative matrix \( \gamma_k \in \mathbb{R}^{n \times n}_+ \) with each column and row summing up to 1. Thus, the
inner supremum in (16) can now be equivalently written as
\[
\sup_{p_1, p_2 \in \mathbb{R}^n_+} \left\{ \sum_{l=1}^n \min \{p_1^l, p_2^l\} - \sum_{k=1}^2 \sum_{l=1}^n p_k^l \min_{1 \leq i \leq n_k} \{\lambda_k c(\hat{\omega}^l_1, \hat{\omega}^l_k) - u_k^l\} \right\}.
\]

It follows that
\[
\sup_{P_1 \in P_1, P_2 \in P_2} \psi(P_1, P_2) \\
\leq \inf_{\lambda_1, \lambda_2 \geq 0} \left\{ \sum_{k=1}^2 \lambda_k \theta_k - \sum_{k=1}^2 \frac{1}{n_k} \sum_{i=1}^{n_k} u_k^i + \sup_{p_1, p_2 \in \mathbb{R}^n_+} \left\{ \sum_{l=1}^n \min \{p_1^l, p_2^l\} \right\} \right. \\
- \sum_{k=1}^2 \sum_{l=1}^n p_k^l \min_{1 \leq i \leq n_k} \{\lambda_k c(\hat{\omega}^l_1, \hat{\omega}^l_k) - u_k^i\} \right\}.
\]

Applying the Lagrangian duality for finite-dimensional convex programming on the right-hand side yields
\[
\sup_{P_1 \in \hat{P}_1, P_2 \in \hat{P}_2} \psi(P_1, P_2) \leq \sup_{P_1 \in \bar{P}_1, P_2 \in \bar{P}_2} \psi(P_1, P_2),
\]

where \(\hat{P}_k := P_k \cap \mathcal{P}(\hat{\Omega})\), \(k = 1, 2\). Observe that both sides have the same objective function, but the feasible region of the right-hand side is a subset of that of the left-hand side, and thus the right-hand side should be no greater than the left-hand side, i.e., the above inequality should hold as equality. Thereby we complete the proof.

A.3 Proof of Theorem 1

Note that from Lemma 2, we have
\[
\sup_{P_1 \in \bar{P}_1, P_2 \in \bar{P}_2} \inf_{\pi: \Omega \to [0,1]} \Phi(\pi; P_1, P_2) = \sup_{P_1 \in P_1, P_2 \in P_2} \inf_{\pi: \Omega \to [0,1]} \Phi(\pi; P_1, P_2) \\
\leq \inf_{\pi: \Omega \to [0,1]} \sup_{P_1 \in \bar{P}_1, P_2 \in \bar{P}_2} \Phi(\pi; P_1, P_2).
\]

Let us prove the other direction.
To begin with, we identify $\hat{\pi} \in [0, 1]^n$ with a function on $\hat{\Omega}$. Using Lemma 8, we have

$$
\sup_{P_1 \in \hat{P}_1} \mathbb{E}_{P_1}[1 - \hat{\pi}] = \inf_{\lambda_1 \geq 0} \left\{ \lambda_1 \theta_1 + \frac{1}{n_1} \sum_{i=1}^{n_1} \max_{1 \leq m \leq n} \left\{ 1 - \hat{\pi}_m - \lambda_1 c(\hat{\omega}_i, \hat{\omega}_m) \right\} \right\},
$$

(17)

$$
\sup_{P_2 \in \hat{P}_2} \mathbb{E}_{P_2}[\hat{\pi}] = \inf_{\lambda_2 \geq 0} \left\{ \lambda_2 \theta_2 + \frac{1}{n_2} \sum_{i=1}^{n_2} \max_{1 \leq m \leq n} \left\{ \hat{\pi}_m - \lambda_2 c(\hat{\omega}_i, \hat{\omega}_m) \right\} \right\}.
$$

Let $\lambda_1^*$ and $\lambda_2^*$ be respectively the minimizers of the two problems in (17). Observe that the right-hand sides of (17) and (8) are identical. Hence (8) implies that $\hat{\pi}^*$ defined in the statement of Theorem 1 satisfies

$$
\mathbb{E}_{P_1^*}[1 - \hat{\pi}^*] = \sup_{P_1 \in \hat{P}_1} \mathbb{E}_{P_1}[1 - \hat{\pi}], \quad \mathbb{E}_{P_2^*}[\hat{\pi}^*] = \sup_{P_2 \in \hat{P}_2} \mathbb{E}_{P_2}[\hat{\pi}],
$$

and thus

$$
\sup_{P_1 \in \hat{P}_1, P_2 \in \hat{P}_2} \Phi(\hat{\pi}^*; P_1, P_2) = \sup_{P_1 \in \hat{P}_1, P_2 \in \hat{P}_2} \Phi(\hat{\pi}; P_1, P_2). \quad (18)
$$

Hence $(\hat{\pi}^*; P_1^*, P_2^*)$ solves the above finite-dimensional convex-concave saddle point problem that always has an optimal solution, which verifies the well-definedness of $\hat{\pi}^*$.

On the other hand, for the $\pi^*$ defined in the statement of Theorem 1, the optimization problem for finding worst-case risk are decoupled and admits the following equivalent reformulations (Lemma 8)

$$
\sup_{P_1 \in P_1} \mathbb{E}_{P_1}[1 - \pi^*(\omega)] = \min_{\lambda_1 \geq 0} \left\{ \lambda_1 \theta_1 + \frac{1}{n_1} \sum_{i=1}^{n_1} \sup_{\omega \in \hat{\Omega}} \left\{ 1 - \pi^*(\omega) - \lambda_1 c(\omega, \hat{\omega}_i) \right\} \right\},
$$

(19)

$$
\sup_{P_2 \in P_2} \mathbb{E}_{P_2}[\pi^*(\omega)] = \min_{\lambda_2 \geq 0} \left\{ \lambda_2 \theta_2 + \frac{1}{n_2} \sum_{i=1}^{n_2} \sup_{\omega \in \hat{\Omega}} \left\{ \pi^*(\omega) - \lambda_2 c(\omega, \hat{\omega}_i) \right\} \right\}.
$$

Comparing (17) and (19), if we can prove $\pi^*$ satisfies

$$
\sup_{\omega \in \hat{\Omega}} \left\{ 1 - \pi^*(\omega) - \lambda_1^* c(\omega, \hat{\omega}_i) \right\} \leq \max_{\omega \in \hat{\Omega}} \left\{ 1 - \hat{\pi}^*(\omega) - \lambda_1^* c(\omega, \hat{\omega}_i) \right\}, \quad \forall 1 \leq i \leq n_1,
$$

$$
\sup_{\omega \in \hat{\Omega}} \left\{ \pi^*(\omega) - \lambda_2^* c(\omega, \hat{\omega}_i) \right\} \leq \max_{\omega \in \hat{\Omega}} \left\{ \hat{\pi}^*(\omega) - \lambda_2^* c(\omega, \hat{\omega}_i) \right\}, \quad \forall 1 \leq i \leq n_2, \quad (20)
$$

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then $\pi^*$ would be an optimal solution to (2.2) since

$$
\inf_{\pi: \Omega \to [0,1]} \sup_{P_1, P_2} \Phi(\pi; P_1, P_2) \leq \sup_{P_1, P_2} \Phi(\pi^*; P_1, P_2) \\
\leq \sup_{P_1, P_2} \Phi(\hat{\pi}; P_1, P_2) \\
= \sup_{P_1, P_2} \inf_{\pi: \Omega \to [0,1]} \Phi(\pi^*; P_1, P_2).
$$

To show (20), for $\pi^*$ restricted on the empirical support $\hat{\Omega}$, we have

$$
\sup_{\omega \in \hat{\Omega}} \{1 - \pi^*(\omega) - \lambda_1^* c(\omega, \hat{\omega}_1^i)\} = \max_{\omega \in \hat{\Omega}} \{1 - \pi^*(\omega) - \lambda_1^* c(\omega, \hat{\omega}_1^i)\}, \quad \forall 1 \leq i \leq n_1,
$$

$$
\sup_{\omega \in \hat{\Omega}} \{\pi^*(\omega) - \lambda_2^* c(\omega, \hat{\omega}_2^i)\} = \max_{\omega \in \hat{\Omega}} \{\pi^*(\omega) - \lambda_2^* c(\omega, \hat{\omega}_2^i)\}, \quad \forall 1 \leq i \leq n_2.
$$

Indeed, this holds by construction $\pi^*(\omega) = \hat{\pi}^*(\omega)$ for $\omega \in \hat{\Omega}$. It remains to show (20) also holds outside of $\hat{\Omega}$:

$$
\sup_{\omega \notin \hat{\Omega}} \{1 - \pi^*(\omega) - \lambda_1^* c(\omega, \hat{\omega}_1^i)\} \leq \max_{\omega \in \hat{\Omega}} \{1 - \pi^*(\omega) - \lambda_1^* c(\omega, \hat{\omega}_1^i)\}, \quad \forall 1 \leq i \leq n_1,
$$

$$
\sup_{\omega \notin \hat{\Omega}} \{\pi^*(\omega) - \lambda_2^* c(\omega, \hat{\omega}_2^i)\} \leq \max_{\omega \in \hat{\Omega}} \{\pi^*(\omega) - \lambda_2^* c(\omega, \hat{\omega}_2^i)\}, \quad \forall 1 \leq i \leq n_2.
$$

To prove this, note that it is equivalent to that $\forall \omega \notin \hat{\Omega}$:

$$
\pi^*(\omega) \geq \min_{\omega \in \hat{\Omega}} \{\pi^*(\omega) + \lambda_1^* c(\omega, \hat{\omega}_1^i)\} - \lambda_1^* c(\omega, \hat{\omega}_1^i), \quad \forall i = 1, \ldots, n_1,
$$

$$
\pi^*(\omega) \leq \lambda_2^* c(\omega, \hat{\omega}_2^j) - \min_{\omega \in \hat{\Omega}} \{\lambda_2^* c(\omega, \hat{\omega}_2^j) - \pi^*(\omega)\}, \quad \forall j = 1, \ldots, n_2. \tag{21}
$$

Observe that $\forall i = 1, \ldots, n_1$ and $\forall j = 1, \ldots, n_2$, we have:

$$
\min_{\omega \in \hat{\Omega}} \{\pi^*(\omega) + \lambda_1^* c(\omega, \hat{\omega}_1^i)\} + \min_{\omega \in \hat{\Omega}} \{\lambda_2^* c(\omega, \hat{\omega}_2^j) - \pi^*(\omega)\}
\leq \begin{cases} 
\pi^*(\hat{\omega}_2^j) + \lambda_1^* c(\hat{\omega}_2^j, \hat{\omega}_1^i) - \pi^*(\hat{\omega}_2^j), & \lambda_1^* \leq \lambda_2^*, \\
\pi^*(\hat{\omega}_1^i) + \lambda_2^* c(\hat{\omega}_1^i, \hat{\omega}_2^j) - \pi^*(\hat{\omega}_1^i), & \lambda_1^* > \lambda_2^*,
\end{cases}
$$

$$
= \min\{\lambda_1^*, \lambda_2^*\} c(\hat{\omega}_1^i, \hat{\omega}_2^j)
$$

$$
\leq \lambda_1^* c(\omega, \hat{\omega}_1^i) + \lambda_2^* c(\omega, \hat{\omega}_2^j), \quad \forall \omega \in \Omega,
$$

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where we have used the triangle inequality of $c$. And we note that

$$\min_{\tilde{\omega} \in \tilde{\Omega}} \{ \pi^*(\tilde{\omega}) + \lambda_1^* c(\omega, \tilde{\omega}_1^i) \} - \lambda_1^* c(\omega, \tilde{\omega}_1^i) \leq \pi^*(\tilde{\omega}_1^i) \leq 1,$$

and

$$\lambda_2^* c(\omega, \tilde{\omega}_2^i) - \min_{\tilde{\omega} \in \tilde{\Omega}} \{ \lambda_2^* c(\omega, \tilde{\omega}_2^i) - \pi^*(\tilde{\omega}) \} \geq \pi^*(\tilde{\omega}_2^i) \geq 0,$$

since $\pi^*(\omega) = \tilde{\pi}^*(\omega) \in [0, 1]$ for $\omega \in \tilde{\Omega}$. Therefore we always have $l(\omega) \leq u(\omega)$ and (21) always admits a feasible solution, as defined in the Theorem statement.

### A.4 Proof of Proposition 1

Given batch samples $\omega_1, \ldots, \omega_m$ sampled i.i.d. from the true distribution $P_1$, define Boolean random variables $\xi_i, 1 \leq i \leq m$ as:

$$\xi_i = \begin{cases} 1 & \pi_1(\omega_i) = 0; \\ 0 & \pi_1(\omega_i) = 1, \end{cases}$$

more specifically, the random variable $\xi_i = 1$ if and only if the test, as applied to observation $\omega_i$, rejects hypothesis $H_0$.

Further, by construction of the Majority test, if the hypothesis $H_0$ is rejected, then the number of $i$’s with $\xi_i = 1$ is at least $m/2$. Thus, the probability to reject $H_0$ is not greater than the probability of the event: in $m$ random Bernoulli trials with probability $\epsilon^*$ of success, the total number of successes is $\geq m/2$. The probability of this event clearly does not exceed:

$$\sum_{m/2 \leq i \leq m} \binom{m}{i} (\epsilon^*)^i (1-\epsilon^*)^{m-i}.$$

When $\epsilon^* < 1/2$, by the Chernoff bound, we have

$$\sum_{m/2 \leq i \leq m} \binom{m}{i} (\epsilon^*)^i (1-\epsilon^*)^{m-i} \leq \exp \{-D(1/2 || \epsilon^*) m\},$$

where $D(1/2 || \epsilon^*) := \frac{1}{2} \log \frac{1}{2\epsilon^*} + \frac{1}{2} \log \frac{1}{2(1-\epsilon^*)}$ is the relative entropy between two Bernoulli distributions with “success” probabilities being $1/2$ and $\epsilon^*$ respectively. It is easy to see that $D(1/2 || \epsilon^*) > 0$. Therefore, the risk goes to 0 exponentially fast, in the order of $\exp \{-D(1/2 || \epsilon^*) m\}$ as $m \to \infty$. 

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B Proofs for Section 4

B.1 Proof of Lemma 3

We first establish an optimality condition (Lemma 4) for the constraint

$$\pi^\circ \in \arg \min_{\pi: \Omega \to [0,1]} \Phi(\pi; P_1, P_2).$$

Without causing confusion, we simply write $$\pi^\circ \in \arg \min_{\pi} \Phi(\pi; P_1, P_2)$$ in subsequent proofs.

**Lemma 4.** Let $$\pi^\circ$$ be the oracle test. For any $$P_1, P_2 \in \mathcal{P}(\Omega),$$ the constraint

$$\pi^\circ \in \arg \min_{\pi: \Omega \to [0,1]} \Phi(\pi; P_1, P_2)$$

holds if and only if

$$\sup_{\alpha_1, \alpha_2 \in B_+(\Omega)} \int_{\Omega} [\alpha_2(\omega)\mathbb{1}_{\Omega_2^c}(\omega) - \alpha_1(\omega)\mathbb{1}_{\Omega_1^c}(\omega)](dP_1 - dP_2)(\omega) = 0. \quad (22)$$

**Proof.** We first prove the necessity. Suppose $$\pi^\circ \in \arg \min_{\pi} \Phi(\pi; P_1, P_2).$$ Then by definition for all randomized test $$\pi,$$ we have

$$\Phi(\pi; P_1, P_2) \geq \Phi(\pi^\circ; P_1, P_2).$$

For any $$\alpha_1, \alpha_2 \in B_+(\Omega),$$ there exists a small enough $$\epsilon > 0$$ such that the following perturbed $$\pi^\circ$$ is still a randomized test:

$$\pi^\circ(\omega) + \epsilon[\alpha_2(\omega)\mathbb{1}_{\Omega_2^c}(\omega) - \alpha_1(\omega)\mathbb{1}_{\Omega_1^c}(\omega)] = \begin{cases} 1 - \epsilon \alpha_1(\omega), & \omega \in \Omega_1^c, \\ \epsilon \alpha_2(\omega), & \omega \in \Omega_2^c, \end{cases}$$

which means that the probability of accepting hypothesis $$H_0$$ is reduced on $$\Omega_1^c,$$ and probability of accepting hypothesis $$H_0$$ is increased on $$\Omega_2^c.$$ Recall $$\alpha = \alpha_2\mathbb{1}_{\Omega_2^c} - \alpha_1\mathbb{1}_{\Omega_1^c}.$$ The optimality of $$\pi^\circ$$ implies that

$$\mathbb{E}_{P_1}[1 - \pi^\circ(\omega) - \epsilon \alpha(\omega)] + \mathbb{E}_{P_2}[\pi^\circ(\omega) + \epsilon \alpha(\omega)] \geq \mathbb{E}_{P_1}[1 - \pi^\circ(\omega)] + \mathbb{E}_{P_2}[\pi^\circ(\omega)].$$

Dividing $$\epsilon$$ on both sides gives $$\mathbb{E}_{P_1}[\alpha(\omega)] - \mathbb{E}_{P_2}[\alpha(\omega)] \leq 0.$$ Moreover, the equality in (22) holds by taking $$\alpha_1 = \alpha_2 \equiv 0,$$ which proves (22).

Next, we prove the sufficiency. Suppose (22) holds. For any randomized test $$\pi,$$ set...
\[ \alpha := \pi - \pi^0. \] Pick \( \alpha_1, \alpha_2 \in \mathcal{B}_+(\Omega) \) such that
\[
\alpha_1(\omega) = \begin{cases} 
1 - \pi(\omega) & \text{if } \omega \in \Omega_1, \\
0 & \text{otherwise;}
\end{cases}
\quad \alpha_2(\omega) = \begin{cases} 
\pi(\omega) & \text{if } \omega \in \Omega_2, \\
0 & \text{otherwise.}
\end{cases}
\]
Then by the definition of \( \pi^0 \), we have \( \alpha(\omega) = \alpha_2(\omega)\mathbb{I}_{\Omega_2}(\omega) - \alpha_1(\omega)\mathbb{I}_{\Omega_1}(\omega) \) for all \( \omega \in \Omega \). It follows that
\[
\mathbb{E}_{P_1}[\alpha(\omega)] - \mathbb{E}_{P_2}[\alpha(\omega)] \leq 0,
\]
and consequently,
\[
\mathbb{E}_{P_1}[1 - \pi(\omega)] + \mathbb{E}_{P_2}[\pi(\omega)] = \mathbb{E}_{P_1}[1 - \pi^0(\omega) - \alpha(\omega)] + \mathbb{E}_{P_2}[\pi^0(\omega) + \alpha(\omega)]
\]
\[
= \mathbb{E}_{P_1}[1 - \pi(\omega)] + \mathbb{E}_{P_2}[\pi(\omega)] - (\mathbb{E}_{P_1}[\alpha(\omega)] - \mathbb{E}_{P_2}[\alpha(\omega)])
\]
\[
\geq \mathbb{E}_{P_1}[1 - \pi(\omega)] + \mathbb{E}_{P_2}[\pi(\omega)].
\]
This indicates that the risk of any test \( \pi \) is greater than or equal to the risk of \( \pi^0 \), implying \( \pi^0 \in \arg \min_{\pi} \Phi(\pi; P_1, P_2) \). Therefore we have completed the proof. \( \square \)

Let us proceed by defining the Lagrangian function
\[
L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2)
:= \sum_{k=1}^{2} \lambda_k \mathcal{W}(P_k, Q_{k,n_k}) + \sum_{k=1}^{2} \sum_{j \neq k} \left\{ \mathbb{E}_{P_k}[\alpha_j(\omega)\mathbb{I}_{\Omega_j^c}(\omega) - \alpha_k(\omega)\mathbb{I}_{\Omega_k^c}(\omega)] \right\}, \tag{23}
\]
where the second term is equivalent to \( \int_{\Omega}[\alpha_2(\omega)\mathbb{I}_{\Omega_2}(\omega) - \alpha_1(\omega)\mathbb{I}_{\Omega_1}(\omega)](dP_1 - dP_2)(\omega) \). Using Lemma 4, if \( \pi^0 \notin \arg \min_{\pi} \Phi(\pi; P_1, P_2) \), then there exists functions \( \alpha_1', \alpha_2' \in \mathcal{B}_+(\Omega) \) such that \( \sum_{k=1}^{2} \sum_{j \neq k} \mathbb{E}_{P_k}[\alpha_j'(\omega)\mathbb{I}_{\Omega_j^c}(\omega) - \alpha_k'(\omega)\mathbb{I}_{\Omega_k^c}(\omega)] > 0 \), whence
\[
\sup_{\alpha_1, \alpha_2 \in \mathcal{B}_+(\Omega)} L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2) \geq \lim_{t \to \infty} L(P_1, P_2; \lambda_1, \lambda_2, t\alpha_1', t\alpha_2') = +\infty.
\]
Therefore, we arrive at an equivalent formulation for the profile function \( F_{n_1,n_2} \) defined in (11):
\[
F_{n_1,n_2} = \inf_{P_1, P_2 \in \mathcal{P}(\Omega)} \sup_{\lambda_1, \lambda_2 \geq 0} \sum_{\lambda_1 + \lambda_2 \leq 1} \mathcal{L}(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2). \tag{24}
\]

In what follows, we prove the strong duality (i.e. exchanging of sup and inf) in five steps. We start by showing the weak duality and simplify the dual formulation of \( F_{n_1,n_2} \). Next, we show that it suffices to restrict the feasible region of \( \alpha_1, \alpha_2 \) from \( \mathcal{B}_+(\Omega) \) to \( \mathcal{B}_+(\Omega) \cap \text{Lip}(\Omega) \), which eventually leads to the set \( \mathcal{A} \) defined in (12), and prove the strong duality by assuming
the support $\Omega$ is compact. Finally, we relax the compactness assumption.

**Step 1** Weak duality.

Exchanging $\inf$ and $\sup$ in Equation (24) yields

$$F_{n_1,n_2} \geq \sup_{\lambda_1,\lambda_2 \geq 0} \inf_{P_1,P_2 \in \mathcal{P}(\Omega)} L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2).$$

(25)

Let us simplify the right-hand side by deriving a closed-form solution to the inner $\inf$ problem. Recall that $\Gamma(P, Q)$ denotes the collection of all Borel probability measures on $\Omega \times \Omega$ with marginal distributions $P$ and $Q$. By the definition of Wasserstein metric, since the empirical distribution $Q_{k,n_k}$ is supported on a finite set $\hat{\Omega}_k = \{\hat{\omega}_1^k, \ldots, \hat{\omega}_{n_k}^k\}$ for $k = 1, 2$, we have

$$\lambda_k \mathcal{W}(P_k, Q_{k,n_k}) = \inf_{\gamma_k \in \Gamma(P_k, Q_{k,n_k})} \left\{ \sum_{i=1}^{n_k} \int_{\Omega} \lambda_k c(\omega, \hat{\omega}_i^k) d\gamma_k(\omega, \hat{\omega}_i^k) \right\}.$$

Moreover, for any distribution $\gamma_k \in \Gamma(P_k, Q_{k,n_k})$, $k = 1, 2$, we have

$$\sum_{j \neq k} \left\{ \mathbb{E}_{P_k}[\alpha_j(\omega) \mathbb{I}_{\Omega_j^k}(\omega)] - \alpha_k(\omega) \mathbb{I}_{\Omega_k^k}(\omega) \right\}$$

$$= \sum_{i=1}^{n_k} \int_{\Omega} \sum_{j \neq k} [\alpha_j(\omega) \mathbb{I}_{\Omega_j^k}(\omega) - \alpha_k(\omega) \mathbb{I}_{\Omega_k^k}(\omega)] d\gamma_k(\omega, \hat{\omega}_i^k).$$

Substituting the above equations to (23), it follows that:

$$L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2)$$

$$= \sum_{k=1}^{2} \inf_{\gamma_k \in \Gamma(P_k, Q_{k,n_k})} \left\{ \sum_{i=1}^{n_k} \int_{\Omega} \left[ \lambda_k c(\omega, \hat{\omega}_i^k) \right. \right.$$

$$+ \left. \sum_{j \neq k} (\alpha_j(\omega) \mathbb{I}_{\Omega_j^k}(\omega) - \alpha_k(\omega) \mathbb{I}_{\Omega_k^k}(\omega)) \right] d\gamma_k(\omega, \hat{\omega}_i^k) \right\}.$$

Thereby for fixed $\lambda_1, \lambda_2, \alpha_1, \alpha_2$, $\inf_{P_1,P_2} L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2)$ can be expressed equivalently as a minimization problem over $\gamma_k$, whose first marginal distribution can be arbitrary
and second marginal is the empirical distribution $Q_{k,n_k}$, $k = 1, 2$:

$$\inf_{P_1, P_2} L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2)$$

$$= \sum_{k=1}^{2} \inf_{\gamma_k \in \Gamma(\cdot, Q_{k,n_k})} \left\{ \sum_{i=1}^{n_k} \int_{\Omega} \left[ \lambda_k c(\omega, \hat{\omega}_k^i) + \sum_{j \neq k} (\alpha_j(\omega) \mathbb{I}_{\Omega_j^k}(\omega) - \alpha_k(\omega) \mathbb{I}_{\Omega_k^k}(\omega)) \right] d\gamma_k(\omega, \hat{\omega}_k^i) \right\}$$

$$= \sum_{k=1}^{2} \frac{1}{n_k} \sum_{i=1}^{n_k} \inf_{\omega \in \Omega} \left\{ \lambda_k c(\omega, \hat{\omega}_k^i) + \sum_{j \neq k} (\alpha_j(\omega) \mathbb{I}_{\Omega_j^k}(\omega) - \alpha_k(\omega) \mathbb{I}_{\Omega_k^k}(\omega)) \right\},$$

where $\Gamma(\cdot, Q_{k,n_k})$ denotes the collection of all Borel probability measures on $\Omega \times \Omega$ with second marginal being $Q_{k,n_k}$, and the last equality is attained by picking

$$\gamma_k(\omega_i, \hat{\omega}_k^i) = \frac{1}{n_k}, \quad i = 1, \ldots, n_k, \quad k = 1, 2,$$

where

$$\omega_i \in \text{arg} \min \omega \in \Omega \left\{ \lambda_k c(\omega, \hat{\omega}_k^i) + \sum_{j \neq k} (\alpha_j(\omega) \mathbb{I}_{\Omega_j^k}(\omega) - \alpha_k(\omega) \mathbb{I}_{\Omega_k^k}(\omega)) \right\}.$$

If the minimizer does not exist, we can argue similarly using a sequence of approximate minimizers. If there are multiple minimizers, we can simply choose one of them or distribute the probability mass $1/n_k$ uniformly on the optimal solution set. Therefore, we have the right-hand side of (25) equals to

$$\sup_{\lambda_1, \lambda_2 \geq 0} \sum_{k=1}^{2} \mathbb{E}_{\hat{\omega}_k \sim Q_{k,n_k}} \left[ \inf_{\omega \in \Omega} \left\{ \lambda_k c(\omega, \hat{\omega}_k) + \sum_{j \neq k} (\alpha_j(\omega) \mathbb{I}_{\Omega_j^k}(\omega) - \alpha_k(\omega) \mathbb{I}_{\Omega_k^k}(\omega)) \right\} \right]. \quad (26)$$

In the sequel, we will refer to the right-hand side of (26) as the dual problem.

**Step 2** Restricting on the subset $\mathcal{A}$ as defined in (12).

We first prove that we can restrict $\alpha_1$ and $\alpha_2$ on the space of Lipschitz continuous functions without affecting the optimal value.

For any feasible solution $(\lambda_1, \lambda_2, \alpha_1, \alpha_2)$ of the dual problem in (26) such that the dual objective is finite, let us construct a modification $(\lambda_1, \lambda_2, \tilde{\alpha}_1, \tilde{\alpha}_2)$ which yields an objective value no worse than $(\lambda_1, \lambda_2, \alpha_1, \alpha_2)$, but enjoys a nicer continuity property. For $i = 1, 2, \ldots, n_1,$
set
\[
\phi_1(\widehat{\omega}_i^1) := \inf_{\omega \in \Omega_1^1}\{\lambda_1 c(\omega, \widehat{\omega}_i^1) + \alpha_2(\omega)\|\omega\|_1^2 - \alpha_1(\omega)\|\omega\|_1^2(\omega)\}
\]
\[
= \min \left\{ \inf_{\omega \in \Omega_1^1}\{\lambda_1 c(\omega, \widehat{\omega}_i^1) - \alpha_1(\omega)\}, \inf_{\omega \in \Omega_1^2}\{\lambda_1 c(\omega, \widehat{\omega}_i^1) + \alpha_2(\omega)\} \right\}.
\]
It follows that
\[
\alpha_1(\omega) \leq \lambda_1 c(\omega, \widehat{\omega}_i^1) - \phi_1(\widehat{\omega}_i^1), \quad \forall \omega \in \Omega_1^1, \forall i = 1, \ldots, n_1.
\] (27)
Define another function \(\tilde{\alpha}_1\) as
\[
\tilde{\alpha}_1(\omega) = \min_{i=1, \ldots, n_1} \{\lambda_1 c(\omega, \widehat{\omega}_i^1) - \phi_1(\widehat{\omega}_i^1)\}, \quad \forall \omega \in \Omega_1^0.
\] (28)
This yields \(\alpha_1(\omega) \leq \tilde{\alpha}_1(\omega)\) for all \(\omega \in \Omega_1^0\), due to (27). Moreover, the objective value in (26) associated with \((\lambda_1, \lambda_2, \tilde{\alpha}_1, \alpha_2)\) is no less than the value associated with \((\lambda_1, \lambda_2, \alpha_1, \alpha_2)\) since
\[
\phi_1(\widehat{\omega}_i^1) \leq \lambda_1 c(\omega, \widehat{\omega}_i^1) - \tilde{\alpha}_1(\omega), \quad \forall \omega \in \Omega_1^0, \forall i = 1, \ldots, n_1,
\]
\[
\lambda_2 c(\omega, \widehat{\omega}_i^2) + \alpha_1(\omega) \leq \lambda_2 c(\omega, \widehat{\omega}_i^2) + \tilde{\alpha}_1(\omega), \quad \forall \omega \in \Omega_1^0, \forall j = i, \ldots, n_2.
\]
Furthermore, the function \(\tilde{\alpha}_1\) defined in this way is Lipschitz with constant \(\lambda_1\). Indeed, for any two points \(\xi, \eta \in \Omega_1^0\), let \(i_1\) and \(i_2\) be the indices at which the minimum are attained in the definition (28) for \(\xi\) and \(\eta\), respectively. We have
\[
\tilde{\alpha}_1(\xi) - \tilde{\alpha}_1(\eta) = [\lambda_1 c(\xi, \widehat{\omega}_i^{1,1}) - \phi_1(\widehat{\omega}_i^{1,1})] - [\lambda_1 c(\eta, \widehat{\omega}_j^{1,2}) - \phi_1(\widehat{\omega}_j^{1,2})]
\]
\[
\leq [\lambda_1 c(\xi, \widehat{\omega}_i^{1,2}) - \phi_1(\widehat{\omega}_i^{1,2})] - [\lambda_1 c(\eta, \widehat{\omega}_j^{1,2}) - \phi_1(\widehat{\omega}_j^{1,2})]
\]
\[
= \lambda_1 [c(\xi, \widehat{\omega}_i^{1,2}) - c(\eta, \widehat{\omega}_j^{1,2})]
\]
\[
\leq \lambda_1 c(\xi, \eta),
\]
where the last inequality is due to the triangle inequality of the metric \(c(\cdot, \cdot)\); and the same inequality holds for \(\tilde{\alpha}_1(\eta) - \tilde{\alpha}_1(\xi)\). In a similar fashion, for \(j = 1, 2, \ldots, n_2\), define
\[
\phi_2(\widehat{\omega}_j^2) := \inf_{\omega}\{\lambda_2 c(\omega, \widehat{\omega}_j^2) + \tilde{\alpha}_1(\omega)\|\omega\|_1^2(\omega) - \alpha_2(\omega)\|\omega\|_2^2(\omega)\}
\]
\[
= \min \left\{ \inf_{\omega \in \Omega_1^1}\{\lambda_2 c(\omega, \widehat{\omega}_j^2) + \tilde{\alpha}_1(\omega)\}, \inf_{\omega \in \Omega_1^2}\{\lambda_2 c(\omega, \widehat{\omega}_j^2) - \alpha_2(\omega)\} \right\},
\]
and set
\[
\tilde{\alpha}_2(\omega) := \min_{j=1, \ldots, n_2} \{\lambda_2 c(\omega, \widehat{\omega}_j^2) - \phi_2(\widehat{\omega}_j^2)\}, \quad \forall \omega \in \Omega_2^0.
\] (29)
Then \(\alpha_2(\omega) \leq \tilde{\alpha}_2(\omega)\) for all \(\omega \in \Omega_2^0\) and the objective value associated with \((\lambda_1, \lambda_2, \tilde{\alpha}_1, \alpha_2)\) is no less than the objective value associated with \((\lambda_1, \lambda_2, \tilde{\alpha}_1, \alpha_2)\); and \(\tilde{\alpha}_2\) is Lipschitz with
constant \( \lambda_2 \). Since we are in the region \( \{ \lambda_1, \lambda_2 \geq 0, \lambda_1 + \lambda_2 \leq 1 \} \), the argument above proves that without loss of generality we can restrict \( \alpha_1, \alpha_2 \) on the set of 1-Lipschitz continuous functions.

Observe that the objective value does not change if we shift \( \alpha_k \) by any constant \( C_k \), \( k = 1, 2 \). Hence, without loss of generality, we can only consider those satisfying \( \alpha_k(\omega_k^0) = 0 \) without affecting the optimal value, where \( \omega_k^0 \in \Omega_k^0, k = 1, 2 \). By the above argument, we have shown that it suffices to restrict the feasible region on \( A \).

**Step 3** Strong duality for compact space.

Now assume \( \Omega \) is compact. We aim to prove the strong duality by applying Sion’s minimax theorem to the Lagrangian \( L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2) \) defined in (23). Observe that \( L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2) \) is convex in \( P_k \), linear in \( \lambda_k \) and \( \alpha_k \); by Prokhorov’s theorem [35], the convex space \( \mathcal{P}(\Omega) \times \mathcal{P}(\Omega) \) is compact since \( \Omega \) is relatively compact with respect to the weak topology; the space \( \{ \lambda_1, \lambda_2 \geq 0, \lambda_1 + \lambda_2 \leq 1 \} \) is also a convex compact space. The feasible region of \( \alpha_k, k = 1, 2 \) belongs to a linear topological space under the sup-norm. This justifies the conditions for Sion’s minimax theorem, thereby we can exchange sup and inf in (23) when \( \Omega \) is compact.

**Step 4** Relaxing the compactness assumption when the cost is bounded.

We now relax the compactness assumption made in the previous step, using a technique similar to the proof of Theorem 1.3 in [46]. We temporarily assume the cost function \( c(\cdot, \cdot) \) is bounded by a positive constant \( C \) and is uniformly continuous. We will relax the bounded assumption later. We already have the weak duality:

\[
v_1 := \inf_{P_1, P_2 \in \mathcal{P}(\Omega)} \sup_{\lambda_1, \lambda_2 \geq 0 \atop \lambda_1 + \lambda_2 \leq 1} \mathcal{A}_{\lambda_1, \lambda_2} =: v_2.
\]

In the following we show that \( v_1 \leq v_2 \).

For any \( \epsilon > 0 \), let \( \Omega^\epsilon \subset \Omega \) be a compact subset sufficiently large, such that \( P_k^\epsilon(\Omega \setminus \Omega^\epsilon) \leq \epsilon \) and \( Q_{k,n_k}(\Omega^\epsilon) = 1, k = 1, 2 \). This is always possible since \( Q_{k,n_k} \) is the empirical distribution
and with finite support. Then the previous steps imply that the strong duality holds on \( \Omega' \):

\[
v_1^\varepsilon := \inf_{P_1, P_2 \in \mathcal{P}(\Omega')} \sup_{\lambda_1, \lambda_2 \geq 0, \lambda_1 + \lambda_2 \leq \epsilon, \alpha_1, \alpha_2 \in B_1(\Omega')} L(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2)
\]

\[
= \sup_{\lambda_1, \lambda_2 \geq 0, \lambda_1 + \lambda_2 \leq \epsilon, \alpha_1, \alpha_2 \in B_1(\Omega')} \sum_{k=1}^{2} \mathbb{E}_{\hat{\omega}_k} \left[ \inf_{\omega \in \Omega'} \left\{ \lambda_k e(\omega, \hat{\omega}_k) + \sum_{\alpha \neq k} [\alpha_j(\omega) I_{\Omega_2^c}(\omega) - \alpha_k(\omega) I_{\Omega_2^c}(\omega)] \right\} \right]
\]

\[
= v_2^\varepsilon.
\]

Consider the inf sup problem defining \( v_1 \). For the optimal solution \((P_1^\varepsilon, P_2^\varepsilon)\) to the inf sup problem that induces \( v_1 \), we define distributions \( \tilde{P}_1, \tilde{P}_2 \) via

\[
\tilde{P}_k(A) = P_k^\varepsilon(\Omega^c) \cdot P_k^\varepsilon(A \cap \Omega^c) + P_k^\varepsilon(A \cap (\Omega \setminus \Omega^c)), \quad \forall \text{ Borel set } A \subset \Omega.
\]

Recall \( \alpha = \alpha_2 I_{\Omega_2^c} - \alpha_1 I_{\Omega_1^c} \). We compare the Lagrangian function \( L \) defined in \((23)\) associated with \((\tilde{P}_1, \tilde{P}_2)\) and \((P_1^\varepsilon, P_2^\varepsilon)\). For the first term in \((23)\), we have that

\[
\mathcal{W}(\tilde{P}_k, Q_{k,n_k}) \leq P_k^\varepsilon(\Omega^c) \mathcal{W}(P_k^\varepsilon, Q_{k,n_k}) + CP_k^\varepsilon(\Omega \setminus \Omega^c) \leq \mathcal{W}(P_k^\varepsilon, Q_{k,n_k}) + C \varepsilon.
\]

For the second term in \((23)\), we have

\[
\int_{\Omega} \alpha(\omega)(\tilde{P}_1 - \tilde{P}_2)(d\omega)
\]

\[
= \int_{\Omega^c} \alpha(\omega)(P_1^\varepsilon(\Omega^c)P_1^\varepsilon - P_2^\varepsilon(\Omega^c)P_2^\varepsilon)(d\omega) + \int_{\Omega \setminus \Omega^c} \alpha(\omega)(P_1^\varepsilon - P_2^\varepsilon)(d\omega).
\]

By definition of \( \Omega_1^c, \Omega_2^c \), we have \( \int_{\Omega \setminus \Omega^c} \alpha(\omega)(P_1^\varepsilon - P_2^\varepsilon)(d\omega) \leq 0 \). Moreover,

\[
\int_{\Omega^c} \alpha(\omega)(P_1^\varepsilon(\Omega^c)P_1^\varepsilon - P_2^\varepsilon(\Omega^c)P_2^\varepsilon)(d\omega)
\]

\[
= \begin{cases} 
P_1^\varepsilon(\Omega^c) \int_{\Omega^c} \alpha(\omega)(P_1^\varepsilon - P_2^\varepsilon)(d\omega) - (P_2^\varepsilon(\Omega^c) - P_1^\varepsilon(\Omega^c))^2 \int_{\Omega^c} \alpha(\omega)P_2^\varepsilon(d\omega), & \text{if } P_1^\varepsilon(\Omega^c) \leq P_2^\varepsilon(\Omega^c); \\
P_2^\varepsilon(\Omega^c) \int_{\Omega^c} \alpha(\omega)(P_1^\varepsilon - P_2^\varepsilon)(d\omega) + (P_1^\varepsilon(\Omega^c) - P_2^\varepsilon(\Omega^c))^2 \int_{\Omega^c} \alpha(\omega)P_2^\varepsilon(d\omega), & \text{if } P_1^\varepsilon(\Omega^c) > P_2^\varepsilon(\Omega^c). 
\end{cases}
\]
By definition \( \int_{\Omega_\epsilon} \alpha(\omega)(P_1^\epsilon - P_2^\epsilon)(d\omega) \leq 0 \) and \( P_k^\epsilon(\Omega^c) \geq 1 - \epsilon \), thereby

\[
P_k^\epsilon(\Omega^c) \int_{\Omega^c} \alpha(\omega)(P_1^\epsilon - P_2^\epsilon)(d\omega) \leq (1 - \epsilon) \int_{\Omega^c} \alpha(\omega)(dP_1^\epsilon - dP_2^\epsilon)(\omega) \leq 0.
\]

Moreover, since \( P_k^\epsilon(\Omega^c) \geq 1 - \epsilon \), we have \( |P_1^\epsilon(\Omega^c) - P_2^\epsilon(\Omega^c)| \leq \epsilon \), consequently we have

\[
|P_1^\epsilon(\Omega^c) - P_2^\epsilon(\Omega^c)| \int_{\Omega^c} \alpha(\omega)dP_k^\epsilon(\omega) \leq \epsilon \int_{\Omega} \alpha(\omega,\omega_k^0)dP_k^\epsilon(\omega) \leq C\epsilon,
\]

where the last inequality is due to the 1-Lipschitz property of \( \alpha_k \) and \( C \) may be a different constant. Combining with previous inequality that \( W(\tilde{P}_k, Q_{k,n_k}) \leq W(P_k^\epsilon, Q_{k,n_k}) + C\epsilon, k = 1, 2 \), we have

\[
v_1 \leq v_1^\epsilon + 2C\epsilon.
\]

Now consider the dual problem defining \( v_2 \). Let \((\alpha_1^\epsilon, \alpha_2^\epsilon)\) be the optimal solution to the dual problem supported on the subset \( \Omega^\epsilon \). We will construct an approximate maximizer \((\tilde{\alpha}_1, \tilde{\alpha}_2)\) of the original dual problem from \((\alpha_1^\epsilon, \alpha_2^\epsilon)\). To this end, let us define

\[
\phi_1(\tilde{\omega}_1^i) : = \min \left\{ \inf_{\omega \in \Omega_1^\epsilon \cap \Omega^c} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) - \alpha_1^\epsilon(\omega) \}, \inf_{\omega \in \Omega_2^\epsilon \cap \Omega^c} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) + \alpha_2^\epsilon(\omega) \} \right\},
\]

\[
\phi_2(\tilde{\omega}_2^j) : = \min \left\{ \inf_{\omega \in \Omega_1^\epsilon \cap \Omega^c} \{ \lambda_2 c(\omega, \tilde{\omega}_2^j) + \alpha_1^\epsilon(\omega) \}, \inf_{\omega \in \Omega_2^\epsilon \cap \Omega^c} \{ \lambda_2 c(\omega, \tilde{\omega}_2^j) - \alpha_2^\epsilon(\omega) \} \right\}.
\]

From the above equations we have that \( \alpha_1^\epsilon, \alpha_2^\epsilon \) satisfy:

\[
\begin{align*}
\alpha_1^\epsilon(\omega) & \leq \lambda_1 c(\omega, \tilde{\omega}_1^i) - \phi_1(\tilde{\omega}_1^i), \quad \forall \omega \in \Omega^\epsilon, \; i = 1, \ldots, n_1, \\
\alpha_2^\epsilon(\omega) & \leq \lambda_2 c(\omega, \tilde{\omega}_2^j) - \phi_2(\tilde{\omega}_2^j), \quad \forall \omega \in \Omega^\epsilon, \; j = 1, \ldots, n_2.
\end{align*}
\]

Define \( \bar{\alpha}_1, \bar{\alpha}_2 \) as

\[
\begin{align*}
\bar{\alpha}_1(\omega) & = \min_{1 \leq i \leq n_1} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) - \phi_1(\tilde{\omega}_1^i) \}, \quad \forall \omega \in \Omega, \\
\bar{\alpha}_2(\omega) & = \min_{1 \leq j \leq n_2} \{ \lambda_2 c(\omega, \tilde{\omega}_2^j) - \phi_2(\tilde{\omega}_2^j) \}, \quad \forall \omega \in \Omega.
\end{align*}
\]

This implies that \( \phi_k(\tilde{\omega}_k^i) \leq \inf_{\omega \in \Omega_\epsilon^\epsilon} \{ \lambda_k c(\omega, \tilde{\omega}_k^i) - \bar{\alpha}_k(\omega) \} \), \( k = 1, 2 \), \( i = 1, \ldots, n_k \). Comparing (31) and (30), we have that \( \bar{\alpha}_k(\omega) \geq \alpha_k^\epsilon(\omega) \), \( k = 1, 2 \), for \( \omega \in \Omega^\epsilon \). Consequently, we have

\[
\begin{align*}
\phi_1(\tilde{\omega}_1^i) & \leq \min \left\{ \inf_{\omega \in \Omega_1^\epsilon \cap \Omega^c} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) - \alpha_1^\epsilon(\omega) \}, \inf_{\omega \in \Omega_2^\epsilon \cap \Omega^c} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) + \alpha_2^\epsilon(\omega) \} \right\}, \\
\phi_2(\tilde{\omega}_2^j) & \leq \min \left\{ \inf_{\omega \in \Omega_1^\epsilon \cap \Omega^c} \{ \lambda_2 c(\omega, \tilde{\omega}_2^j) + \alpha_1^\epsilon(\omega) \}, \inf_{\omega \in \Omega_2^\epsilon \cap \Omega^c} \{ \lambda_2 c(\omega, \tilde{\omega}_2^j) - \alpha_2^\epsilon(\omega) \} \right\}.
\end{align*}
\]
Moreover, we can choose $\Omega^c$ sufficiently large so that for every $\omega \in \Omega^c \cap (\Omega \setminus \Omega^c)$,

$$\lambda_1 c(\omega, \tilde{\omega}_1^i) + \tilde{\alpha}_2 (\omega) = \lambda_1 c(\omega, \tilde{\omega}_1^i) + \lambda_2 c(\omega, \tilde{\omega}_2^j) - \tilde{\phi}^j_2(\tilde{\omega}_2^j)$$

$$\geq \inf_{\omega \in \Omega^c \cap (\Omega \setminus \Omega^c)} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) + \tilde{\alpha}_2 (\omega) \} \geq \phi^i_1(\tilde{\omega}_1^i),$$

where $j$ is the minimizer in the definition (31). Combining these together, we have

$$\phi^i_1(\tilde{\omega}_1^i) \leq \min \left\{ \inf_{\omega \in \Omega^c} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) - \tilde{\alpha}_1 (\omega) \}, \inf_{\omega \in \Omega^c} \{ \lambda_1 c(\omega, \tilde{\omega}_1^i) + \tilde{\alpha}_2 (\omega) \} \right\},$$

$$\phi^j_2(\tilde{\omega}_2^j) \leq \min \left\{ \inf_{\omega \in \Omega^c} \{ \lambda_2 c(\omega, \tilde{\omega}_2^j) + \tilde{\alpha}_1 (\omega) \}, \inf_{\omega \in \Omega^c} \{ \lambda_2 c(\omega, \tilde{\omega}_2^j) - \tilde{\alpha}_2 (\omega) \} \right\}.$$

Therefore, from $\tilde{\alpha}_1, \tilde{\alpha}_2$ defined in (31), we see $v_2 \geq v^*_2$. Combine with previous argument, we have

$$v^*_2 \leq v_2 \leq v_1 \leq v^*_1 + 2C\epsilon.$$

By letting $\epsilon \to 0$, we have shown the strong duality, provided that the cost function is bounded.

**Step 5** Relaxing the bounded cost assumption.

Next, we turn to the general case with cost function by writing $c := \sup_m c_m$, where $c_m(x, y) = \min \{ c(x, y), m \}$ is the truncated cost function that are bounded for each $m \in \mathbb{N}$. Let $v^*_1$ be the optimal value of the primal problem under cost $c_m$, and $v^*_2$ denote the optimal value of the dual problem under cost $c_m$. More specifically, let

$$L^m(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2)$$

$$:= \sum_{k=1}^2 \lambda_k W^m(P_k, Q_{k,n_k}) + \sum_{k=1}^2 \sum_{j \neq k} \left\{ E_{P_k} [\alpha_j (\omega) I_{\Omega^c_j} (\omega) - \alpha_k (\omega) I_{\Omega^c_k} (\omega)] \right\},$$

where $W^m(P_k, Q_{k,n_k})$ is the Wasserstein distance associated with cost function $c_m(\cdot, \cdot)$. Define

$$v^*_1 := \inf_{P_1, P_2 \in \mathcal{P}(\Omega)} \sup_{\lambda_1, \lambda_2 \geq 0 \atop \lambda_1 + \lambda_2 \leq 1} \inf_{\alpha_1, \alpha_2 \in \mathcal{B}_+ (\Omega)} L^m(P_1, P_2; \lambda_1, \lambda_2, \alpha_1, \alpha_2)$$

$$= \sup_{\lambda_1, \lambda_2 \geq 0 \atop \lambda_1 + \lambda_2 \leq 1} \sum_{k=1}^2 E_{\tilde{\omega}_k \sim Q_{k,n_k}} \left[ \inf_{\omega \in \Omega} \left\{ \lambda_k c_m (\omega, \tilde{\omega}_k) + \sum_{j \neq k} [\alpha_j (\omega) I_{\Omega^c_j} (\omega) - \alpha_k (\omega) I_{\Omega^c_k} (\omega)] \right\} \right]$$

$$=: v^*_2.$$
We have proved $v_1^m = v_2^m$ in previous steps. And clearly we have $v_2^m \le v_2$ since $c_m \le c$, leading to $v_1^m = v_2^m \le v_2 \le v_1$, so we only need to show $v_1 = \sup_m v_1^m$.

Observe that $W_m(P_k, Q_{k,n_k})$ is a non-decreasing sequence bounded above by $W(P_k, Q_{k,n_k})$. If $\{(P_{1,t}^m, P_{2,t}^m)\}_{t \in \mathbb{N}}$ is a minimizing sequence for the problem $v_1^m$, then we can extract a subsequence that converges weakly to some probability measure $P_1^m, P_2^m$ [46].

We claim that the sequence $\{P_{m,k}\}_{m \in \mathbb{N}}$ is relatively compact with respect to the weak topology, $k = 1, 2$. To show this, suppose $\{P_{m,k}\}_{m \in \mathbb{N}}$ is not relatively compact, then there exists $\epsilon > 0$ such that for any compact set $A$ and any $m_0 \in \mathbb{N}$, there exists $m > m_0$ such that $P_m^m(A) \ge \epsilon$. We choose $m_0 = \lceil W(Q_{k,n_k}, P_k) / \epsilon \rceil$ and a set $A$ such that $\inf_{\omega \in A, \hat{\omega} \in \hat{\Omega}} c(\omega, \hat{\omega}) \ge m_0$. Then for any $m > m_0$, we have

$$W_m(Q_{k,n_k}, P_k) = \min_{\gamma \in \Gamma(P_k^m, Q_{k,n_k})} \{ E(\omega, \omega') \sim \gamma [c_m(\omega, \omega')] \} > m_0 P_k^m(A) \ge m_0 \epsilon \ge W(Q_{k,n_k}, P_k^0),$$

while at the same time we have

$$W_m(Q_{k,n_k}, P_1^m) \le W_m(Q_{k,n_k}, P_1^0) \le W(Q_{k,n_k}, P_1^0),$$

which is a contradiction. Therefore $\{P_k^m\}_{m \in \mathbb{N}}$ is relatively compact and we can extract a subsequence that converges to some probability measure $P_k^*$. For any $m_1 > m_2$, we have $W_{m_1}(P_k^m, Q_{k,n_k}) \ge W_{m_2}(P_k^m, Q_{k,n_k})$, and

$$\lim_{m_1 \to \infty} \sup_{m_1} W_{m_1}(P_k^m, Q_{k,n_k}) \ge \lim_{m_1 \to \infty} \sup_{m_1} W_{m_2}(P_k^m, Q_{k,n_k}) \ge W_{m_2}(P_k^*, Q_{k,n_k}).$$

Moreover, $W_{m_2}(P_k^*, Q_{k,n_k})$ is a non-decreasing sequence and converges to $W(P_k^*, Q_{k,n_k})$ as $m_2 \to \infty$, hence:

$$\lim_{m \to \infty} v_1^m = \lim_{m \to \infty} W_m(P_k^m, Q_{k,n_k}) \ge W(P_k^*, Q_{k,n_k}) = v_1.$$

Thereby we complete the proof. $\square$

### B.2 Proof of Theorem 2

Our analysis starts from the observation that

$$F_{1,n_1 n_2} \le \sup_{\alpha \in A} G_{1,n_1 n_2}(\alpha).$$
First recall that $A$ is defined in (12) as:

$$A = \{ \alpha = \alpha_2 \mathbb{I}_{\Omega_2} - \alpha_1 \mathbb{I}_{\Omega_1} : \alpha_k \in B_+(\Omega_k^*) \cap \text{Lip}(\Omega_k^*), \alpha(\omega_k^*) = 0, k = 1, 2 \}.$$ 

We then provide an upper bound on $\sup_{\alpha \in A} G_{n_1, n_2}(\alpha)$ detailed as follows. By definition of $A$, $\alpha(\hat{\omega}_1^i) \leq 0$ for $\hat{\omega}_1^i \in \Omega_1^i$ and $\alpha(\hat{\omega}_2^i) \geq 0$ for $\hat{\omega}_2^i \in \Omega_2^i$. Therefore, to maximize $G_{n_1, n_2}(\alpha)$, we should let $\alpha(\hat{\omega}_1^i) = 0$ for $\hat{\omega}_1^i \in \Omega_1^i$ and $\alpha(\hat{\omega}_2^i) = 0$ for $\hat{\omega}_2^i \in \Omega_2^i$. In addition, since $\alpha_1, \alpha_2$ are 1-Lipschitz, we have $\alpha(\hat{\omega}_1^i) \leq \min_{j: \hat{\omega}_2^j \in \Omega_2^i} c(\hat{\omega}_1^i, \hat{\omega}_2^j)$ for $\hat{\omega}_1^i \in \Omega_2^i$ and $\alpha(\hat{\omega}_2^i) \geq -\min_{i: \hat{\omega}_1^i \in \Omega_1^i} c(\hat{\omega}_2^i, \hat{\omega}_1^i)$ for $\hat{\omega}_2^i \in \Omega_1^i$. Hence we have

$$\sup_{\alpha \in A} G_{n_1, n_2}(\alpha) = \frac{1}{n_1} \sum_{i: \hat{\omega}_1^i \in \Omega_2^i} \min_{j: \hat{\omega}_2^j \in \Omega_2^i} c(\hat{\omega}_1^i, \hat{\omega}_2^j) + \frac{1}{n_2} \sum_{i: \hat{\omega}_1^i \in \Omega_1^i} \min_{j: \hat{\omega}_2^j \in \Omega_1^i} c(\hat{\omega}_2^i, \hat{\omega}_1^i).$$

(32)

Note that the summation equals 0 if there is no point $\hat{\omega}_1^i$ falling into the set $\Omega_2^i$ and no point $\hat{\omega}_2^i$ falling into the set $\Omega_1^i$.

In light of above, in order to obtain the asymptotic upper bound on the profile function $F_{n_1, n_2}$, we study the right-hand side of the above inequality instead, which is relatively simpler since it only involves the minimum distance type statistics of two sample sets. We state the following lemma, whose proof is adapted from the asymptotic moments of near-neighbour distance distributions in [32, 48, 33].

**Lemma 5.** Let $\{x_1, \ldots, x_n\}$ be a set of points selected independently at random from $\Omega \subset \mathbb{R}^d$ according to the sampling distribution $F$ with density function $f$. Let $x$ be a random variable sampled from the distribution $G$ with density function $g$. Suppose that $f(x), g(x)$ are densities with

$$\int_{\Omega} g(x)f(x)^{-1/d} dx < \infty,$$

and for some $\epsilon > 0$ we have $\sup_{n \in \mathbb{N}} \mathbb{E}_{f, x_1, \ldots, x_n \sim g} [(n^{1/d} \min_{1 \leq i \leq n} \|x - x_i\|)^{1+r}] < \infty$. Then

$$n^{1/d} \mathbb{E}\{\min_{1 \leq i \leq n} \|x - x_i\|\} \rightarrow \frac{\Gamma(1 + 1/d)}{V_d^{1/d}} \int_{\mathbb{R}^d} g(x)f(x)^{-1/d} dx,$$

as $n \rightarrow \infty$, where $V_d = \pi^{d/2}/\Gamma(1 + d/2)$ is the volume of the unit ball in $\mathbb{R}^d$.

**Proof of Lemma 5.** The proof is based on a conditioning argument following [33, Theorem 2.1], [48, Theorem 2], and [32, Theorem 2.3]. Let $x$ be the random variable with density function $g$, and $X_n = \{x_1, \ldots, x_n\}$ be a set of $n$ i.i.d. samples from the distribution $f$. Denote $\xi(x; X_n)$ as the minimum distance from $x$ to the $n$ points within $X_n$. For any fixed $x$, it has been shown in Lemma 3.2 of [33] that the expectation of $n^{1/d}\{\min_{1 \leq i \leq n} \|x - x_i\|\}$
and the second term on the right-hand side of (32) can be treated similarly: 

\[
\lim_{n \to \infty} \mathbb{E}[\xi_\infty(\mathcal{P}_{f(x)})] = \mathbb{E}[\xi_\infty(\mathcal{P}_{f(x)})] = \mathbb{E}[\xi_\infty(\mathcal{P}_{f(x)})] = \mathbb{E}[\xi_\infty(\mathcal{P}_{f(x)})]
\]

Therefore, under the assumption that \( \lim_{n_1, n_2 \to \infty} n_2/n_1 = c > 0 \), in the asymptotic regime we roughly have \( n_2 \sim cn_1 \) for fixed constants \( c > 0 \), and the expectation of the minimum distance is asymptotically of the order \( \mathcal{O}(n_1^{-1/d}) \) if we do not impose any further conditions for the data-generating distributions. Observe that in our case the first term on the right-hand side of (32) is a variant of the minimum distance in Lemma 5 in terms that we restrict our attention to points in the subset \( \hat{\mathcal{O}}^c_2 \). Therefore, by restricting the support of the integral we have that:

\[
(cn_1)^{1/d} \mathbb{E}_{\hat{\omega}_1 \sim P_{\hat{\mathcal{O}}^c_1}} \left[ \min_{j: \hat{\omega}_j \in \hat{\mathcal{O}}^c_2} c(\hat{\omega}_1, \hat{\omega}_j) \right] \to \frac{\Gamma(1 + 1/d)}{V_1^{1/d}} \int_{\hat{\mathcal{O}}^c_2} \frac{f_1(x)}{[f_2(x)]^{1/d}} dx,
\]

and the second term on the right-hand side of (32) can be treated similarly:

\[
(n_1)^{1/d} \mathbb{E}_{\hat{\omega}_2 \sim P_{\hat{\mathcal{O}}^c_2}} \left[ \min_{i: \hat{\omega}_{i} \in \hat{\mathcal{O}}^c_1} c(\hat{\omega}_1, \hat{\omega}_i) \right] \to \frac{\Gamma(1 + 1/d)}{V_1^{1/d}} \int_{\hat{\mathcal{O}}^c_1} \frac{f_2(x)}{[f_1(x)]^{1/d}} dx.
\]

Then we apply a refined law-of-large-numbers-type argument to show the desired results in the theorem. Here we observe the key challenge is that the sample average is taken for dependent random variables. In particular, for fixed sample points \( \{\hat{\omega}_1, \ldots, \hat{\omega}_2 \} \) and two i.i.d. observations \( \hat{\omega}_1 \) and \( \hat{\omega}_1' \), the variables \( \min_{j: \hat{\omega}_j \in \hat{\mathcal{O}}^c_2} c(\hat{\omega}_1, \hat{\omega}_j) \) and \( \min_{j: \hat{\omega}_j \in \hat{\mathcal{O}}^c_2} c(\hat{\omega}_1', \hat{\omega}_j) \) are \textit{dependent} since they rely on the common sample set \( \{\hat{\omega}_1, \ldots, \hat{\omega}_2 \} \). To address this issue, we can apply the coupling argument used in the proof to [33, Theorem 2.1]. More specifically, for fixed \( \hat{\omega}_1 \) and \( \hat{\omega}_1' \), we can separate the space into two half-spaces: \( F_{\hat{\omega}_1} \) that contains all points closer to \( \hat{\omega}_1 \) than to \( \hat{\omega}_1' \), and \( F_{\hat{\omega}_1'} \) that contains all points closer to \( \hat{\omega}_1' \) than to \( \hat{\omega}_1 \). Given these two half-spaces, we can construct two independent homogeneous Poisson process of intensity \( f_1(\hat{\omega}_1) \) and \( f_1(\hat{\omega}_1') \), respectively. Then by the coupling argument, it was shown in
\[ \frac{1}{n_1} \sum_{i: \hat{\omega}_1^i \in \Omega_2^i} (cn_1)^{1/d} \min_{j: \hat{\omega}_2^j \in \Omega_2^j} c(\hat{\omega}_1^i, \hat{\omega}_2^j) \to \frac{\Gamma(1 + 1/d)}{V_d^{1/d}} \int_{\Omega_2^i} \frac{f_1(x)}{[f_2(x)]^{1/d}} dx, \quad \text{in } L^1, \]  

and

\[ \frac{1}{n_2} \sum_{j: \hat{\omega}_2^j \in \Omega_2^j} (n_1)^{1/d} \min_{i: \hat{\omega}_1^i \in \Omega_1^i} c(\hat{\omega}_2^j, \hat{\omega}_1^i) \to \frac{\Gamma(1 + 1/d)}{V_d^{1/d}} \int_{\Omega_1^i} \frac{f_2(x)}{[f_1(x)]^{1/d}} dx, \quad \text{in } L^1. \]  

Finally, note that for any sequences of random variable \( X_n, Y_n \), if \( X_n \to X \) in \( L^1 \) and \( Y_n \to Y \) in \( L^1 \), then \( X_n + Y_n \to X + Y \) in \( L^1 \). By combining (33) and (34), we prove the theorem.

C Auxiliary Results

C.1 Kantorovich duality

Lemma 6 (Theorem 5.10, [47]). Let \((\mathcal{X}, \mu)\) and \((\mathcal{Y}, \nu)\) be two Polish probability spaces and let \( c: \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \cup \{+\infty\} \) be a lower semicontinuous cost function. Then we have the duality

\[ \min_{\gamma \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\gamma(x, y) = \sup_{\substack{\phi, \psi \in L^1(\mu) \times L^1(\nu) \\ \phi(x) + \psi(y) \leq c(x, y) \quad \forall x, y}} \left( \int_{\mathcal{X}} \phi(x) d\mu + \int_{\mathcal{Y}} \psi(y) d\nu \right), \]

where \( \gamma \in \Pi(\mu, \nu) \) denotes the joint distribution on \( \mathcal{X} \times \mathcal{Y} \), with marginal distributions \( \mu \) and \( \nu \), respectively.

Note that when \( \mu \) (or \( \nu \)) is a discrete distribution on \( \{x_1, \ldots, x_m\} \), then the function \( \phi(x) \) can be viewed as a vector \( \xi \in \mathbb{R}^m \). And the above dual formulation will be reduced to

\[ \min_{\gamma \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\gamma(x, y) = \sup_{\substack{\xi \in \mathbb{R}^m, \psi \in L^1(\nu) \\ \xi_i + \psi(y) \leq c(x_i, y) \quad \forall i \leq m, \forall y}} \left( \sum_{i=1}^{m} \xi_i \mu(x_i) + \int_{\mathcal{Y}} \psi(y) d\nu \right), \]  

this is what we have used in the proof of Lemma 2.

C.2 Interchangeability principle

Before introducing the principle, we recall the definition for decomposable spaces. Assume a probability space \((\Omega, \mathcal{F}, P)\). A linear space \( \mathcal{M} \) of \( \mathcal{F} \)-measurable functions \( \psi: \Omega \to \mathbb{R}^d \) is
decomposable if for every $\psi \in \mathcal{M}$ and $A \in \mathcal{F}$, and every bounded $\mathcal{F}$-measurable function $\phi : \Omega \to \mathbb{R}^d$, the space $\mathcal{M}$ also contains the function $\eta(\cdot) = \mathbb{I}_{\Omega \setminus A}(\cdot) \psi(\cdot) + \mathbb{I}_A(\cdot) \phi(\cdot)$.

**Lemma 7** (Theorem 7.80, [41]). Let $\mathcal{M}$ be a decomposable space and $f : \mathbb{R}^d \times \Omega \to \mathbb{R}$ be a random lower semicontinuous function. Then

$$
\mathbb{E} \left[ \inf_{x \in \mathbb{R}^d} f(x, \omega) \right] = \inf_{\chi \in \mathcal{M}} \mathbb{E}[F_{\chi}],
$$

(36)

where $F_{\chi} := f(\chi(\omega), \omega)$, provided that the right-hand side of (36) is less than $+\infty$. Moreover, if the common value of the both sides in (36) is not $-\infty$, then

$$
\tilde{\chi} \in \operatorname{arg\,min}_{\chi \in \mathcal{M}} \mathbb{E}[F_{\chi}] \text{ iff } \tilde{\chi}(\omega) \in \operatorname{arg\,min}_{x \in \mathbb{R}^d} f(x, \omega) \text{ for a.e. } \omega \in \Omega \text{ and } \tilde{\chi} \in \mathcal{M}.
$$

### C.3 Wasserstein distributionally robust optimization

The following result is a special case of Theorem 1 in [15] by choosing the Wasserstein metric of order 1.

**Lemma 8** (Theorem 1, [15])). For $\nu = \frac{1}{N} \sum_{i=1}^{N} \delta_{\hat{\xi}_i}$ and $\theta > 0$, we have:

$$
\sup_{\mu \in \mathcal{P}(\nu, \theta)} \int_{\Omega} \Phi(\xi)d\mu(\xi) = \min_{\lambda \geq 0} \left\{ \lambda \theta - \frac{1}{N} \sum_{i=1}^{N} \inf_{\xi \in \Omega} [\lambda c(\hat{\xi}_i, \xi) - \Phi(\xi)] \right\},
$$

where $\mathcal{P}(\nu, \theta)$ is the uncertainty set induced by Wasserstein metric [15] as defined in (2):

$$
\mathcal{P}(\nu, \theta) = \{ \mu \in \mathcal{P}(\Omega) : W(\mu, \nu) \leq \theta \}. 
$$