

Multivariate Distribution-free Testing using Optimal Transport

Bodhisattva Sen¹
Department of Statistics
Columbia University, New York

**ICERM workshop on “Optimal Transport in Data Science”
Brown University
May 08, 2023**

¹Supported by NSF grant DMS-2015376

Multivariate two-sample testing

- **Data:** $\{X_i\}_{i=1}^m$ iid P_1 on \mathbb{R}^d ; $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$
- Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

Multivariate two-sample testing

- **Data:** $\{X_i\}_{i=1}^m$ iid P_1 on \mathbb{R}^d ; $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$

- Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

- When $d = 1$: Student (1908), Wilcoxon (1945), Cramér von-Mises (1928), Smirnov (1939), Wald and Wolfowitz (1940), Mann and Whitney (1947), Anderson (1962), ...
- When $d > 1$: Hotelling (1931), Weiss (1960), Bickel (1969), Friedman and Rafsky (1979), Schilling (1986), Henze (1988), Liu and Singh (1993), Székely (2003), Rosenbaum (2005), Gretton et al. (2012), Chen and Friedman (2017), Bhattacharya (2019), ...

Multivariate two-sample testing

- **Data:** $\{X_i\}_{i=1}^m$ iid P_1 on \mathbb{R}^d ; $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$

- Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

- When $d = 1$: Student (1908), Wilcoxon (1945), Cramér von-Mises (1928), Smirnov (1939), Wald and Wolfowitz (1940), Mann and Whitney (1947), Anderson (1962), ...
- When $d > 1$: Hotelling (1931), Weiss (1960), Bickel (1969), Friedman and Rafsky (1979), Schilling (1986), Henze (1988), Liu and Singh (1993), Székely (2003), Rosenbaum (2005), Gretton et al. (2012), Chen and Friedman (2017), Bhattacharya (2019), ...

What is the **distribution-free** analogue of **Hotelling's test** when $d > 1$?

When $d = 1$

Two-sample t -test

- **Two-sample t -test:** Compares $\bar{X}_m = \frac{1}{m} \sum_{i=1}^m X_i$ & $\bar{Y}_n = \frac{1}{n} \sum_{j=1}^n Y_j$

When $d = 1$

Two-sample t -test

- **Two-sample t -test:** Compares $\bar{X}_m = \frac{1}{m} \sum_{i=1}^m X_i$ & $\bar{Y}_n = \frac{1}{n} \sum_{j=1}^n Y_j$
- Under H_0 , the t -statistic has approximately t_{m+n-2} distribution
- **Approximate** (not valid for small sample sizes) level α test; requires **moment** assumptions; not **robust** to **outliers**

When $d = 1$

Two-sample t -test

- **Two-sample t -test:** Compares $\bar{X}_m = \frac{1}{m} \sum_{i=1}^m X_i$ & $\bar{Y}_n = \frac{1}{n} \sum_{j=1}^n Y_j$
- Under H_0 , the t -statistic has approximately t_{m+n-2} distribution
- **Approximate** (not valid for small sample sizes) level α test; requires **moment** assumptions; not **robust** to **outliers**

Question: Can we find a **distribution-free** test that is **robust** to **outliers** and **heavy-tailed** distributions and is also **efficient**?

When $d = 1$

Two-sample t -test

- **Two-sample t -test:** Compares $\bar{X}_m = \frac{1}{m} \sum_{i=1}^m X_i$ & $\bar{Y}_n = \frac{1}{n} \sum_{j=1}^n Y_j$
- Under H_0 , the t -statistic has approximately t_{m+n-2} distribution
- **Approximate** (not valid for small sample sizes) level α test; requires **moment** assumptions; not **robust** to **outliers**

Question: Can we find a **distribution-free** test that is **robust** to **outliers** and **heavy-tailed** distributions and is also **efficient**?

Answer: **Wilcoxon rank-sum test** (WRS) [Wilcoxon (1945)]

WRS test is **distribution-free**: **null distribution** is **universal** — does **not depend** on the distribution of the data (if it is a continuous dist.)

Wilcoxon rank-sum test (WRS)

- **Pool** $\{X_1, \dots, X_m, Y_1, \dots, Y_n\}$ to obtain **rank**s $\hat{R}_{m,n}(X_i)$'s and $\hat{R}_{m,n}(Y_j)$'s:

$$\text{WRS} = \frac{1}{n} \sum_{j=1}^n \hat{R}_{m,n}(Y_j) - \frac{1}{m} \sum_{i=1}^m \hat{R}_{m,n}(X_i)$$

- WRS test is **distribution-free** and **exact** for all $P_1 = P_2$ **continuous**

Wilcoxon rank-sum test (WRS)

- **Pool** $\{X_1, \dots, X_m, Y_1, \dots, Y_n\}$ to obtain **rank**s $\hat{R}_{m,n}(X_i)$'s and $\hat{R}_{m,n}(Y_j)$'s:

$$\text{WRS} = \frac{1}{n} \sum_{j=1}^n \hat{R}_{m,n}(Y_j) - \frac{1}{m} \sum_{i=1}^m \hat{R}_{m,n}(X_i)$$

- WRS test is **distribution-free** and **exact** for all $P_1 = P_2$ **continuous**
- Under H_0 , $(\hat{R}_{m,n}(X_1), \dots, \hat{R}_{m,n}(X_m), \hat{R}_{m,n}(Y_1), \dots, \hat{R}_{m,n}(Y_n))$ distributed **uniformly** over all $(m+n)!$ **permutations** of $\left\{ \frac{1}{m+n}, \frac{2}{m+n}, \dots, 1 \right\}$

Wilcoxon rank-sum test (WRS)

- **Pool** $\{X_1, \dots, X_m, Y_1, \dots, Y_n\}$ to obtain **rank**s $\hat{R}_{m,n}(X_i)$'s and $\hat{R}_{m,n}(Y_j)$'s:

$$\text{WRS} = \frac{1}{n} \sum_{j=1}^n \hat{R}_{m,n}(Y_j) - \frac{1}{m} \sum_{i=1}^m \hat{R}_{m,n}(X_i)$$

- WRS test is **distribution-free** and **exact** for all $P_1 = P_2$ **continuous**
- Under H_0 , $(\hat{R}_{m,n}(X_1), \dots, \hat{R}_{m,n}(X_m), \hat{R}_{m,n}(Y_1), \dots, \hat{R}_{m,n}(Y_n))$ distributed **uniformly** over all $(m+n)!$ **permutations** of $\left\{ \frac{1}{m+n}, \frac{2}{m+n}, \dots, 1 \right\}$

- **WRS**: **Exact** test valid for **all sample sizes**
- **Robust** to outliers; does **not** need moment assumptions
- Based on **univariate ranks** — advent of **classical nonparametrics**

Efficiency of the WRS test

Test if the two samples came from the same distribution, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

Comparison of WRS test with t -test (under location shift alternatives)

- WRS test has 0.95 Pitman efficiency w.r.t t -test when P_1 is Gaussian

Efficiency of the WRS test

Test if the two samples came from the same distribution, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

Comparison of WRS test with t -test (under location shift alternatives)

- WRS test has 0.95 Pitman efficiency w.r.t t -test when P_1 is Gaussian
- Non-trivial efficiency lower bound of 0.864 w.r.t t -test [Hodges and Lehmann (1956)]; efficiency can be $+\infty$ (for heavy-tailed dist.)

Efficiency of the WRS test

Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

Comparison of WRS test with t -test (under location shift alternatives)

- WRS test has **0.95 Pitman efficiency** w.r.t t -test when P_1 is **Gaussian**
- Non-trivial efficiency **lower bound** of **0.864** w.r.t t -test [Hodges and Lehmann (1956)]; efficiency can be $+\infty$ (for heavy-tailed dist.)
- Non-trivial efficiency **lower bound** of **1** w.r.t t -test [Chernoff and Savage (1958)] when the following revised statistic is used:

$$\frac{1}{n} \sum_{j=1}^n \Phi^{-1}(\hat{R}_{m,n}(Y_j)) - \frac{1}{m} \sum_{i=1}^m \Phi^{-1}(\hat{R}_{m,n}(X_i))$$

Generalize all these properties to **multivariate** data

Question: How to construct **efficient** **distribution-free** **multivariate** tests?

- When $d = 1$ tests based on “**ranks**” are distribution-free
- How to define **multivariate ranks** that lead to distribution-free tests?

Optimal transport!

- 1 Optimal Transport: Monge's Problem
 - Introduction
 - Multivariate Ranks via Optimal Transport
- 2 Multivariate Two-sample Goodness-of-fit Testing
 - Distribution-free Testing — Hotelling T^2 and Rank Hotelling
 - Lower bounds on Asymptotic (Pitman) Relative Efficiency
- 3 Other Applications of Distribution-free Inference
 - Testing for Mutual Independence
 - Testing for Symmetry

1 Optimal Transport: Monge's Problem

- Introduction
- Multivariate Ranks via Optimal Transport

2 Multivariate Two-sample Goodness-of-fit Testing

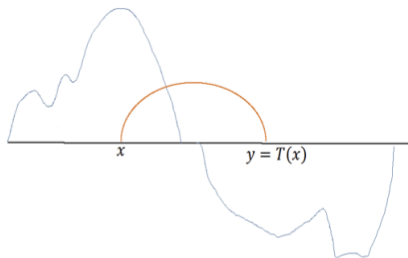
- Distribution-free Testing — Hotelling T^2 and Rank Hotelling
- Lower bounds on Asymptotic (Pitman) Relative Efficiency

3 Other Applications of Distribution-free Inference

- Testing for Mutual Independence
- Testing for Symmetry

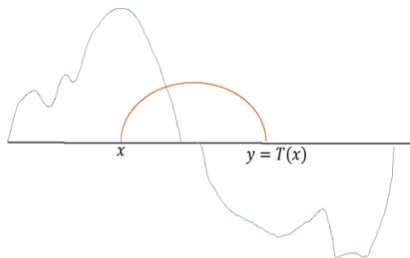
Optimal transport: Monge's problem

Gaspard Monge (1781): What is the cheapest way to **transport** a pile of sand to cover a sinkhole?



Optimal transport: Monge's problem

Gaspard Monge (1781): What is the cheapest way to **transport** a pile of sand to cover a sinkhole?



Goal: $\inf_{T: T(X) \sim \mu} \mathbb{E}_{\nu}[c(X, T(X))] \quad X \sim \nu$

- ν (“data” dist.) and μ (“reference” dist.)
- $c(x, y) \geq 0$: **cost of transporting** x to y (e.g., $c(x, y) = \|x - y\|^2$)
- T **transports** ν to μ : $T\#\nu = \mu$ (i.e., $T(X) \sim \mu$ where $X \sim \nu$)

Rank function as the optimal transport (OT) map: when $d = 1$

- $X \sim \nu$ (continuous dist.) on \mathbb{R} , $F \equiv F_\nu$ c.d.f. of ν
- **Rank:** The population rank of $x \in \mathbb{R}$ is $F(x)$ (a.k.a. the c.d.f. at x)
- **Property:** $F(X) \sim \text{Uniform}([0, 1]) \equiv \mu$; i.e., F transports ν to μ

Rank function as the optimal transport (OT) map: when $d = 1$

- $X \sim \nu$ (continuous dist.) on \mathbb{R} , $F \equiv F_\nu$ c.d.f. of ν
- **Rank:** The population rank of $x \in \mathbb{R}$ is $F(x)$ (a.k.a. the c.d.f. at x)
- **Property:** $F(X) \sim \text{Uniform}([0, 1]) \equiv \mu$; i.e., F transports ν to μ
- If $\mathbb{E}_\nu[X^2] < \infty$, the c.d.f F is the optimal transport (OT) map as

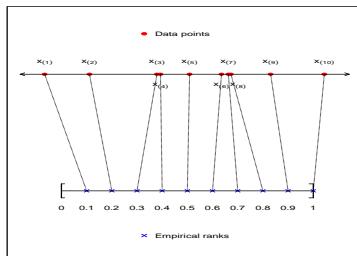
$$F = \arg \min_{T: T\# \nu = \mu} \mathbb{E}_\nu[(X - T(X))^2]$$

where we take

$$c(x, y) = (x - y)^2$$

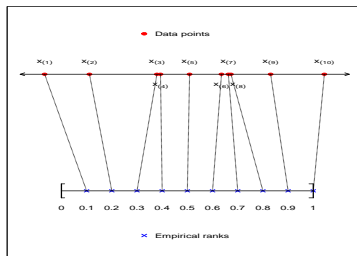
Sample rank map: when $d = 1$

- **Data:** X_1, \dots, X_n iid ν (cont. distribution) on \mathbb{R}
- **Sample rank map:** $\hat{R}_n : \{X_1, X_2, \dots, X_n\} \longrightarrow \{\frac{1}{n}, \frac{2}{n}, \dots, \frac{n}{n}\}$



Sample rank map: when $d = 1$

- **Data:** X_1, \dots, X_n iid ν (cont. distribution) on \mathbb{R}
- **Sample rank map:** $\hat{R}_n : \{X_1, X_2, \dots, X_n\} \longrightarrow \{\frac{1}{n}, \frac{2}{n}, \dots, \frac{n}{n}\}$



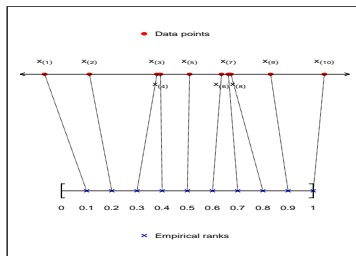
Sample rank map \hat{R}_n is the OT map that transports

$$\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i} \quad \text{to} \quad \mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{\frac{j}{n}},$$

$$\text{i.e., } \hat{R}_n := \arg \min_{T: T\# \nu_n = \mu_n} \frac{1}{n} \sum_{i=1}^n |X_i - T(X_i)|^2$$

Sample rank map: when $d = 1$

- **Data:** X_1, \dots, X_n iid ν (cont. distribution) on \mathbb{R}
- **Sample rank map:** $\hat{R}_n : \{X_1, X_2, \dots, X_n\} \longrightarrow \{\frac{1}{n}, \frac{2}{n}, \dots, \frac{n}{n}\}$



Sample rank map \hat{R}_n is the OT map that transports

$$\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i} \quad \text{to} \quad \mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{\frac{j}{n}},$$

$$\text{i.e., } \hat{R}_n := \arg \min_{T: T\# \nu_n = \mu_n} \frac{1}{n} \sum_{i=1}^n |X_i - T(X_i)|^2 = \arg \max_{T: T\# \nu_n = \mu_n} \frac{1}{n} \sum_{i=1}^n X_{(i)} \cdot T(X_{(i)})$$

1 Optimal Transport: Monge's Problem

- Introduction
- Multivariate Ranks via Optimal Transport

2 Multivariate Two-sample Goodness-of-fit Testing

- Distribution-free Testing — Hotelling T^2 and Rank Hotelling
- Lower bounds on Asymptotic (Pitman) Relative Efficiency

3 Other Applications of Distribution-free Inference

- Testing for Mutual Independence
- Testing for Symmetry

- $X \sim \nu$; ν is a probability measure (abs. cont.) in \mathbb{R}^d ($d \geq 1$)
- **Reference dist.:** $U \sim \mu$ on $\mathcal{S} \subset \mathbb{R}^d$ ($\mu = \text{Unif}([0, 1]^d), N(0, I_d)$)
- Find OT map T s.t. $T(X) \stackrel{d}{=} U \sim \mu$ (μ abs. cont.)

- $X \sim \nu$; ν is a probability measure (abs. cont.) in \mathbb{R}^d ($d \geq 1$)
- **Reference dist.:** $U \sim \mu$ on $\mathcal{S} \subset \mathbb{R}^d$ ($\mu = \text{Unif}([0, 1]^d), N(0, I_d)$)
- Find **OT map** T s.t. $T(X) \stackrel{d}{=} U \sim \mu$ (μ abs. cont.)

Population rank function [Hallin (2017), Chernozhukov et al. (2017)]

If $\mathbb{E}_\nu \|X\|^2 < \infty$, **rank function** $R: \mathbb{R}^d \rightarrow \mathcal{S}$ is the **OT map** s.t.

$$R := \arg \min_{T: T\# \nu = \mu} \mathbb{E}_\nu \|X - T(X)\|^2$$

- $X \sim \nu$; ν is a probability measure (abs. cont.) in \mathbb{R}^d ($d \geq 1$)
- **Reference dist.:** $U \sim \mu$ on $\mathcal{S} \subset \mathbb{R}^d$ ($\mu = \text{Unif}([0, 1]^d), N(0, I_d)$)
- Find **OT map** T s.t. $T(X) \stackrel{d}{=} U \sim \mu$ (μ abs. cont.)

Population rank function [Hallin (2017), Chernozhukov et al. (2017)]

If $\mathbb{E}_\nu \|X\|^2 < \infty$, **rank function** $R: \mathbb{R}^d \rightarrow \mathcal{S}$ is the **OT map** s.t.

$$R := \arg \min_{T: T\# \nu = \mu} \mathbb{E}_\nu \|X - T(X)\|^2$$

Properties of population rank function [Brenier (1991), McCann (1995)]

- $R(\cdot)$ **characterizes** distribution: $R_1(x) = R_2(x) \forall x \in \mathbb{R}^d$ iff $P_1 = P_2$

- $X \sim \nu$; ν is a probability measure (abs. cont.) in \mathbb{R}^d ($d \geq 1$)
- **Reference dist.:** $U \sim \mu$ on $\mathcal{S} \subset \mathbb{R}^d$ ($\mu = \text{Unif}([0, 1]^d), N(0, I_d)$)
- Find **OT map** T s.t. $T(X) \stackrel{d}{=} U \sim \mu$ (μ abs. cont.)

Population rank function [Hallin (2017), Chernozhukov et al. (2017)]

If $\mathbb{E}_\nu \|X\|^2 < \infty$, **rank function** $R : \mathbb{R}^d \rightarrow \mathcal{S}$ is the **OT map** s.t.

$$R := \arg \min_{T: T\# \nu = \mu} \mathbb{E}_\nu \|X - T(X)\|^2$$

Properties of population rank function [Brenier (1991), McCann (1995)]

- $R(\cdot)$ **characterizes** distribution: $R_1(x) = R_2(x) \forall x \in \mathbb{R}^d$ iff $P_1 = P_2$
- $R(\cdot)$ is **invertible**, i.e., there exists unique $Q(\cdot)$ s.t.

$$R \circ Q(u) = u \quad (\mu\text{-a.e.}) \quad \text{and} \quad Q \circ R(x) = x \quad (\nu\text{-a.e.})$$

- $X \sim \nu$; ν is a probability measure (abs. cont.) in \mathbb{R}^d ($d \geq 1$)
- **Reference dist.:** $U \sim \mu$ on $\mathcal{S} \subset \mathbb{R}^d$ ($\mu = \text{Unif}([0, 1]^d), N(0, I_d)$)
- Find **OT map** T s.t. $T(X) \stackrel{d}{=} U \sim \mu$ (μ abs. cont.)

Population rank function [Hallin (2017), Chernozhukov et al. (2017)]

If $\mathbb{E}_\nu \|X\|^2 < \infty$, **rank function** $R : \mathbb{R}^d \rightarrow \mathcal{S}$ is the **OT map** s.t.

$$R := \arg \min_{T: T\# \nu = \mu} \mathbb{E}_\nu \|X - T(X)\|^2$$

Properties of population rank function [Brenier (1991), McCann (1995)]

- $R(\cdot)$ **characterizes** distribution: $R_1(x) = R_2(x) \forall x \in \mathbb{R}^d$ iff $P_1 = P_2$
- $R(\cdot)$ is **invertible**, i.e., there exists unique $Q(\cdot)$ s.t.

$$R \circ Q(u) = u \quad (\mu\text{-a.e.}) \quad \text{and} \quad Q \circ R(x) = x \quad (\nu\text{-a.e.})$$

- Both $R(\cdot)$ and $Q(\cdot)$ and **gradients** of **convex functions**

- If $\mathbb{E}_\nu \|X\|^2 < \infty$, the population rank function $R(\cdot)$ is defined as

$$R := \arg \min_{T: T \# \nu = \mu} \mathbb{E}_\nu \|X - T(X)\|^2 \quad (1)$$

- Even when $\mathbb{E}_\nu \|X\|^2 = +\infty$, $R(\cdot)$ can still be defined

- If $\mathbb{E}_\nu \|X\|^2 < \infty$, the **population rank function** $R(\cdot)$ is defined as

$$R := \arg \min_{T: T\#\nu=\mu} \mathbb{E}_\nu \|X - T(X)\|^2 \quad (1)$$

- Even when $\mathbb{E}_\nu \|X\|^2 = +\infty$, $R(\cdot)$ can still be defined

Characterization of the population rank function [McCann (1995)]

Suppose $X \sim \nu$ **abs. cont.** on \mathbb{R}^d . Then \exists ν -a.e. **unique** meas. mapping $R: \mathbb{R}^d \rightarrow \mathcal{S}$, transporting ν to μ (i.e., $R\#\nu = \mu$), of the form

$$R(x) = \nabla \varphi(x), \quad \text{for } \nu\text{-a.e. } x, \quad (2)$$

where $\varphi: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ is a **convex** function (**cf. when** $d = 1$).

- If $\mathbb{E}_\nu \|X\|^2 < \infty$, the **population rank function** $R(\cdot)$ is defined as

$$R := \arg \min_{T: T\#\nu=\mu} \mathbb{E}_\nu \|X - T(X)\|^2 \quad (1)$$

- Even when $\mathbb{E}_\nu \|X\|^2 = +\infty$, $R(\cdot)$ can still be defined

Characterization of the population rank function [McCann (1995)]

Suppose $X \sim \nu$ **abs. cont.** on \mathbb{R}^d . Then \exists ν -a.e. **unique** meas. mapping $R: \mathbb{R}^d \rightarrow \mathcal{S}$, transporting ν to μ (i.e., $R\#\nu = \mu$), of the form

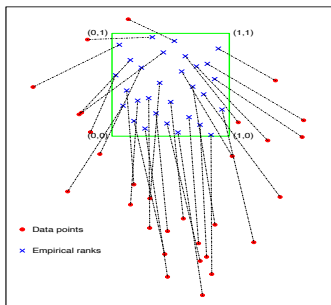
$$R(x) = \nabla \varphi(x), \quad \text{for } \nu\text{-a.e. } x, \quad (2)$$

where $\varphi: \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ is a **convex** function (**cf. when** $d = 1$).

Moreover, when $\mathbb{E}_\nu \|X\|^2 < \infty$, $R(\cdot)$ as defined in (2) also satisfies (1).

- $X_1, \dots, X_n \stackrel{iid}{\sim} \nu$ on \mathbb{R}^d (abs. cont.); $\mu \sim \text{Unif}([0, 1]^d)$
- Empirical rank map $\hat{R}_n: \{X_1, \dots, X_n\} \rightarrow \{c_1, \dots, c_n\} \subset [0, 1]^d$ — sequence of “uniform-like” points (or quasi-Monte Carlo sequence)

- $X_1, \dots, X_n \stackrel{iid}{\sim} \nu$ on \mathbb{R}^d (abs. cont.); $\mu \sim \text{Unif}([0, 1]^d)$
- Empirical rank map $\hat{R}_n: \{X_1, \dots, X_n\} \rightarrow \{c_1, \dots, c_n\} \subset [0, 1]^d$ — sequence of “uniform-like” points (or quasi-Monte Carlo sequence)



- Sample multivariate rank map \hat{R}_n is defined as the OT map s.t.

$$\hat{R}_n := \arg \min_{T: T\# \nu_n = \mu_n} \frac{1}{n} \sum_{i=1}^n \|X_i - T(X_i)\|^2$$

where T transports $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$ to $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$

- Assignment problem (can be reduced to a linear program — $O(n^3)$)

Distribution-free property [Hallin (2017), Deb and S. (2019)]

Suppose that X_1, \dots, X_n iid on \mathbb{R}^d with abs. cont. distribution. Then,

$$(\hat{R}_n(X_1), \dots, \hat{R}_n(X_n))$$

is uniformly distributed over the $n!$ permutations of $\{c_1, \dots, c_n\}$.

Distribution-free property [Hallin (2017), Deb and S. (2019)]

Suppose that X_1, \dots, X_n iid on \mathbb{R}^d with **abs. cont.** distribution. Then,

$$(\hat{R}_n(X_1), \dots, \hat{R}_n(X_n))$$

is **uniformly distributed** over the $n!$ permutations of $\{c_1, \dots, c_n\}$.

The **first** step to obtaining **distribution-free** tests [Hallin et al. (2021)]

Distribution-free property [Hallin (2017), Deb and S. (2019)]

Suppose that X_1, \dots, X_n iid on \mathbb{R}^d with **abs. cont.** distribution. Then,

$$(\hat{R}_n(X_1), \dots, \hat{R}_n(X_n))$$

is **uniformly distributed** over the $n!$ permutations of $\{c_1, \dots, c_n\}$.

The **first** step to obtaining **distribution-free** tests [Hallin et al. (2021)]

Consistency [Deb and S. (2019), Deb, Bhattacharya and S. (2021)]

X_1, \dots, X_n iid ν (abs. cont.). If $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j} \xrightarrow{d} \mu$ (abs. cont.), then

$$\frac{1}{n} \sum_{i=1}^n \|\hat{R}_n(X_i) - R(X_i)\|^2 \xrightarrow{p} 0$$

Regularity to the empirical multivariate **rank/OT** map

Question: What is the **rate of convergence** of \hat{R}_n ?

- **Recall:** $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$, $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$
- **OT maps:** $R \# \nu = \mu$, $\hat{R}_n \# \nu_n = \mu_n$
- Assume $\int \|x\|^2 d\nu(x) < \infty$, $\int \|y\|^2 d\mu(y) < \infty$

Rate of convergence [Deb, Ghosal and S. (2021)] Proof of this result

Suppose the population rank map $R(\cdot)$ is **Lipschitz**. Then, under appropriate conditions on μ_n ,

$$\mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n \|\hat{R}_n(X_i) - R(X_i)\|^2 \right] \lesssim \begin{cases} n^{-1/2} & d = 2, 3, \\ n^{-1/2} \log n & d = 4, \\ n^{-2/d} & d > 4. \end{cases}$$

Question: What is the **rate of convergence** of \hat{R}_n ?

- **Recall:** $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$, $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$
- **OT maps:** $R \# \nu = \mu$, $\hat{R}_n \# \nu_n = \mu_n$
- Assume $\int \|x\|^2 d\nu(x) < \infty$, $\int \|y\|^2 d\mu(y) < \infty$

Rate of convergence [Deb, Ghosal and S. (2021)]

Proof of this result

Suppose the population rank map $R(\cdot)$ is **Lipschitz**. Then, under appropriate conditions on μ_n ,

$$\mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n \|\hat{R}_n(X_i) - R(X_i)\|^2 \right] \lesssim \begin{cases} n^{-1/2} & d = 2, 3, \\ n^{-1/2} \log n & d = 4, \\ n^{-2/d} & d > 4. \end{cases}$$

This is the **optimal** rate for $d \geq 4$ [Hütter & Rigollet (2021)]

Question: What is the **rate of convergence** of \hat{R}_n ?

- **Recall:** $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$, $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$
- **OT maps:** $R\#\nu = \mu$, $\hat{R}_n\#\nu_n = \mu_n$
- Assume $\int \|x\|^2 d\nu(x) < \infty$, $\int \|y\|^2 d\mu(y) < \infty$

Rate of convergence [Deb, Ghosal and S. (2021)] Proof of this result

Suppose the population rank map $R(\cdot)$ is **Lipschitz**. Then, under appropriate conditions on μ_n ,

$$\mathbb{E} \left[\frac{1}{n} \sum_{i=1}^n \|\hat{R}_n(X_i) - R(X_i)\|^2 \right] \lesssim \begin{cases} n^{-1/2} & d = 2, 3, \\ n^{-1/2} \log n & d = 4, \\ n^{-2/d} & d > 4. \end{cases}$$

This is the **optimal** rate for $d \geq 4$ [Hütter & Rigollet (2021)]

Connection to **estimation** of the **OT** map R ($R\#\nu = \mu$)

References: Hütter & Rigollet (2021), Ghosal and S. (2019), Manole et al. (2021), Pooladian and Niles-Weed (2022), Gunsilius (2022), ...

- 1 Optimal Transport: Monge's Problem
 - Introduction
 - Multivariate Ranks via Optimal Transport
- 2 Multivariate Two-sample Goodness-of-fit Testing
 - Distribution-free Testing — Hotelling T^2 and Rank Hotelling
 - Lower bounds on Asymptotic (Pitman) Relative Efficiency
- 3 Other Applications of Distribution-free Inference
 - Testing for Mutual Independence
 - Testing for Symmetry

1 Optimal Transport: Monge's Problem

- Introduction
- Multivariate Ranks via Optimal Transport

2 Multivariate Two-sample Goodness-of-fit Testing

- Distribution-free Testing — Hotelling T^2 and Rank Hotelling
- Lower bounds on Asymptotic (Pitman) Relative Efficiency

3 Other Applications of Distribution-free Inference

- Testing for Mutual Independence
- Testing for Symmetry

Multivariate two-sample goodness-of-fit test

Testing for equality of two multivariate distributions

- **Data:** $\{X_i\}_{i=1}^m$ iid P_1 on \mathbb{R}^d ; $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$
- Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

Multivariate two-sample goodness-of-fit test

Testing for equality of two multivariate distributions

- **Data:** $\{X_i\}_{i=1}^m$ iid P_1 on \mathbb{R}^d ; $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$
- Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

- **Hotelling T^2 statistic** [**Hotelling (1931)**]: The **multivariate analogue** of Student's **t -statistic**, given by

$$T_{m,n}^2 := \frac{mn}{m+n} (\bar{X} - \bar{Y})^\top S_{m,n}^{-1} (\bar{X} - \bar{Y});$$

where $S_{m,n}$ is **pooled covariance matrix**

Multivariate two-sample goodness-of-fit test

Testing for equality of two multivariate distributions

- **Data:** $\{X_i\}_{i=1}^m$ iid P_1 on \mathbb{R}^d ; $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$
- Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

- **Hotelling T^2 statistic** [Hotelling (1931)]: The **multivariate analogue** of Student's **t -statistic**, given by

$$T_{m,n}^2 := \frac{mn}{m+n} (\bar{X} - \bar{Y})^\top S_{m,n}^{-1} (\bar{X} - \bar{Y});$$

where $S_{m,n}$ is **pooled covariance matrix**

- Reject H_0 iff $T_{m,n}^2 > c_\alpha$ [**asympt. cut-off** c_α : $(1 - \alpha)$ quantile of χ_d^2]
- **Consistency:** $\mathbb{P}(T_{m,n}^2 > c_\alpha) \rightarrow 1$ when $\mathbb{E}[X_1] \neq \mathbb{E}[Y_1]$

Multivariate two-sample goodness-of-fit test

Testing for equality of two multivariate distributions

- **Data:** $\{X_i\}_{i=1}^m$ iid P_1 on \mathbb{R}^d ; $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$
- Test if the **two samples** came from the **same distribution**, i.e.,

$$H_0 : P_1 = P_2 \quad \text{versus} \quad H_1 : P_1 \neq P_2$$

- **Hotelling T^2 statistic** [Hotelling (1931)]: The **multivariate analogue** of Student's **t -statistic**, given by

$$T_{m,n}^2 := \frac{mn}{m+n} (\bar{X} - \bar{Y})^\top S_{m,n}^{-1} (\bar{X} - \bar{Y});$$

where $S_{m,n}$ is **pooled covariance matrix**

- Reject H_0 iff $T_{m,n}^2 > c_\alpha$ [**asympt. cut-off** c_α : $(1 - \alpha)$ quantile of χ_d^2]
- **Consistency:** $\mathbb{P}(T_{m,n}^2 > c_\alpha) \rightarrow 1$ when $\mathbb{E}[X_1] \neq \mathbb{E}[Y_1]$

Question: What is the **distribution-free** analogue of **Hotelling's T^2** ?

Data: $\{X_i\}_{i=1}^m$ iid P_1 (abs. cont.), $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$
Reference dist.: μ on $\mathcal{S} \subset \mathbb{R}^d$ (abs. cont.; $\mu = \text{Unif}([0, 1]^d)$ or $N(0, I_d)$)

Proposed test [Deb, Bhattacharya and S. (2021)]

- **Joint rank map:** The sample ranks of the **pooled** observations:

$$\hat{R}_{m,n} : \{X_1, \dots, X_m, Y_1, \dots, Y_n\} \rightarrow \{c_1, \dots, c_{m+n}\} \subset \mathcal{S}$$

- **Rank Hotelling:** $\text{RT}_{m,n}^2 := T_{m,n}^2 \left(\{\hat{R}_{m,n}(X_i)\}, \{\hat{R}_{m,n}(Y_j)\} \right)$

Data: $\{X_i\}_{i=1}^m$ iid P_1 (abs. cont.), $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$

Reference dist.: μ on $\mathcal{S} \subset \mathbb{R}^d$ (abs. cont.; $\mu = \text{Unif}([0, 1]^d)$ or $N(0, I_d)$)

Proposed test [Deb, Bhattacharya and S. (2021)]

- **Joint rank map:** The sample ranks of the **pooled** observations:

$$\hat{R}_{m,n} : \{X_1, \dots, X_m, Y_1, \dots, Y_n\} \rightarrow \{c_1, \dots, c_{m+n}\} \subset \mathcal{S}$$

- **Rank Hotelling:** $\text{RT}_{m,n}^2 := T_{m,n}^2 \left(\{\hat{R}_{m,n}(X_i)\}, \{\hat{R}_{m,n}(Y_j)\} \right)$

This yields the **Wilcoxon rank-sum** test when applied to the **t-test**

General principle [Deb and S. (2019)]

Start with any “**good**” test & **replace** X_i ’s & Y_j ’s with **pooled OT ranks**

Data: $\{X_i\}_{i=1}^m$ iid P_1 (abs. cont.), $\{Y_j\}_{j=1}^n$ iid P_2 on \mathbb{R}^d , $d \geq 1$
Reference dist.: μ on $\mathcal{S} \subset \mathbb{R}^d$ (abs. cont.; $\mu = \text{Unif}([0, 1]^d)$ or $N(0, I_d)$)

Proposed test [Deb, Bhattacharya and S. (2021)]

- **Joint rank map:** The sample ranks of the **pooled** observations:

$$\hat{R}_{m,n} : \{X_1, \dots, X_m, Y_1, \dots, Y_n\} \rightarrow \{c_1, \dots, c_{m+n}\} \subset \mathcal{S}$$

- **Rank Hotelling:** $\text{RT}_{m,n}^2 := T_{m,n}^2 \left(\{\hat{R}_{m,n}(X_i)\}, \{\hat{R}_{m,n}(Y_j)\} \right)$

This yields the **Wilcoxon rank-sum** test when applied to the **t-test**

General principle [Deb and S. (2019)]

Start with any “**good**” test & **replace** X_i ’s & Y_j ’s with **pooled OT ranks**

Distribution-freeness: Under H_0 , the dist. of $\text{RT}_{m,n}^2$ is **free** of $P_1 \equiv P_2$

The **only** known **efficient**, computationally feasible, **distribution-free** analogue of Hotelling’s T^2 ; cf. **Puri & Sen (1971)**, **Hallin et al. (2020)**, ...

Rank Hotelling test

Rank Hotelling test: $\phi_{m,n} \equiv \mathbf{1}\{\text{RT}_{m,n}^2 > \kappa_{\alpha}^{(m,n)}\}$ — distribution-free

$\kappa_{\alpha}^{(m,n)}$ depends on c_j 's, m, n and d

Rank Hotelling test

Rank Hotelling test: $\phi_{m,n} \equiv \mathbf{1}\{\text{RT}_{m,n}^2 > \kappa_{\alpha}^{(m,n)}\}$ — **distribution-free**

$\kappa_{\alpha}^{(m,n)}$ depends on c_j 's, m, n and d

Asymptotic null distribution [Deb, Bhattacharya, and S. (2021)]

Under H_0 , if $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j} \xrightarrow{d} \mu$, then,

$$\text{RT}_{m,n}^2 \xrightarrow{d} \chi_d^2 \quad \text{as } \min\{m, n\} \rightarrow \infty.$$

The choice of the c_j 's have **no effect** for **large** m, n

Rank Hotelling test

Rank Hotelling test: $\phi_{m,n} \equiv \mathbf{1}\{\text{RT}_{m,n}^2 > \kappa_\alpha^{(m,n)}\}$ — **distribution-free**

$\kappa_\alpha^{(m,n)}$ depends on c_j 's, m, n and d

Asymptotic null distribution [Deb, Bhattacharya, and S. (2021)]

Under H_0 , if $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j} \xrightarrow{d} \mu$, then,

$$\text{RT}_{m,n}^2 \xrightarrow{d} \chi_d^2 \quad \text{as } \min\{m, n\} \rightarrow \infty.$$

The choice of the c_j 's have **no effect** for **large** m, n

Consistency [Deb, Bhattacharya, and S. (2021)]

Under **location shift** alternatives ($P_1 \neq P_2$), if (i) $\mu_n \xrightarrow{d} \mu$, and
(ii) $\frac{m}{m+n} \rightarrow \lambda \in (0, 1)$, then,

$$\lim_{m,n \rightarrow \infty} \mathbb{E}_{H_1}[\phi_{m,n}] = 1.$$

Rank Hotelling test

Rank Hotelling test: $\phi_{m,n} \equiv \mathbf{1}\{\text{RT}_{m,n}^2 > \kappa_{\alpha}^{(m,n)}\}$ — **distribution-free**

$\kappa_{\alpha}^{(m,n)}$ depends on c_j 's, m, n and d

Asymptotic null distribution [Deb, Bhattacharya, and S. (2021)]

Under H_0 , if $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j} \xrightarrow{d} \mu$, then,

$$\text{RT}_{m,n}^2 \xrightarrow{d} \chi_d^2 \quad \text{as } \min\{m, n\} \rightarrow \infty.$$

The choice of the c_j 's have **no effect** for **large** m, n

Consistency [Deb, Bhattacharya, and S. (2021)]

Under **location shift** alternatives ($P_1 \neq P_2$), if (i) $\mu_n \xrightarrow{d} \mu$, and
(ii) $\frac{m}{m+n} \rightarrow \lambda \in (0, 1)$, then,

$$\lim_{m,n \rightarrow \infty} \mathbb{E}_{H_1}[\phi_{m,n}] = 1.$$

Question: How does the **efficiency** of $\text{RT}_{m,n}^2$ compare with $\text{T}_{m,n}^2$?

1 Optimal Transport: Monge's Problem

- Introduction
- Multivariate Ranks via Optimal Transport

2 Multivariate Two-sample Goodness-of-fit Testing

- Distribution-free Testing — Hotelling T^2 and Rank Hotelling
- Lower bounds on Asymptotic (Pitman) Relative Efficiency

3 Other Applications of Distribution-free Inference

- Testing for Mutual Independence
- Testing for Symmetry

- **Question:** How to compare two consistent tests S_N and T_N ?
- **Asymptotic relative (Pitman) efficiency (ARE)** [Pitman (1948), Serfling (1980), Lehmann & Romano (2005), van der Vaart (1998)]

- **Question:** How to compare two **consistent** tests S_N and T_N ?
- **Asymptotic relative (Pitman) efficiency (ARE)** [Pitman (1948), Serfling (1980), Lehmann & Romano (2005), van der Vaart (1998)]
- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$; $\frac{m}{N} \approx \lambda \in (0, 1)$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family

- **Question:** How to compare two **consistent** tests S_N and T_N ?
- **Asymptotic relative (Pitman) efficiency (ARE)** [Pitman (1948), Serfling (1980), Lehmann & Romano (2005), van der Vaart (1998)]
- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$; $\frac{m}{N} \approx \lambda \in (0, 1)$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family
- **Test** $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + \Delta$; $\Delta \rightarrow 0$

- **Question:** How to compare two **consistent** tests S_N and T_N ?
- **Asymptotic relative (Pitman) efficiency (ARE)** [Pitman (1948), Serfling (1980), Lehmann & Romano (2005), van der Vaart (1998)]
- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$; $\frac{m}{N} \approx \lambda \in (0, 1)$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family
- **Test** $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + \Delta$; $\Delta \rightarrow 0$
- Fix $\alpha \in (0, 1)$ (level) and $\beta \in (\alpha, 1)$ (power)

- **Question:** How to compare two **consistent** tests S_N and T_N ?
- **Asymptotic relative (Pitman) efficiency (ARE)** [Pitman (1948), Serfling (1980), Lehmann & Romano (2005), van der Vaart (1998)]
- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$; $\frac{m}{N} \approx \lambda \in (0, 1)$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family
- **Test** $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + \Delta$; $\Delta \rightarrow 0$
- Fix $\alpha \in (0, 1)$ (level) and $\beta \in (\alpha, 1)$ (power)
- Let $N_\Delta(T.) \equiv N_\Delta$ denote the **minimum** number of **samples** s.t.:

$$\mathbb{E}_{H_0}[T_{N_\Delta}] = \alpha \quad \text{and} \quad \mathbb{E}_{H_1}[T_{N_\Delta}] \geq \beta$$

- **Question:** How to compare two **consistent** tests S_N and T_N ?
- **Asymptotic relative (Pitman) efficiency (ARE)** [Pitman (1948), Serfling (1980), Lehmann & Romano (2005), van der Vaart (1998)]
- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$; $\frac{m}{N} \approx \lambda \in (0, 1)$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family

- **Test** $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + \Delta$; $\Delta \rightarrow 0$
- Fix $\alpha \in (0, 1)$ (level) and $\beta \in (\alpha, 1)$ (power)
- Let $N_\Delta(T.) \equiv N_\Delta$ denote the **minimum** number of **samples** s.t:

$$\mathbb{E}_{H_0}[T_{N_\Delta}] = \alpha \quad \text{and} \quad \mathbb{E}_{H_1}[T_{N_\Delta}] \geq \beta$$

- The **asymptotic (Pitman) efficiency** of S_N w.r.t T_N is given by

$$\text{ARE}(S_N, T_N) := \lim_{\Delta \rightarrow 0} \frac{N_\Delta(T.)}{N_\Delta(S.)}$$

- **Question:** How to compare two **consistent** tests S_N and T_N ?
- **Asymptotic relative (Pitman) efficiency** (**ARE**) [Pitman (1948), Serfling (1980), Lehmann & Romano (2005), van der Vaart (1998)]
- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$; $\frac{m}{N} \approx \lambda \in (0, 1)$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “**smooth**” (satisfies DQM) parametric family

- **Test** $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + \Delta$; $\Delta \rightarrow 0$
- Fix $\alpha \in (0, 1)$ (**level**) and $\beta \in (\alpha, 1)$ (**power**)
- Let $N_\Delta(T.) \equiv N_\Delta$ denote the **minimum** number of **samples** s.t:

$$\mathbb{E}_{H_0}[T_{N_\Delta}] = \alpha \quad \text{and} \quad \mathbb{E}_{H_1}[T_{N_\Delta}] \geq \beta$$

- The **asymptotic (Pitman) efficiency** of S_N w.r.t T_N is given by

$$\text{ARE}(S_N, T_N) := \lim_{\Delta \rightarrow 0} \frac{N_\Delta(T.)}{N_\Delta(S.)}$$

$\text{ARE}(S_N, T_N)$ can depend on α and β , but in some cases **it doesn't!**

Hotelling T^2 : $T_{m,n}^2(\{X_i\}, \{Y_j\}) = \frac{mn}{m+n} (\bar{X} - \bar{Y})^\top S_{m,n}^{-1} (\bar{X} - \bar{Y})$

Rank Hotelling: $RT_{m,n}^2 = T_{m,n}^2(\{\hat{R}_{m,n}(X_i)\}, \{\hat{R}_{m,n}(Y_j)\})$

- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family
- Consider $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + hN^{-1/2}$; $h \neq 0 \in \mathbb{R}^p$

$\text{ARE}(RT_{m,n}^2, T_{m,n}^2)$ can be derived under the above alternatives

Hotelling T^2 : $T_{m,n}^2(\{X_i\}, \{Y_j\}) = \frac{mn}{m+n} (\bar{X} - \bar{Y})^\top S_{m,n}^{-1} (\bar{X} - \bar{Y})$

Rank Hotelling: $RT_{m,n}^2 = T_{m,n}^2(\{\hat{R}_{m,n}(X_i)\}, \{\hat{R}_{m,n}(Y_j)\})$

- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family
- Consider $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + hN^{-1/2}$; $h \neq 0 \in \mathbb{R}^p$

$\text{ARE}(RT_{m,n}^2, T_{m,n}^2)$ can be derived under the above alternatives

Some observations

- Expression of $\text{ARE}(RT_{m,n}^2, T_{m,n}^2)$ does not depend on α and β
- Asymp. dist. of $RT_{m,n}^2$ can depend on choice of μ (reference dist.)

Hotelling T^2 : $T_{m,n}^2(\{X_i\}, \{Y_j\}) = \frac{mn}{m+n} (\bar{X} - \bar{Y})^\top S_{m,n}^{-1} (\bar{X} - \bar{Y})$

Rank Hotelling: $RT_{m,n}^2 = T_{m,n}^2(\{\hat{R}_{m,n}(X_i)\}, \{\hat{R}_{m,n}(Y_j)\})$

- $X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1}$ & $Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}$; $N = m + n$
- $\{P_\theta\}_{\theta \in \Theta \subset \mathbb{R}^p}$: “smooth” (satisfies DQM) parametric family
- Consider $H_0 : \theta_2 = \theta_1$ vs. $H_1 : \theta_2 = \theta_1 + hN^{-1/2}$; $h \neq 0 \in \mathbb{R}^p$

$\text{ARE}(RT_{m,n}^2, T_{m,n}^2)$ can be derived under the above alternatives

Some observations

- Expression of $\text{ARE}(RT_{m,n}^2, T_{m,n}^2)$ does not depend on α and β
- Asymp. dist. of $RT_{m,n}^2$ can depend on choice of μ (reference dist.)

Can we lower bound ARE for sub-classes of multivariate dists., i.e.,

$$\min_{\mathcal{F}} \text{ARE}(RT_{m,n}^2, T_{m,n}^2) = ??$$

$$X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1} \text{ \& } Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}; \quad N = m + n$$

Independent coordinates case (location shift family)

$$\mathcal{F}_{\text{ind}} = \{P_\theta\}_{\theta \in \Theta} \text{ has density } p_\theta(z_1, \dots, z_d) = \prod_{i=1}^d f_i(z_i - \theta_i), \quad \theta \in \mathbb{R}^d$$

Theorem [Deb, Bhattacharya, and S. (2021)]

Suppose $\frac{m}{N} \rightarrow \lambda \in (0, 1)$. If $\mu_N := \frac{1}{N} \sum_{j=1}^N \delta_{c_j} \xrightarrow{d} \text{Unif}([0, 1]^d) \equiv \mu$, then

$$\min_{\mathcal{F}_{\text{ind}}} \text{ARE}(\text{RT}_{m,n}^2, \text{T}_{m,n}^2) = 0.864.$$

$$X_1, \dots, X_m \stackrel{iid}{\sim} P_{\theta_1} \text{ \& } Y_1, \dots, Y_n \stackrel{iid}{\sim} P_{\theta_2}; \quad N = m + n$$

Independent coordinates case (location shift family)

$$\mathcal{F}_{\text{ind}} = \{P_\theta\}_{\theta \in \Theta} \text{ has density } p_\theta(z_1, \dots, z_d) = \prod_{i=1}^d f_i(z_i - \theta_i), \quad \theta \in \mathbb{R}^d$$

Theorem [Deb, Bhattacharya, and S. (2021)]

Suppose $\frac{m}{N} \rightarrow \lambda \in (0, 1)$. If $\mu_N := \frac{1}{N} \sum_{j=1}^N \delta_{c_j} \xrightarrow{d} \text{Unif}([0, 1]^d) \equiv \mu$, then

$$\min_{\mathcal{F}_{\text{ind}}} \text{ARE}(\text{RT}_{m,n}^2, T_{m,n}^2) = 0.864.$$

If $\mu_N \xrightarrow{d} N(0, I_d) \equiv \mu$, then

$$\min_{\mathcal{F}_{\text{ind}}} \text{ARE}(\text{RT}_{m,n}^2, T_{m,n}^2) = 1.$$

$$X_1, \dots, X_m \stackrel{iid}{\sim} \mathbf{P}_{\theta_1} \text{ \& } Y_1, \dots, Y_n \stackrel{iid}{\sim} \mathbf{P}_{\theta_2}; \quad N = m + n$$

Independent coordinates case (location shift family)

$$\mathcal{F}_{\text{ind}} = \{P_\theta\}_{\theta \in \Theta} \text{ has density } p_\theta(z_1, \dots, z_d) = \prod_{i=1}^d f_i(z_i - \theta_i), \quad \theta \in \mathbb{R}^d$$

Theorem [Deb, Bhattacharya, and S. (2021)]

Suppose $\frac{m}{N} \rightarrow \lambda \in (0, 1)$. If $\mu_N := \frac{1}{N} \sum_{j=1}^N \delta_{c_j} \xrightarrow{d} \text{Unif}([0, 1]^d) \equiv \mu$, then

$$\min_{\mathcal{F}_{\text{ind}}} \text{ARE}(\text{RT}_{m,n}^2, \text{T}_{m,n}^2) = 0.864.$$

If $\mu_N \xrightarrow{d} N(0, I_d) \equiv \mu$, then

$$\min_{\mathcal{F}_{\text{ind}}} \text{ARE}(\text{RT}_{m,n}^2, \text{T}_{m,n}^2) = 1.$$

- Generalizes Hodges & Lehmann (1956), Chernoff & Savage (1958)
- ARE can be arbitrarily large (can tend to $+\infty$) for heavy tailed dists.

Elliptically symmetric distributions

$\mathcal{F}_{\text{ell}} = \{P_\theta\}_{\theta \in \Theta}$ is class of **elliptically symmetric** distributions on \mathbb{R}^d , i.e.,

$$p_\theta(x) \propto (\det(\Sigma))^{-\frac{1}{2}} \underline{f}\left((x - \theta)^\top \Sigma^{-1}(x - \theta)\right), \quad \text{for all } x \in \mathbb{R}^d$$

Elliptically symmetric distributions

$\mathcal{F}_{\text{ell}} = \{P_\theta\}_{\theta \in \Theta}$ is class of **elliptically symmetric** distributions on \mathbb{R}^d , i.e.,

$$p_\theta(x) \propto (\det(\Sigma))^{-\frac{1}{2}} \underline{f}((x - \theta)^\top \Sigma^{-1}(x - \theta)), \quad \text{for all } x \in \mathbb{R}^d$$

Theorem [Deb, Bhattacharya, and S. (2021)]

Suppose: (i) $\mu_N \xrightarrow{d} N(0, I_d) \equiv \mu$, (ii) $\frac{m}{N} \rightarrow \lambda \in (0, 1)$. Then,

$$\min_{\mathcal{F}_{\text{ell}}} \text{ARE}(\text{RT}_{m,n}^2, \text{T}_{m,n}^2) = 1.$$

- This generalizes the famous result of **Chernoff and Savage (1958)**

Elliptically symmetric distributions

$\mathcal{F}_{\text{ell}} = \{P_\theta\}_{\theta \in \Theta}$ is class of **elliptically symmetric** distributions on \mathbb{R}^d , i.e.,

$$p_\theta(x) \propto (\det(\Sigma))^{-\frac{1}{2}} \underline{f}((x - \theta)^\top \Sigma^{-1}(x - \theta)), \quad \text{for all } x \in \mathbb{R}^d$$

Theorem [Deb, Bhattacharya, and S. (2021)]

Suppose: (i) $\mu_N \xrightarrow{d} N(0, I_d) \equiv \mu$, (ii) $\frac{m}{N} \rightarrow \lambda \in (0, 1)$. Then,

$$\min_{\mathcal{F}_{\text{ell}}} \text{ARE}(\text{RT}_{m,n}^2, T_{m,n}^2) = 1.$$

- This generalizes the famous result of **Chernoff and Savage (1958)**
- **Lower bounds** can also be obtained for other **sub-classes** of multivariate distributions (e.g., the model for **ICA**)

Outline

- 1 Optimal Transport: Monge's Problem
 - Introduction
 - Multivariate Ranks via Optimal Transport
- 2 Multivariate Two-sample Goodness-of-fit Testing
 - Distribution-free Testing — Hotelling T^2 and Rank Hotelling
 - Lower bounds on Asymptotic (Pitman) Relative Efficiency
- 3 Other Applications of Distribution-free Inference
 - Testing for Mutual Independence
 - Testing for Symmetry

1 Optimal Transport: Monge's Problem

- Introduction
- Multivariate Ranks via Optimal Transport

2 Multivariate Two-sample Goodness-of-fit Testing

- Distribution-free Testing — Hotelling T^2 and Rank Hotelling
- Lower bounds on Asymptotic (Pitman) Relative Efficiency

3 Other Applications of Distribution-free Inference

- Testing for Mutual Independence
- Testing for Symmetry

Testing for Mutual Independence

- $(X, Y) \sim P$ on $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$; $d_1, d_2 \geq 1$
- **Data:** n iid observations $\{(X_i, Y_i)\}_{i=1}^n$ from P
- Test if X is independent of Y , i.e.,

$$H_0 : X \perp\!\!\!\perp Y \quad \text{versus} \quad H_1 : X \not\perp\!\!\!\perp Y$$

Testing for Mutual Independence

- $(X, Y) \sim P$ on $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$; $d_1, d_2 \geq 1$
- **Data:** n iid observations $\{(X_i, Y_i)\}_{i=1}^n$ from P
- Test if X is independent of Y , i.e.,

$$H_0 : X \perp\!\!\!\perp Y \quad \text{versus} \quad H_1 : X \not\perp\!\!\!\perp Y$$

- When $d_1 = d_2 = 1$: Pearson (1904), Spearman (1904), Kendall (1938), Hoeffding (1948), Blomqvist (1950), Blum et al. (1961), Rosenblatt (1975), Feuerverger (1993), ...
- When $d_1 > 1$ or $d_2 > 1$: Friedman and Rafsky (1979), Székely et al. (2007), Gretton et al. (2008), Oja (2010), Heller et al. (2013), Biswas et al. (2016), Berrett and Samworth (2019), ...

- $(X, Y) \sim P$ on $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$, $X \sim P_X$, $Y \sim P_Y$, $d_1, d_2 \geq 1$
- **Data:** $\{(X_i, Y_i) : 1 \leq i \leq n\}$ iid P
- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$

- $(X, Y) \sim P$ on $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$, $X \sim P_X$, $Y \sim P_Y$, $d_1, d_2 \geq 1$
- **Data:** $\{(X_i, Y_i) : 1 \leq i \leq n\}$ iid P
- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$

Distance Covariance [Szekely et al. (2007, 2009), Feuerverger (1993)]

- **Characterizes** independence: $\text{dCov}(X, Y) = 0$ iff $X \perp\!\!\!\perp Y$

- $(X, Y) \sim P$ on $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$, $X \sim P_X$, $Y \sim P_Y$, $d_1, d_2 \geq 1$
- **Data:** $\{(X_i, Y_i) : 1 \leq i \leq n\}$ iid P
- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$

Distance Covariance [Szekely et al. (2007, 2009), Feuerverger (1993)]

- **Characterizes** independence: $\text{dCov}(X, Y) = 0$ iff $X \perp\!\!\!\perp Y$
- **Sample distance covariance:** dCov_n (V-statistic)
- **Distance covariance test:** Reject H_0 if

$$\text{dCov}_n(\{(X_i, Y_i)\}_{i=1}^n) > c_\alpha$$

- Critical value c_α **depends** on n , P_X , P_Y ! (can use permutation test)

- $(X, Y) \sim P$ on $\mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$, $X \sim P_X$, $Y \sim P_Y$, $d_1, d_2 \geq 1$
- **Data:** $\{(X_i, Y_i) : 1 \leq i \leq n\}$ iid P
- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$

Distance Covariance [Szekely et al. (2007, 2009), Feuerverger (1993)]

- **Characterizes** independence: $\text{dCov}(X, Y) = 0$ iff $X \perp\!\!\!\perp Y$
- **Sample distance covariance:** dCov_n (V-statistic)
- **Distance covariance test:** Reject H_0 if

$$\text{dCov}_n(\{(X_i, Y_i)\}_{i=1}^n) > c_\alpha$$

- Critical value c_α **depends** on n, P_X, P_Y ! (can use permutation test)

Question: What is the **distribution-free** analogue of **distance covariance**?

- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$
- Take $\mu_1 = \text{Uniform}([0, 1]^{d_1})$ and $\mu_2 = \text{Uniform}([0, 1]^{d_2})$

Rank distance covariance [Deb and S. (2019)]

- OT rank of X_i : $\hat{R}_n^X : \{X_1, \dots, X_n\} \rightarrow \{c_1^{(1)}, \dots, c_n^{(1)}\} \subset [0, 1]^{d_1}$
- OT rank of Y_i : $\hat{R}_n^Y : \{Y_1, \dots, Y_n\} \rightarrow \{c_1^{(2)}, \dots, c_n^{(2)}\} \subset [0, 1]^{d_2}$

- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$
- Take $\mu_1 = \text{Uniform}([0, 1]^{d_1})$ and $\mu_2 = \text{Uniform}([0, 1]^{d_2})$

Rank distance covariance [Deb and S. (2019)]

- **OT rank** of X_i : $\hat{R}_n^X : \{X_1, \dots, X_n\} \rightarrow \{c_1^{(1)}, \dots, c_n^{(1)}\} \subset [0, 1]^{d_1}$
- **OT rank** of Y_i : $\hat{R}_n^Y : \{Y_1, \dots, Y_n\} \rightarrow \{c_1^{(2)}, \dots, c_n^{(2)}\} \subset [0, 1]^{d_2}$
- **Rank distance cov.:** $\text{RdCov}_n = \text{dCov}_n \left(\left\{ (\hat{R}_n^X(X_i), \hat{R}_n^Y(Y_i)) \right\}_{i=1}^n \right)$

Distribution-freeness [Deb and S. (2019)]

X and Y abs. cont. Under H_0 , the dist. of RdCov_n is free of P_X and P_Y .

- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$
- Take $\mu_1 = \text{Uniform}([0, 1]^{d_1})$ and $\mu_2 = \text{Uniform}([0, 1]^{d_2})$

Rank distance covariance [Deb and S. (2019)]

- **OT rank** of X_i : $\hat{R}_n^X : \{X_1, \dots, X_n\} \rightarrow \{c_1^{(1)}, \dots, c_n^{(1)}\} \subset [0, 1]^{d_1}$
- **OT rank** of Y_i : $\hat{R}_n^Y : \{Y_1, \dots, Y_n\} \rightarrow \{c_1^{(2)}, \dots, c_n^{(2)}\} \subset [0, 1]^{d_2}$
- **Rank distance cov.:** $\text{RdCov}_n = \text{dCov}_n \left(\left\{ (\hat{R}_n^X(X_i), \hat{R}_n^Y(Y_i)) \right\}_{i=1}^n \right)$

Distribution-freeness [Deb and S. (2019)]

X and Y abs. cont. Under H_0 , the dist. of RdCov_n is **free** of P_X and P_Y .

Leads to a test that is also: (i) **consistent** (against all **fixed** alternatives),
 (ii) **computationally feasible**, and (iii) has **non-trivial efficiency**

- **Test:** $H_0 : X \perp\!\!\!\perp Y$ vs. $H_1 : X \not\perp\!\!\!\perp Y$
- Take $\mu_1 = \text{Uniform}([0, 1]^{d_1})$ and $\mu_2 = \text{Uniform}([0, 1]^{d_2})$

Rank distance covariance [Deb and S. (2019)]

- **OT rank** of X_i : $\hat{R}_n^X : \{X_1, \dots, X_n\} \rightarrow \{c_1^{(1)}, \dots, c_n^{(1)}\} \subset [0, 1]^{d_1}$
- **OT rank** of Y_i : $\hat{R}_n^Y : \{Y_1, \dots, Y_n\} \rightarrow \{c_1^{(2)}, \dots, c_n^{(2)}\} \subset [0, 1]^{d_2}$
- **Rank distance cov.:** $\text{RdCov}_n = \text{dCov}_n \left(\left\{ (\hat{R}_n^X(X_i), \hat{R}_n^Y(Y_i)) \right\}_{i=1}^n \right)$

Distribution-freeness [Deb and S. (2019)]

X and Y abs. cont. Under H_0 , the dist. of RdCov_n is **free** of P_X and P_Y .

Leads to a test that is also: (i) **consistent** (against all **fixed** alternatives),
 (ii) **computationally feasible**, and (iii) has **non-trivial efficiency**

Our **general principle** could have been used with any other procedure for mutual independence testing, e.g., the **HSIC statistic** [Gretton et al. (2005)] which uses ideas from the theory of **RKHS**, ...

1 Optimal Transport: Monge's Problem

- Introduction
- Multivariate Ranks via Optimal Transport

2 Multivariate Two-sample Goodness-of-fit Testing

- Distribution-free Testing — Hotelling T^2 and Rank Hotelling
- Lower bounds on Asymptotic (Pitman) Relative Efficiency

3 Other Applications of Distribution-free Inference

- Testing for Mutual Independence
- Testing for Symmetry

Testing for Symmetry

Data: $\{X_i\}_{i=1}^n$ iid $X \sim P$ (abs. cont.) on \mathbb{R}

Test the hypothesis of *symmetry*, i.e.,

$$H_0 : X \stackrel{d}{=} -X \quad \text{versus} \quad H_1 : \text{not } H_0 \quad (\star)$$

Testing for Symmetry

Data: $\{X_i\}_{i=1}^n$ iid $X \sim P$ (abs. cont.) on \mathbb{R}

Test the hypothesis of **symmetry**, i.e.,

$$H_0 : X \stackrel{d}{=} -X \quad \text{versus} \quad H_1 : \text{not } H_0 \quad (\star)$$

Distribution-free testing for symmetry

- **Sign** test [**Arbuthnott (1710)**]: "... the **first** use of **significance tests** ..." (first **nonparametric** test)
- **Wilcoxon signed-rank** (WSR) test [**Wilcoxon (1945)**]: Created the field of (classical) nonparametrics
- Arises with **paired** (matched) data; when **normality** can be violated

Testing for Symmetry

Data: $\{X_i\}_{i=1}^n$ iid $X \sim P$ (abs. cont.) on \mathbb{R}

Test the hypothesis of **symmetry**, i.e.,

$$H_0 : X \stackrel{d}{=} -X \quad \text{versus} \quad H_1 : \text{not } H_0 \quad (\star)$$

Distribution-free testing for symmetry

- **Sign** test [**Arbuthnott (1710)**]: "... the **first** use of **significance tests** ..." (first **nonparametric** test)
- **Wilcoxon signed-rank** (WSR) test [**Wilcoxon (1945)**]: Created the field of (classical) nonparametrics
- Arises with **paired** (matched) data; when **normality** can be violated
- **Result** [**van der Vaart (1998)**]: Under H_0 , the (i) **signs** are iid **Bernoulli**($\frac{1}{2}$), and (ii) **signs** and **signed-ranks** are **independent**

Goal: Develop **multivariate distribution-free** testing procedures for (\star)

Testing Multivariate Symmetry

There are **many** notions of **symmetry** in \mathbb{R}^d , for $d \geq 2$:

- **Central symmetry:** $H_0 : X \stackrel{d}{=} -X$
- **Sign symmetry:** $H_0 : X \stackrel{d}{=} DX$, $D = \text{diag}(\pm 1, \dots, \pm 1)$
- **Spherical symmetry:** $H_0 : X \stackrel{d}{=} QX$, Q **orthogonal** matrix

Testing Multivariate Symmetry

There are **many** notions of **symmetry** in \mathbb{R}^d , for $d \geq 2$:

- **Central symmetry:** $H_0 : X \stackrel{d}{=} -X$
- **Sign symmetry:** $H_0 : X \stackrel{d}{=} DX$, $D = \text{diag}(\pm 1, \dots, \pm 1)$
- **Spherical symmetry:** $H_0 : X \stackrel{d}{=} QX$, Q **orthogonal** matrix

Our framework

- $O(d)$: **group** of all **orthogonal** matrices on $\mathbb{R}^{d \times d}$
- \mathcal{G} : compact **subgroup** of $O(d)$
- **Test:** $H_0 : X \stackrel{d}{=} QX \quad \forall Q \in \mathcal{G}$, versus $H_1 : \text{not } H_0$

Testing Multivariate Symmetry

There are **many** notions of **symmetry** in \mathbb{R}^d , for $d \geq 2$:

- **Central symmetry:** $H_0 : X \stackrel{d}{=} -X$
- **Sign symmetry:** $H_0 : X \stackrel{d}{=} DX$, $D = \text{diag}(\pm 1, \dots, \pm 1)$
- **Spherical symmetry:** $H_0 : X \stackrel{d}{=} QX$, Q **orthogonal** matrix

Our framework

- $O(d)$: **group** of all **orthogonal** matrices on $\mathbb{R}^{d \times d}$
- \mathcal{G} : compact **subgroup** of $O(d)$
- **Test:** $H_0 : X \stackrel{d}{=} QX \quad \forall Q \in \mathcal{G}$, versus $H_1 : \text{not } H_0$

Results [Huang and S. (2023+)]

- Construct **distribution-free analogues** of **signs** and **signed-ranks**
- Generalized **Wilcoxon signed-rank test** for \mathcal{G} -symmetry
- Derive **consistency**, **efficiency lower bounds**, etc.
- Distribution-free **confidence sets** for the **center** of \mathcal{G} -symmetry

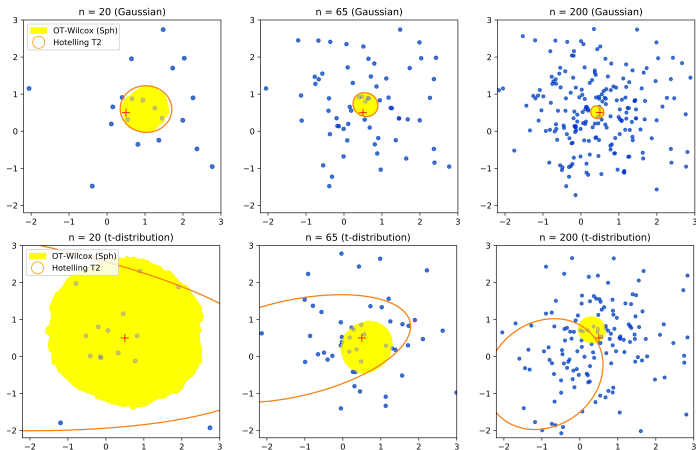


Figure: Confidence sets for center of $O(d)$ -symmetry (spherical symmetry) as the sample size n varies, obtained from (i) normal data (first row) and (ii) data from multivariate t -distribution with 1 degree of freedom (second row).

Summary

- Proposed a **multivariate** analogue of the **Wilcoxon rank-sum** test
- Studied its **distribution-freeness** and **efficiency** properties

Summary

- Proposed a **multivariate** analogue of the **Wilcoxon rank-sum** test
- Studied its **distribution-freeness** and **efficiency** properties
- Proposed a **general framework** — **multivariate distribution-free** testing procedures based on **optimal transport**; other examples may include testing for **symmetry**, testing the **equality of K -distributions**, **independence testing** of K -vectors, ...
- The proposed tests are: (i) **distribution-free** and have good efficiency, (ii) computationally feasible, (iii) more powerful for distributions with **heavy tails**, and (iv) **robust** to **outliers** & **contamination**

Ghosal and S. (2019). <https://arxiv.org/abs/1905.05340> (AoS)

Deb and S. (2019). <https://arxiv.org/pdf/1909.08733> (JASA)

Deb, Ghosal and S. (2021). <https://arxiv.org/pdf/2107.01718>. NeurIPS

Deb, Bhattacharya and S. (2021). <https://arxiv.org/abs/2104.01986>

Huang and S. (2023). <https://arxiv.org/abs/2305.01839>

Deb, Bhattacharya and S. (2023+). (working paper)

Thank you very much!

Questions?

Bhaswar Bhattacharya (UPenn)



Promit Ghosal (MIT)



Nabarun Deb (Columbia)



Zhen Huang (Columbia)



- $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}, \quad \mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$

- **OT maps:** $R \# \nu = \mu, \quad \hat{R}_n \# \nu_n = \mu_n$

- $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}, \quad \mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$

- **OT maps:** $R \# \nu = \mu, \quad \hat{R}_n \# \nu_n = \mu_n$

- Suppose $R = \nabla \varphi$, where $\varphi : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ is convex

- **Legendre-Fenchel dual of φ :** $\varphi^*(y) := \sup_{x \in \mathbb{R}^d} [x^\top y - \varphi(x)]$

- **Fact 1:** R is $\frac{1}{\lambda}$ -Lipschitz iff φ^* is λ -strongly convex

- φ^* is λ -strongly convex if, for all $x, y \in \text{Dom}(\varphi^*)$,

$$\varphi^*(y) \geq \varphi^*(x) + \nabla \varphi^*(x)^\top (y - x) + \frac{\lambda}{2} \|y - x\|^2$$

- $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}, \quad \mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$

- **OT maps:** $R \# \nu = \mu, \quad \hat{R}_n \# \nu_n = \mu_n$

- Suppose $R = \nabla \varphi$, where $\varphi : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ is convex

- **Legendre-Fenchel dual of φ :** $\varphi^*(y) := \sup_{x \in \mathbb{R}^d} [x^\top y - \varphi(x)]$

- **Fact 1:** R is $\frac{1}{\lambda}$ -Lipschitz iff φ^* is λ -strongly convex

- φ^* is λ -strongly convex if, for all $x, y \in \text{Dom}(\varphi^*)$,

$$\varphi^*(y) \geq \varphi^*(x) + \nabla \varphi^*(x)^\top (y - x) + \frac{\lambda}{2} \|y - x\|^2.$$

- **Fact 2:** $\nabla \varphi^*(R(x)) = x$ a.e.

- The 2-Wasserstein distance (squared) between ν and μ is defined as:

$$W_2^2(\nu, \mu) := \min_{\pi \in \Pi(\nu, \mu)} \int \|x - y\|^2 d\pi(x, y),$$

where $\Pi(\nu, \mu) := \{\text{distributions on } \mathbb{R}^d \times \mathbb{R}^d \text{ with marginals } \nu \text{ \& } \mu\}$

If the population rank map $R(\cdot)$ is $\frac{1}{\lambda}$ -Lipschitz, then

$$\lambda \int \|\hat{R}_n(x) - R(x)\|^2 d\nu_n(x) \leq W_2^2(\nu_n, \tilde{\mu}_n) - W_2^2(\nu_n, \mu_n) + 2 \int g d(\mu_n - \tilde{\mu}_n)$$

where $\tilde{\mu}_n := \frac{1}{n} \sum_{i=1}^n \delta_{R(x_i)}$ and $g(y) := \varphi^*(y) - \frac{1}{2}\|y\|^2$.

If the population rank map $R(\cdot)$ is $\frac{1}{\lambda}$ -Lipschitz, then

$$\lambda \int \|\hat{R}_n(x) - R(x)\|^2 d\nu_n(x) \leq W_2^2(\nu_n, \tilde{\mu}_n) - W_2^2(\nu_n, \mu_n) + 2 \int g d(\mu_n - \tilde{\mu}_n)$$

where $\tilde{\mu}_n := \frac{1}{n} \sum_{i=1}^n \delta_{R(x_i)}$ and $g(y) := \varphi^*(y) - \frac{1}{2}\|y\|^2$.

- Then, recalling $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ and $\mu_n := \frac{1}{n} \sum_{j=1}^n \delta_{c_j}$,

$$\begin{aligned} D_1 &:= \int \varphi^* d\mu_n - \int \varphi^* d\tilde{\mu}_n \\ &= \int [\varphi^*(\hat{R}_n(x)) - \varphi^*(R(x))] d\nu_n(x) \quad (\text{as } \hat{R}_n \# \nu_n = \mu_n) \\ &\stackrel{(a)}{\geq} \int \left\{ \nabla \varphi^*(R(x))^\top (\hat{R}_n(x) - R(x)) + \frac{\lambda}{2} \|\hat{R}_n(x) - R(x)\|^2 \right\} d\nu_n(x) \\ &\stackrel{(b)}{=} \underbrace{\int x^\top (\hat{R}_n(x) - R(x)) d\nu_n(x)}_{D_2} + \frac{\lambda}{2} \int \|\hat{R}_n(x) - R(x)\|^2 d\nu_n(x) \end{aligned}$$

- Fact 3:** $2D_2 = W_2^2(\nu_n, \tilde{\mu}_n) - W_2^2(\nu_n, \mu_n) + \int \|y\|^2 d(\mu_n - \tilde{\mu}_n)(y)$