Optimal transport in statistics and Pitman efficient multivariate distribution-free testing

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Multivariate distribution-free nonparametric testing

Consider the following nonparametric hypothesis testing problem:

Testing for equality of distributions (two-sample goodness-of-fit (GoF))

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

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- When $d = 1$: Student's t-test (1908), Wilcoxon rank-sum (1947), Cramér-von Mises (1928), Wald and Wolfowitz (1940), Mann and Whitney (1947), Kolmogorov-Smirnov (1939)
- When $d > 1$: Hotelling's T^2-statistic (1931), Weiss (1960), Anderson (1962), Friedman and Raksky (1979), Schilling (1986), Rosenbaum (2005), **Gretton et al. (2012), Szekely and Rizzo (2013),** Biswas et al. (2014), Li and Yuan (2019)

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- They are exact tests and valid for all sample sizes
- Based on univariate ranks — advent of classical nonparametrics

Comparison of Wilcoxon rank-sum (WRS) test with two-sample t-test

Pool $(X_1, \ldots, X_m, Y_1, \ldots, Y_n)$: (scaled) ranks $\hat{R}_{m,n}(X_i)$'s and $\hat{R}_{m,n}(Y_j)$'s

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

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Comparison of Wilcoxon rank-sum (WRS) test with two-sample t-test

Pool $(X_1; : : : ; X_m; Y_1; : : : ; Y_n)$: (scaled) ranks $\hat{R}_{m;n}(X_i)$'s and $\hat{R}_{m;n}(Y_j)$'s

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- Non-trivial efficiency lower bound of 0.864 w.r.t. t-test [Hodges and Lehmann (1956)]; efficiency can be $+1$ (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:

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

Generalize distribution-freeness, e ciency to multivariate data

Question

Can we construct multivariate nonparametric distribution-free tests?

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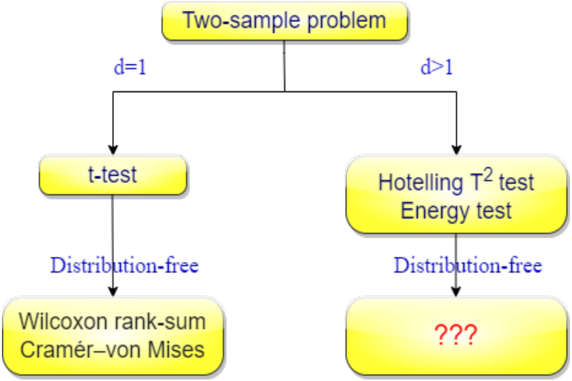

Good news

Tests based on *\ranks"* **are distribution-free**

Bad news

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How do we define multivariate ranks which lead to distribution-free tests?

What about their statistical efficiency?

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Optimal transport!

Outline

1. A (very) brief introduction to optimal transport

2. Multivariate ranks using optimal transport

3. Multivariate distribution-free tests using optimal transport
   - Rank Hotelling T^2 test and Pitman e ciency
   - Pitman e ciency, comparison with Hotelling T^2

Outline

Optimal (measure) transportation

$$\mathrm{KL}(P\|Q) = \int \log\left(\frac{p}{q}\right) p = 1$$

$$TV(P;Q) = \frac{1}{2}\int |p - q| = 1$$

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Need a notion of distance that is sensitive to geometry

Monge's approach (1781): Given probability measures $P; Q$ on $\mathbb{R}^d$, find an "optimal" map $T_0 : \mathbb{R}^d \to \mathbb{R}^d$ satisfying

$$\min_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x); \quad T\#P = Q, \quad X \sim P; \; T(X) \sim Q$$

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Monge's approach (1781): Given probability measures P, Q on $\mathbb{R}^d$, find an "optimal" map $T_0 : \mathbb{R}^d \to \mathbb{R}^d$ satisfying

$$W_2^2(P,Q) = \min_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x), \quad \left(T\#P = Q \iff X \sim P,\ T(X) \sim Q\right)$$

Call optimizer $T_0^{P,Q} \equiv T_0$ (if it exists) — optimal transport (OT) map

$W_2^2(P,Q)$ — squared Wasserstein distance

Optimal (Measure) Transportation

$$W_2^2(P; Q) = \|b - a\|^2, \; W_2^2(P; R) = \|c - a\|^2$$

Optimal (Measure) Transportation

$$W_2^2(P;Q) = kb \quad ak^2, \; W_2^2(P;R) = kc \quad ak^2$$

$$T_0^{P;Q}(x) = x + b \quad a, \; T_0^{P;R}(x) = x + c \quad a$$

Applications of optimal transport | $X \quad P;\ T(X) \quad Q$

How to estimate the optimal transport map?

Estimation | a plug-in approach

$$T_0 = \arg\min_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x); \quad \left(T\#P = Q \;, \quad X \sim P;\ T(X) \sim Q \right)$$

T_0 is unique (P a.s.) if $P; Q$ are absolutely continuous (McCann (1995))

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Data: $X_1, X_2, \ldots, X_m$ iid P (unknown, absolutely continuous) and $Y_1, \ldots, Y_n$ iid Q (unknown, absolutely continuous)

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Recall $T\#P_n = Q_n$ means if $X \sim P_n$, then $T(X) \sim Q_n$

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$T\#P_n = Q_n$: $(T(X_1), \ldots, T(X_n))$ is some permutation of $(Y_1, \ldots, Y_n)$

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Assignment problem (linear program – exact algorithm with complexity $O(n^3)$; parallel computing – Date and Nagi (2016))

Estimation | a plug-in approach (Continued)

What happens when $m < n$?

Can we still define

$$\hat{T} := \arg\min_{T\#P_m = Q_n} \int \|x - T(x)\|^2 \, dP_m(x)??$$

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NOT FEASIBLE!

There is no function T such that $T \# P_m = Q_n$

(Kantorovic relaxation)
Let $(P;Q)$ be the set of probability measures (coupling) on $\mathbb{R}^d \quad \mathbb{R}^d$, with marginals $P;Q$.
Then

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Examples: $P \quad Q$,
$(x;y) / \ 1(y = T_0(x))$

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Examples: $\quad P \quad Q$,
$(x; y) / \quad 1(y = T_0(x))$

Always has a minimizer which matches T_0 if P is absolutely continuous

Solve

$$b \in \arg\min_{\in (P_m, Q_n)} \int \|x - y\|^2 \, d(x; y)$$

via a linear program

Solve

$$\hat{\pi} \in \arg\min_{\pi \in \Pi(P_m, Q_n)} \int \|x - y\|^2 \, d\pi(x, y)$$

via a linear program

D., Ghosal, and Sen (NeurIPS, 2021): Define our estimator (barycentric projection) as

$$\hat{T}(x) = \mathbb{E}_{\hat{\pi}}[Y \mid X = x] = \frac{\int_y y \, d\hat{\pi}(x, y)}{\int_y d\hat{\pi}(x, y)}.$$

Both definitions coincide when $m = n$

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When $m = n$ ...

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Population OT map:

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Different parameter spaces

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Rate of convergence (D., Ghosal, and Sen (NeurIPS, 2021))

Assume that T_0 is Lipschitz, and both P and Q are compactly supported (can be relaxed). Then, for $d \geq 4$,

$$\frac{1}{m}\sum_{i=1}^{m} E\|\hat{T}(X_i) - T_0(X_i)\|^2 \lesssim m^{-\frac{2}{d}} + n^{-\frac{2}{d}}.$$

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The proof requires convex analysis, chaining and Talagrand's concentration arguments

Minimax optimal for $d \geq 4$ (Hütter and Rigollet (2019))

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- For $d = 1, 2, 3$, $m = n$, rates are $n^{-4/5}$, $n^{-2/3}$, $n^{-4/7}$ (ongoing work)
- The proof requires convex analysis, chaining and Talagrand's concentration arguments
- Minimax optimal for $d \geq 4$ (Hütter and Rigollet (2019))
- These are the first rates for a practically computable estimator of the OT map T_0 (note $\hat{T}$ requires no tuning) skip

Question

Can we construct multivariate distribution-free tests?

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2. Multivariate ranks using optimal transport

3. Multivariate distribution-free tests using optimal transport
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Ranks: When $d = 1$

Rank map $\widehat{R}_n$ assigns $\{X_1, X_2, \ldots, X_n\}$ to elements of $\{\frac{1}{n}, \frac{2}{n}, \ldots, \frac{n}{n}\}$

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Define $\mu_n := \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}$ and $\nu_n := \frac{1}{n}\sum_{j=1}^{n} \delta_{\frac{j}{n}}$

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$\widehat{R}_n$ is the empirical OT map from $_n$ to $_n$

Multivariate ranks ($d \geq 1$)

Empirical rank map assigns $\{X_1, \ldots, X_n\} \to \{c_1, \ldots, c_n\} \subset \mathbb{R}^d$ — grid of "reference" points (e.g., a random sample from $\mathrm{Unif}[0,1]^d$, $N(0, I_d)$ distribution, deterministic quasi-Monte Carlo sequences)

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Sample rank map (Hallin (2017)) is defined as the empirical OT map:

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Multivariate rank function as an OT map

X ; is a probability measure in $\mathbb{R}^d$ (abs. cont.)

Reference dist. U on S $\mathbb{R}^d$ (= Unif($[0;1]^d$), $N(0; I_d)$)

Find OT map T s.t. $T(X) \stackrel{d}{=} U$ (abs. cont.)

Multivariate rank function as an OT map

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Population rank function (a.k.a OT map) [Chernozhukov et al. (2017)]

If $E\|X\|^2 < \infty$, rank fn. $R : \mathbb{R}^d \to S$ is the population transport map

$$R := \arg\min_{T : T\# \; = } E\|X \quad T(X)\|^2$$

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

$R(\ )$ characterizes distribution: $R_1(x) = R_2(x)\ 8\ x\ 2\ R^d$ i $P_1 = P_2$

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When $d = 1$, $R(\ )$ is the CDF of X, when $= \mathrm{Unif}([0;1])$

Properties [D. and Sen (JASA 2020); D., Bhattacharya, and Sen (202

Distribution-freeness: If is absolutely continuous, then

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

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

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

Consistency: If $_n := \frac{1}{n}\sum_{j=1}^{n} {}_{c_j} \xrightarrow{d}$ (abs. cont.), then

$$\frac{1}{n}\sum_{i=1}^{n} \|\widehat{R}_n(X_i) - R(X_i)\|^2 \xrightarrow{p} 0 \qquad \text{as } n \to \infty \;;$$

where R is the unique OT map from to .

No moment assumptions needed on the model

Outline

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1 A (very) brief introduction to optimal transport

2 Multivariate ranks using optimal transport

3 Multivariate distribution-free tests using optimal transport
 Rank Hotelling T^2 test and Pitman e ciency
 Pitman e ciency, comparison with Hotelling T^2

Testing for equality of two multivariate distributions

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

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

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

$$T^2_{m,n} := \frac{mn}{m+n} \left(\bar{X} - \bar{Y}\right)^\top S^{-1}_{m,n} \left(\bar{X} - \bar{Y}\right),$$

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

Reject H_0 iff $T^2_{m,n} > c_\alpha$ [asymp. cut-off c_α : $(1 - \alpha)$ quantile of χ^2_d]

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Consistency: $P(T^2_{m,n} > c_\alpha) \to 1$ when $E[X_1] \neq E[Y_1]$

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

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

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General principle: Start with a "good" test and replace the X_i's and Y_j's with their pooled multivariate ranks

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Distribution-freeness [D. & Sen (JASA, 2020)]

Under H_0, distributions of $RT^2_{m,n}$ are free of $P \quad Q$

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Under location shift alternatives, we have

$$\lim_{m,n \to \infty} E_{H_1}[\phi_{m,n}] = 1.$$

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Goal

How does rank Hotelling test compare with Hotelling T^2 test?

Outline

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)]

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In principle, ARE $(S_N; T_N)$ can depend on and , but in many interesting cases they don't

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Consider $H_0 : \ _2 = \ _1$ vs. $H_1 : \ _2 = \ _1 + hN^{\ 1=2}$; $\quad h \ne 0 \ 2\ R^p$

ARE $(RT^2_{m;n}; T^2_{m;n})$ can be derived from the distribution of both test statistics under above alternatives

$X_1;\ldots;X_m \overset{iid}{\sim} P_{\theta_1}$ & $Y_1;\ldots;Y_n \overset{iid}{\sim} P_{\theta_2}$; $N = m + n$

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Some observations

Expression of ARE $(RT^2_{m;n}; T^2_{m;n})$ does not depend on and

Asymp. dist. of $RT^2_{m;n}$ can depend on the choice of

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Some observations

- Expression of ARE $(RT^2_{m,n}, T^2_{m,n})$ does not depend on and
- Asymp. dist. of $RT^2_{m,n}$ can depend on the choice of

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

$$\min_F \text{ARE}\,(RT^2_{m,n}, T^2_{m,n}) = ??$$

$X_1; : : : ; X_m \overset{iid}{} P_{1}$ & $Y_1; : : : ; Y_n \overset{iid}{} P_{2}$; $N = m + n$

Independent coordinates case

$F_{ind} = f P\ g_{2}$ has density $p\ (z_1; : : : ; z_d) = \prod_{i=1}^{d} f_i\,(z_i \quad {}_i)$, $\ 2\ R^d$

Theorem (D., Bhattacharya, and Sen (2021))

Suppose $\frac{m}{N}\ !\quad 2\ (0; 1)$. If $\ _N := \frac{1}{N} \sum_{j=1}^{N}\ c_j\ !^{d}\ \mathrm{Unif}\,([0; 1]^d)$, then

$$\min_{F_{ind}} \mathrm{ARE}\,(RT^2_{m;n}; T^2_{m;n}) = 0{:}864$$

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Independent coordinates case

$F_{ind} = \{P \in \mathcal{P}_2$ has density $p(z_1, \dots, z_d) = \prod_{i=1}^{d} f_i(z_i)$, $\in \mathbb{R}^d\}$

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Suppose $\frac{m}{N} \to \in (0, 1)$. If $_N := \frac{1}{N} \sum_{j=1}^{N} c_j \xrightarrow{d}$ Unif$([0, 1]^d)$, then

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

If $_N \xrightarrow{d} N(0, I_d)$, then

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

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If ${}_N \stackrel{d}{\to} N(0, I_d)$, then

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Generalizes Hodges & Lehmann (1956), Chernoff & Savage (1958)

ARE can be arbitrarily large (can tend to $+\infty$) for heavy tailed dists.

Elliptically symmetric distributions

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

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

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$$p(x) \propto (\det())^{-\frac{1}{2}} f\left((x -)^{\top} {}^{-1} (x -)\right), \quad \text{for all } x \in R^d.$$

Theorem (D., Bhattacharya, and Sen (2021))

Suppose: (i) $_N \to^d N(0; I_d)$, (ii) $\frac{m}{N} \to \in (0;1)$. Then,

$$\min_{F_{ell}} \mathrm{ARE}\,(RT^2_{m;n}; T^2_{m;n}) = 1.$$

This generalizes the famous result of Cherno and Savage (1958)

Model for Independent Component Analysis (ICA)

$F_{ICA} = \{ f_1(\cdot) : f_1 \in F \}_{\cdot \in \mathbb{R}^d}$ where $f_1 \in F$ has the form

$$f_1(x_1, \ldots, x_d) = \prod_{i=1}^{d} \tilde{f}_i\left(\sum_{j=1}^{d} a_{ji} x_j \right)$$

where $\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_d$ are univariate densities, and $A = (a_{ij})_{d \times d}$ is an orthogonal matrix (unknown)

Thus, f_1 is the density of $X_{d \times 1}$ where

$$X = AW$$

with $W_{d \times 1}$ having independent components

Model for Independent Component Analysis (ICA)

$F_{ICA} = \{ f_1(\quad) : f_1 \in F \}_{\in \mathbb{R}^d}$ where $f_1 \in F$ has the form

$$f_1(x_1, \ldots, x_d) = \prod_{i=1}^{d} \tilde{f}_i \left(\sum_{j=1}^{d} a_{ji} x_j \right)$$

where $\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_d$ are univariate densities, and $A = (a_{ij})_{d \quad d}$ is an orthogonal matrix (unknown)

Thus, f_1 is the density of $X_{d \quad 1}$ where

$$X = AW$$

with $W_{d \quad 1}$ having independent components

Theorem (D., Bhattacharya, and Sen (2021))

Suppose: (i) $_N \xrightarrow{d} N(0, I_d)$, (ii) $\frac{m}{N} \to \quad \in (0, 1)$. Then,

$$\min_{F_{ICA}} \mathrm{ARE}\,(RT^2_{m,n}, T^2_{m,n}) = 1$$

Recap

Exact distribution-free, nonparametric test, gives uniformly level test and high e ciency compared to Hotelling T^2 test

Provides the rst comprehensive extension of classical nonparametric testing to the multivariate setting skip

Using Gaussian reference distribution ensures ARE $(RT^2_{m;n}; T^2_{m;n})$ 1 for many popular subfamilies. Note that the test is agnostic to the underlying subfami skip

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Thank you. Questions?

Multivariate two-sample goodness-of- t test

Recall general strategy: Start with a \good" test and replace the X_i's and Y_j's with their pooled multivariate ranks

Multivariate two-sample goodness-of- t test

Start with a \good" consistent test, say the energy statistic (Szekely and Rizzo, 2013) and apply our general strategy

Multivariate two-sample goodness-of-fit test

Start with a “good” consistent test, say the energy statistic (Székely and Rizzo, 2013) and apply our general strategy

Suppose $X; X' \overset{iid}{\sim} P$, $Y; Y' \overset{iid}{\sim} Q$, $K(s; t) := \|s - t\|$, then energy dist. (or kernel MMD (see Gretton et al., 2008)):

$$E^2(P; Q) := 2\,\mathbb{E}K(X; Y) - \mathbb{E}K(X; X') - \mathbb{E}K(Y; Y') \geq 0$$

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Characterizes equality of distributions: $E(P,Q) = 0$ iff $P = Q$

E-statistic : $E^2_{m,n}\left(\{X_i\}_{i=1}^m, \{Y_j\}_{j=1}^n\right) := 2A - B - C$ where

$$A = \frac{1}{mn}\sum_{i,j=1}^{m,n} K(X_i, Y_j); \quad B = \frac{1}{m^2}\sum_{i,j=1}^{m} K(X_i, X_j); \quad C = \frac{1}{n^2}\sum_{i,j=1}^{n} K(Y_i, Y_j)$$

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Energy test: Reject H_0 if $\mathcal{E}_{m,n}\left(\{X_i\}_{i=1}^m, \{Y_j\}_{j=1}^n\right) >$ (depends on P; we can use permutation test)

Proposed statistic

Rank energy statistic [D. and Sen (JASA, 2020)]

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

$$\hat{R}_{m,n} : \{X_1, \ldots, X_m, Y_1, \ldots, Y_n\} \to \{c_1, \ldots, c_{m+n}\} \subseteq [0,1]^d$$

Rank energy: $RE^2_{m,n} := E^2_{m,n}\left(\{\hat{R}_{m,n}(X_i)\}_{i=1}^m, \{\hat{R}_{m,n}(Y_j)\}_{j=1}^n\right)$

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Distribution-freeness

Under H_0, distribution of $RE_{m,n}$ is free of $P \quad Q$, if P is abs. cont.

Dist. of $RE_{m,n}$ just depends on c_i's, m, n and d

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Simplification when $d = 1$

$RE^2_{m,n}$ is exactly equivalent to the two-sample Cramér-von Mises statistic

Power [D. and Sen (JASA, 2020)]

Under (ii) and $P \neq Q$, if $\frac{m}{m+n} \quad \in (0,1)$ then,

$$P(\mathrm{RE}_{m,n} > {}^{(m,n)}) \to 1 \quad \text{as } m,n \to \infty \quad .$$

Proposed test has asymptotic power 1, against all fixed alternatives

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Proposed test has asymptotic power 1, against all fixed alternatives

Limiting distribution under H_0 [D. and Sen (JASA, 2020)]

If (i) $P \ll Q$ is abs. cont., and

(ii) $\frac{1}{N}\sum_{i=1}^{N} \delta_{c_i} \xrightarrow{d} \ \text{a.s.} \ (N = m+n)$

Then, under H_0, $\exists$ a universal distribution s.t.

$$\frac{mn}{m+n} RE^2_{m,n} \xrightarrow{d} \sum_{j=1}^{\infty} \lambda_j Z_j^2 \quad \text{as } \min\{m,n\} \to \infty \quad \text{where } \lambda_j \geq 0.$$

Pitman e ciency

Some observations

E ciency of $RE_{m;n}$ w.r.t. $E_{m;n}$ depends on the type I error and power , which makes it hard obtain e ciency lower bounds

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Rank Energy $RE_{m;n}$ [D., Bhattacharya, and Sen (working paper)]

$$\lim_{m;n!1} P_{H_1}(RE_{m;n} \text{ rejects } H_0) >$$

Only consistent, exactly dist.-free test that can distinguish H_0 & H_1

Summary

Introduced optimal transport and obtained rst tuning-free, minimax optimal estimator of optimal transport map

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Tuning-free, robust, computationally feasible procedures, performs particularly well under heavy-tailed data skip

Summary

References

D. and Sen, (2020). https://arxiv.org/pdf/1909.08733 (JASA, to appear)

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Nonparametric association/conditional association

Suppose

$$\begin{matrix}X\\Y\end{matrix} \quad N_2 \quad \begin{matrix}0\\0\end{matrix} ; \quad \begin{matrix}1 & \\ & 1\end{matrix}$$

The correlation measures association (linear) between X and Y

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Goal: Given random elements $(X_1; Y_1); \dots; (X_n; Y_n) \; {}^{i.i.d.} \; (X; Y)$, de ne $T(X; Y)$ and T_n (estimator), such that:

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Measure of Association

We answer this question in the a rmative by combining ideas from reproducing kernel Hilbert spaces (RKHS) and geometric graphs (e.g., nearest neighbors, minimum spanning trees), to come up with a large class of such measures

Our measures are completely nonparametric (unlike)e

We can also extend this to measuring conditional association with applications in variable selection, conditional independence testing ...

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Huang, D., and Sen (2021). https://arxiv.org/pdf/2012.14804.pdf (JMLR, to appear)

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Other works

Applied probability (Ising type models):

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(JASA, published online)

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skip

Rate of convergence result

$$T_0 = \arg\min_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x);$$

$$W_2^2(P;Q) = \min_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x)$$

Data: $X_1; X_2; \ldots; X_n$ iid P and $Y_1; \ldots; Y_n$ iid Q

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Rate of convergence (D., Ghosal, Sen, NeurIPS, 2021)

Assume that T_0 is Lipschitz, and both P and Q are compactly supported (can be relaxed). Then,

$$\frac{1}{n} \sum_{i=1}^{n} \|\hat{T}(X_i) - T_0(X_i)\|^2 \lesssim n^{-\frac{2}{d}}$$

for $d \geq 4$. For $d = 1; 2; 3$, the rates are n^{-1}, $n^{-2/3}$ and $n^{-4/7}$.

Nonparametric regression: Say $Y_i = f_0(X_i) + \epsilon_i$, $i = 1, \dots, n$, where ϵ_i's are iid $N(0, 1)$, and $f_0 \in \mathcal{F}$

$$\hat{f}_n := \arg\min_{f \in \mathcal{F}} \sum_{i=1}^{n} (Y_i - f(X_i))^2$$

Both $\hat{f}_n$ and f_0 belong to $\mathcal{F}$, which yields the basic inequality:

$$\sum_{i=1}^{n} (Y_i - \hat{f}_n(X_i))^2 \le \sum_{i=1}^{n} (Y_i - f_0(X_i))^2$$

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$$\sum_{i=1}^{n} (f_0(X_i) - \hat{f}_n(X_i))^2 \le 2 \sum_{i=1}^{n} \epsilon_i (\hat{f}_n(X_i) - f_0(X_i))$$

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OT problem:

$$\hat{T} := \arg\min_{T \# P_n = Q_n} \int \|x - T(x)\|^2 \, dP_n(x)$$

Constraint set: $\mathcal{T}_n := \{T : T \# P_n = Q_n\}$.

$\hat{T}_n \in \mathcal{T}_n$ but $T_0 \notin \mathcal{T}_n$

Dual form

Alternatively,

$$W_2^2(P_n; Q_n) = \min_{T\,\#\,P_n = Q_n} \int \|x - T(x)\|^2 \, dP_n(x) = {\color{red} \min_{f;g} \int f \, dP_n + \int g \, dQ_n}$$

such that $f(x) + g(y) \leq \|x - y\|^2$ for all $x; y \in \mathbb{R}^d$.

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$$W_2^2(P_n;Q_n) = \min_{T\#P_n=Q_n} \int \|x - T(x)\|^2 \, dP_n(x) = \min_{f,g} \int f \, dP_n + \int g \, dQ_n$$

such that $f(x) + g(y) \geq \|x - y\|^2$ for all $x, y \in \mathbb{R}^d$.

Note that the constraints are not data driven.

Basic inequality (D., Ghosal and Sen, 2021)

Suppose T_0 is Lipschitz. Write $T_0 = \nabla \varphi_0$ and $Q_n := T_0 \# P_n$. Then,

$$\frac{1}{n}\sum_{i=1}^{N} \|\hat{T}_n(X_i) - T_0(X_i)\|^2 \lesssim W_2^2(P_n;Q_n) - W_2^2(P_n;Q_n) + \int g \, d(Q_n - Q_n)$$

where $g(y) = \varphi_0^*(y) - (1/2)\|y\|^2$, $\varphi_0^*(y) := \sup_{x \in \mathbb{R}^d}(\langle x, y\rangle - \varphi_0(x))$ (Legendre-Fenchel dual of $\varphi_0(\cdot)$)

Proof requires arguments from convex analysis

Dual form

Alternatively,

$$W_2^2(P_n; Q_n) = \max_{f;g} \int f \, dP_n + \int g \, dQ_n$$

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Note that the constraints are not data driven.

Basic inequality (D., Ghosal and Sen, 2021)

Suppose T_0 is Lipschitz. Write $T_0 = \nabla \varphi_0$ and $Q_n := T_0 \# P_n$. Then,

$$\frac{1}{n} \sum_{i=1}^{N} \|\hat{T}_n(X_i) - T_0(X_i)\|^2 \lesssim W_2^2(P_n; Q_n) - W_2^2(P_n; Q_n) + \int g \, d(Q_n - Q_n)$$

where $g(y) = \varphi_0^*(y) - (1/2)\|y\|^2$, $\varphi_0^*(y) := \sup_{x \in \mathbb{R}^d}(\langle x; y \rangle - \varphi_0(x))$ (Legendre-Fenchel dual of $\varphi_0(\cdot)$)

Proof requires arguments from convex analysis

Using the dual form of $W_2^2(\cdot\,;\cdot)$, coupled with chaining and Talagrand's concentration inequality proves the rate of convergence result

Thank you. Questions?

Properties

$$T_0 \overset{???}{:=} \arg\min_{T \# P = Q} \int \|x - T(x)\|^2 \, dP(x); \quad \left(T \# P = Q, \quad X \sim P; \ T(X) \sim Q \right):$$

Does a solution always exist?

Is the solution unique?

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Does a solution always exist?

No! Take $P = \quad_0$ and $Q = \mathrm{Unif}[0;1]$.

Is the solution unique?

No! Take $P = 0{:}5 \ _p + 0{:}5 \ _p$ and $Q = 0{:}5 \ _q + 0{:}5 \ _q$.

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Crossmatch test (Rosenbaum 2005)

Pitman asymptotics for crossmatch test (Rosenbaum 2005)

Consider the testing set-up from before (with additional regularity assumptions). Then, for any h, we have:

$$\lim_{m,n\to\infty} P_{H_1}(T_{m,n} \text{ rejects } H_0) = \quad :$$

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$$\lim_{m,n\to\infty} P_{H_1}(T_{m,n} \text{ rejects } H_0) = \quad :$$

Therefore, crossmatch test does not distinguish between the null and the alternative at the contiguous scale

The same phenomena happens for many other graph-based asymptotically distribution-free tests, see Bhattacharya (2019, Theorem 3.1)

Power plot with varying sample size

Figure: X_1, Y_1 are i.i.d. Epanechnikov with location parameters 0 and 1.0 respectively. X_2, X_3 X_1; Y_2, Y_3 Y_1 and $X := (X_1, X_2, X_3)$, $Y := (Y_1, Y_2, Y_3)$. Here

$$e(\text{RankUnif}; \text{Hotelling}) = 0.864$$

and $e(\text{RankGaussian}; \text{Hotelling}) > 1$ skip

Power plot with varying location parameter

Log-normal location problem (slightly heavy-tailed)

Figure: $U_1; U_2$ are iid standard normal, and $V_1; V_2$ are normal with variance 1 and varying mean. De ne $X_i := \exp(U_i)$ and $Y_i := \exp(V_i)$. Set $X := (X_1; X_2)$ and $Y := (Y_1; Y_2)$ | sample size $n = 200$ skip

Power plot with varying location parameter

Figure: (Left panel) $X_1; Y_1$ are i.i.d. normal with mean 0 and respectively (and unit variance). $X_2; X_3$ $X_1; Y_2; Y_3$ Y_1 and $X := (X_1; X_2; X_3)$. Similarly de ne Y. skip
(Right panel) $U := (U_1; U_2; U_3)$ and $V := (V_1; V_2; V_3)$ where $U_i = \exp(X_i)$, $V_i = \exp(Y_i)$ and $X_1; X_2; X_3; Y_1; Y_2; Y_3$ has the same distribution as above.
Red - Rank energy, Black - Crossmatch, Blue - Energy, Green - HHG.

More simulations

	(RB)	(HHG)	(EN)	(REN)
V1	0.13	0.15	0.13	0.34
V2	0.34	0.94	0.94	0.89
V3	0.41	0.34	0.34	0.46
V4	0.34	0.31	0.33	0.32
V5	0.73	0.70	0.56	0.93
V6	0.90	0.88	0.82	0.99
V7	0.13	0.51	0.65	0.63
V8	0.11	0.39	0.35	0.43
V9	0.06	1.00	0.97	1.00
V10	0.28	0.99	1.00	0.59

Table: Proportion of times the null hypothesis was rejected across 10 settings. Here $n = 200$, $d = 3$. Here RB - Rosenbaum's crossmatch test (Rosenbaum, 2005), HHG - Heller, Heller and Gor ne (Heller et al., 2013), En - energy statistic (Szekely and Rizzo, 2013).

Asymptotic stabilization

	(100)	(300)	(500)	(700)	(900)
0.05	0.39	0.40	0.39	0.40	0.40
0.1	0.36	0.36	0.36	0.36	0.36

Table: Thresholds for $= 0.05$, 0.1 and $n = 100; 300; 500; 700; 900$, $d = 2$.

	(100)	(300)	(500)	(700)	(900)
0.05	1.37	1.38	1.38	1.38	1.38
0.1	1.34	1.35	1.35	1.35	1.35

Table: Thresholds for $= 0.05$, 0.1 and $n = 100; 300; 500; 700; 900$, $d = 8$.

What happens for $d = 1$?

$$T_0 \overset{???}{:=} \arg\min_{T\#P=Q} \int |x - T(x)|^2 \, dP(x).$$

Assume $Q = \mathrm{Unif}[0;1]$ and $X \sim P$ with cdf F

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Given $x_1 \leq x_2 \in \mathbb{R}$, note that

$$(x_1 - T_0(x_1))^2 + (x_2 - T_0(x_2))^2 \leq (x_1 - T_0(x_2))^2 + (x_2 - T_0(x_1))^2$$
$$\iff T_0(x_1) \leq T_0(x_2)$$

Expect $T_0(\cdot)$ to be monotone and $T_0(X) \overset{d}{=} \mathrm{Unif}[0,1]$.

$T_0(\cdot)$ is the distribution function of X, say $F(\cdot)$

What happens for $d = 1$?

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$$(x_1 - T_0(x_1))^2 + (x_2 - T_0(x_2))^2 \le (x_1 - \textcolor{red}{T_0(x_2)})^2 + (x_2 - \textcolor{red}{T_0(x_1)})^2$$
$$\Leftrightarrow \quad T_0(x_1) \le T_0(x_2)$$

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Note that increasing functions can be viewed as "derivatives" of convex functions.

Suppose T_0 2 C (Hölder or Sobolev class), > 1

The minimax rate of convergence is

$$n^{\frac{2}{2\quad 2+d}} + n^{1}$$

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In ongoing work, we can show that using a kernel density based estimator yields the optimal rate (up to log-factors)

$$\frac{1}{n}\sum_{i=1}^{n} E\|\hat{T}(X_i) \quad T_0(X_i)\|^2 \lesssim n^{\frac{2}{2 \quad 2+d}} + n^{\ 1}$$

In Manole et al. (2021), Hütter and Rigollet (2019), wavelet based estimators have been used to get optimal rat

$T_0(X) \quad Y$, X with density f, Y with density g. Then change of variable formula implies

$$g(T(x))\det(J_{T_0}(x)) = f(x)$$

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(Ca arelli Regularity, 1992, 1996) | $T_0 \; 2 \; C$ corresponds to $f; g \; 2 \; C \quad ^1$, $> \; 1$

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Goal is to estimate the anti-derivative of $C^{\quad 1}$ functions

(Müller and Gasser, 1979) — optimal minimax lower bounds for estimating k-th derivative of $\quad$-smooth functions is

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(Müller and Gasser, 1979) — optimal minimax lower bounds for estimating k-th derivative of -smooth functions is

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Use $=$ 1 and $k =$ 1 (anti-derivative), the lower bound reduces to $\frac{2}{2\quad 2+d}$ skip

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Modified Rank Hotelling T^2:

$$RT^2_{m,n} := T^2_{m,n} \quad \frac{X_1}{\|X_1\|} G_{m,n}(\|X_1\|), \ldots, \frac{Y_1}{\|Y_1\|} G_{m,n}(\|Y_1\|), \ldots,$$

Test is distribution-free | if $Y \overset{d}{=} X$ then detection boundary at $\| \ \|$ $\sqrt{d/n}$ skip

$d > 1$ | A step in the right direction

Brenier, '91, McCann '95, Polar Factorization Theorem

Assume that P is absolutely continuous on $\mathbb{R}^d$, Then there exists a unique (P a.s.) $T_0 : \mathbb{R}^d \to \mathbb{R}^d$ such that $T_0(\cdot)$ is the gradient of a convex function and

$$T_0 \# P = Q.$$

If both P and Q have finite second moments, then $T_0(\cdot)$ solves

$$\min_{T \# P = Q} \int \|x - T(x)\|^2 \, dP(x).$$

- Existence of $T_0(\cdot)$ does not require any moment assumptions
- Uniqueness: $T_0 \# P = Q$ and $T_0 \# R = Q$ will imply $P = R$

Rank functions as transport maps: When $d = 1$

$X \sim F$ on $\mathbb{R}$, F abs. cont. c.d.f.

Rank: The rank of $x \in \mathbb{R}$ is $F(x)$ (aka the c.d.f. at x)

Property : $F(X) \sim \text{Uniform}([0, 1])$

Thus, F transports the distribution of X to $U \sim \text{Uniform}([0, 1])$

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In fact, if $E[X^2] < \infty$, c.d.f. F is the optimal transport map as

$$F = \mathop{\arg\min}_{T : T(X) \stackrel{d}{=} U} E|X - T(X)|^2$$

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Sample rank map (aka empirical c.d.f.) is also a transport map:

$$\hat{R}_n := \arg\min_{\sigma \in S_n} \frac{1}{n} \sum_{i=1}^{n} \left(X_i - \frac{\sigma(i)}{n} \right)^2 = \arg\min_{T} \frac{1}{n} \sum_{i=1}^{n} |X_i - T(X_i)|^2$$

where T transports $\frac{1}{n} \sum_{i=1}^{n} \delta_{X_i}$ to $\frac{1}{n} \sum_{i=1}^{n} \delta_{\frac{i}{n}}$

Multivariate rank functions as transport maps

X ; is a probability measure in $\mathbb{R}^d$ (abs. cont.)

U Uniform$([0;1]^d)$

Goal: Find the \optimal" transport map T s.t. $T(X) \stackrel{d}{=} U$

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Goal: Find the \optimal" transport map T s.t. $T(X) \stackrel{d}{=} U$

If $E\|X\|^2 < 1$, the population rank function $R(\ )$ is the transport map s.t.

$$R := \mathop{\arg\min}_{T : T(X) \stackrel{d}{=} U;\ X} E\|X \quad T(X)\|^2$$

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Data: $X_1, \ldots, X_n$ iid (abs. cont.) on $\mathbb{R}^d$

$\{c_1, \ldots, c_n\}$ $\mathbb{R}^d$ — grid of "reference" points

Sample multivariate rank map is defined as the tranport map s.t.

$$\hat{R}_n = \underset{\in S_n}{\arg\min} \frac{1}{n}\sum_{i=1}^{n} \|X_i \quad c_{(i)}\|^2 \quad \underset{T}{\arg\min} \frac{1}{n}\sum_{i=1}^{n} \|X_i \quad T(X_i)\|^2$$

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Even when $EkXk^2 = +1$, population rank function $R( )$ can also be de ned More details

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

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Sample multivariate rank map $\hat{\mathbf{R}}_\mathbf{n}(\cdot)$ is defined as

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Regularity: L_2-convergence [D. and Sen, JASA 2020]

$X_1, \ldots, X_n$ iid $\sim \mu$ (abs. cont.). If $\frac{1}{n}\sum_{i=1}^{n} \delta_{c_i} \xrightarrow{w}$ Unif$([0,1]^d)$, then

$$\frac{1}{n}\sum_{i=1}^{n} \|\hat{\mathbf{R}}_n(X_i) - \mathbf{R}(X_i)\| \xrightarrow{a.s.} 0 \quad \text{as } n \to \infty.$$

Result gives the required regularity of the empirical multivariate rank map

Population version

Assume $m/(m+n) = \quad 2\ (0;1)$.

Rank energy distance [D. and Sen, JASA 2020]

- Joint rank map: The "pooled" population rank map:

$$\mathrm{R} \quad : \mathrm{R} \quad (\mathbf{Z}) \qquad \mathrm{Uniform}([0;1]^d)$$

where $\mathbf{Z} \qquad P + (1 \qquad)Q$.

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- Our general principle could have been used with any other procedure for testing equality of distributions, e.g., the MMD statistic [Gretton et al. (2008)] which uses ideas from RKHS, ...

- For $d = 1$, we prove that $\mathrm{RE}^2_{m;n}$ and RE^2 are exactly equivalent to the sample and population two-sample Cramér-von Mises statistic.

Pitman efficiency

Consider $X_1, \ldots, X_n$ P $_1$ and $Y_1, \ldots, Y_m$ P $_2$, with $m/(m+n) = \quad 2\ (0,1)$. We want to test:

$$\mathrm{H}_0 : \ _2 \quad _1 = 0 \qquad \text{versus} \qquad \mathrm{H}_1 : \ _2 \quad _1 = h(m+n)^{\ 1/2}.$$

Pitman efficiency

Consider $X_1, \ldots, X_n \quad P_{\ 1}$ and $Y_1, \ldots, Y_m \quad P_{\ 2}$, with $m/(m+n) = \quad 2\ (0, 1)$. We want to test:

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Fix (size) and > (power).

Two test functions $T_{m,n}$ and $S_{m,n}$.

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$K(T_{m;n})$ denotes minimum number of samples such that:

$$\mathrm{E}_{\mathrm{H}_0}(T_{m;n}) \qquad \text{and} \qquad \mathrm{E}_{\mathrm{H}_1}(T_{m;n}) \qquad :$$

Pitman efficiency

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$$\mathrm{E}_{\mathrm{H}_0}(T_{m,n}) \qquad \text{and} \qquad \mathrm{E}_{\mathrm{H}_1}(T_{m,n}) \qquad .$$

The Pitman efficiency of $S_{m,n}$ with respect to $T_{m,n}$ is given by

$$\lim_{m+n \to \infty} \frac{K(T_{m,n})}{K(S_{m,n})}.$$