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

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Kantorovich Initiative Retreat
March 18, 2022

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), Székely and Rizzo (2013),** Biswas et al. (2014), Li and Yuan (2019)

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- Based on univariate ranks — advent of classical nonparametrics

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

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

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

Generalize distribution-freeness, efficiency to multivariate data

Question

Can we construct multivariate nonparametric distribution-free tests?

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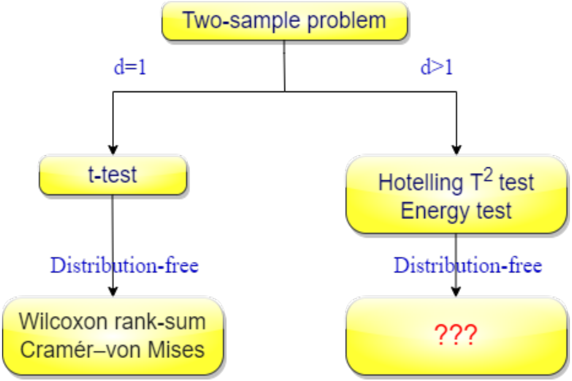

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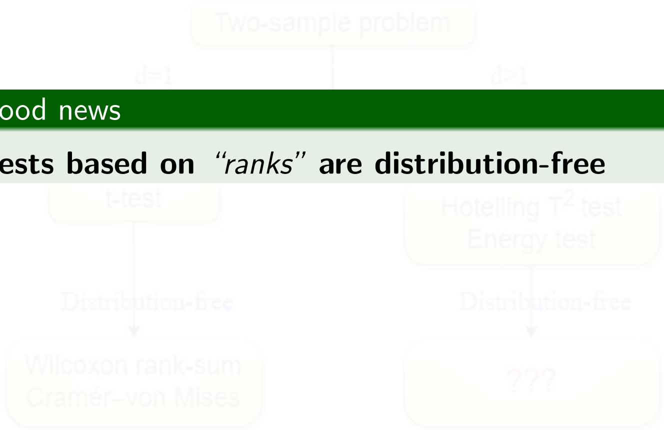

Good news

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

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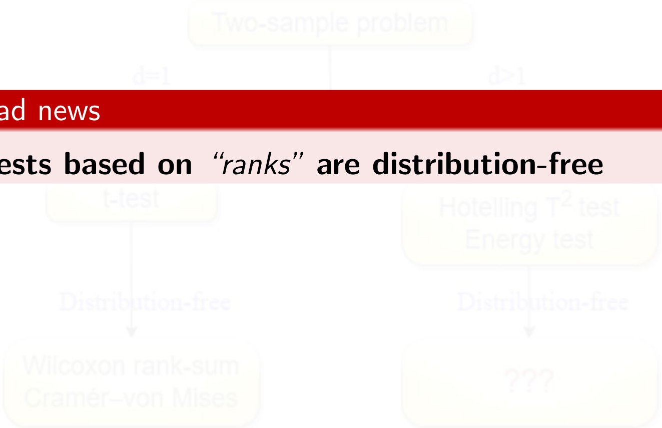

Bad news

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

What about their statistical efficiency?

Wilcoxon rank-sum
Cramér–von Mises

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Optimal transport!

Wilcoxon rank-sum
Cramér–von Mises

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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 efficiency
    - Pitman efficiency, comparison with Hotelling T^2

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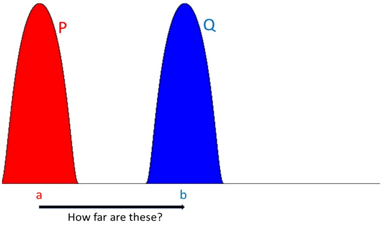
Optimal (measure) transportation



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

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

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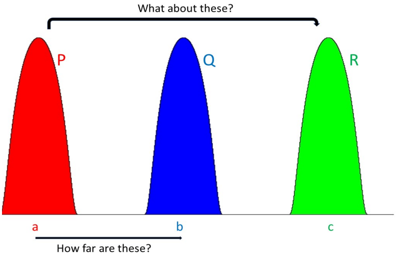

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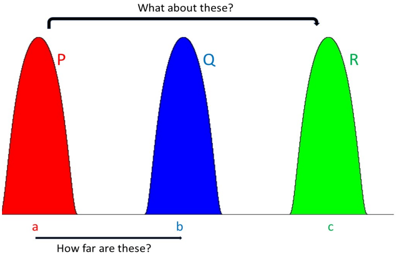

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Need a notion of distance that is sensitive to geometry

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

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

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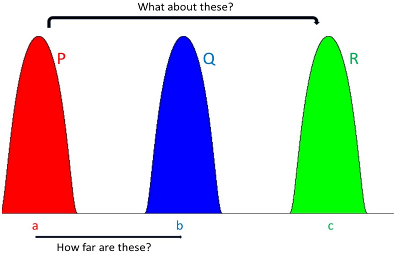

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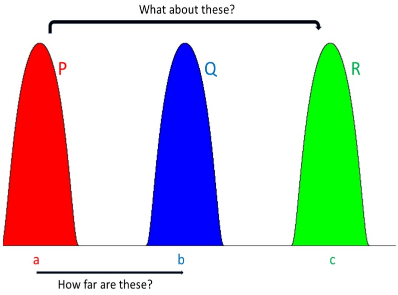
$$\mathbf{W}_2^2(P,Q) = \min_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x), \quad T\#P = Q \Leftrightarrow X \sim P,\ T(X) \sim Q$$

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

$\mathbf{W}_2^2(P,Q)$ — squared Wasserstein distance

Optimal (Measure) Transportation



- $\mathbf{W}_2^2(P, Q) = \|b - a\|^2$, $\mathbf{W}_2^2(P, R) = \|c - a\|^2$

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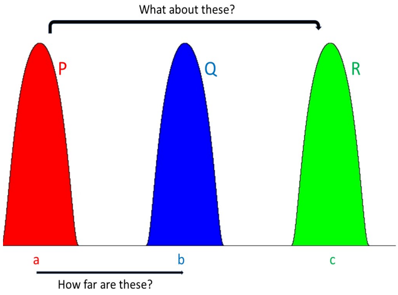
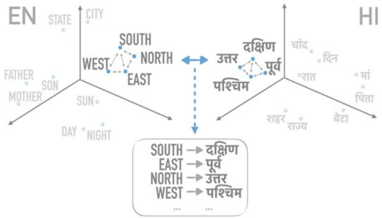


- $\mathbf{W}_2^2(P, Q) = \|b - a\|^2$, $\mathbf{W}_2^2(P, R) = \|c - a\|^2$
- $T_0^{P,Q}(x) = x + b - a$, $T_0^{P,R}(x) = x + c - a$

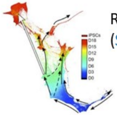
Applications of optimal transport — $X \sim P, \; T(X) \sim Q$



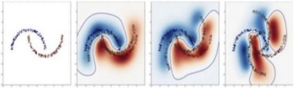
Translation (Mellis and Jaakkola, 2019)

Generative Modelling (Rout et al., 2021)

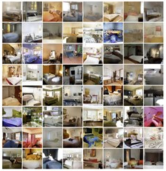
Color transfer (Rabin et al., 2010)



RNA sequencing (Schiebinger et al., 2019)



Domain adaptation (Courty et al., 2017)



Wasserstein GAN (Arjovsky et al., 2017)

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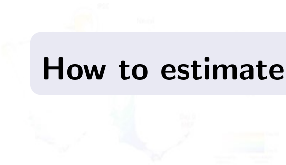

(Schiebinger et al, 2019)

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How to estimate the optimal transport map?

Domain adaptation (Courty et al, 2017)

Image retrieval (Papadakis, 2015)

Estimation — a plug-in approach

$$T_0 = \operatorname*{arg\,min}_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x), \quad T\#P = Q \Leftrightarrow X \sim P,\ T(X) \sim Q$$

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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

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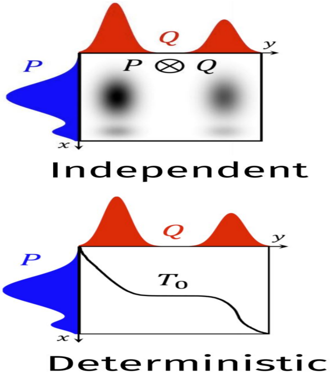
NOT FEASIBLE!

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

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

  $$W_2^2(P, Q) = \inf_{\gamma \in \Pi(P,Q)} \int \|x - y\|^2 \, d\gamma(x, y)$$

  Examples: $\pi \equiv P \otimes Q$,
  $\pi(x, y) \propto \mathbf{1}(y = T_0(x))$



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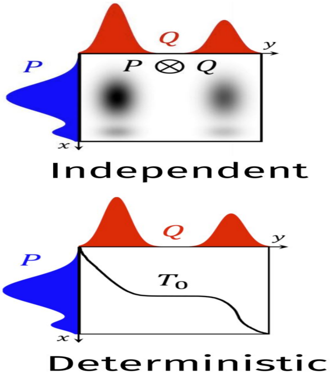
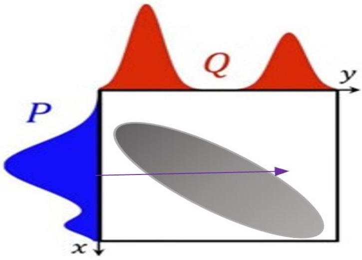
- Always has a minimizer which matches T_0 if P is absolutely continuous



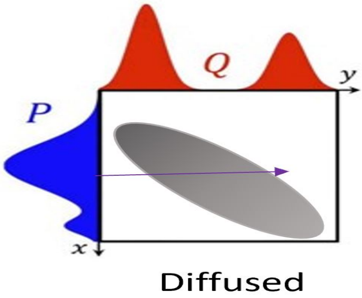


Diffused

- Solve

$$\widehat{\gamma} \in \underset{\gamma \in \Pi(P_m, Q_n)}{\arg\min} \int \|x - y\|^2 \, d\gamma(x, y)$$

via a linear program



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

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

Both definitions coincide when $m = n$

What is the rate of convergence of $\hat{T}$ to T_0?

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When $m = n$ ...

Empirical OT map:

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Population OT map:

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

What is the rate of convergence of $\hat{T}$ to T_0?

When $m = n$ ...

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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 $d \geq 4$,

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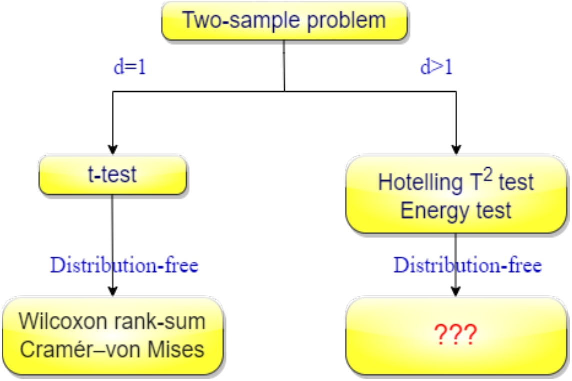
- For $d = 1, 2, 3$, $m = n$, rates are $n^{-4/5}$, $n^{-2/3}$, $n^{-4/7}$ (ongoing work)
- The proof requires convex analysis, chaining and Talagrand's concentration arguments
- Minimax optimal for $d \geq 4$ (Hütter and Rigollet (2019))
- These are the first rates for a practically computable estimator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

Question

Can we construct multivariate distribution-free tests?



Outline

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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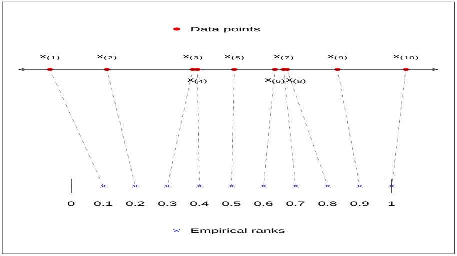

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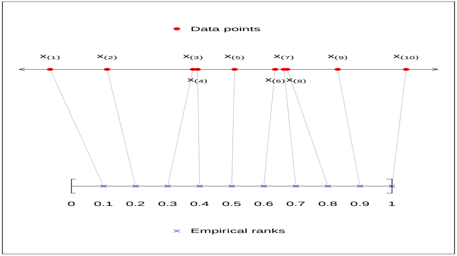

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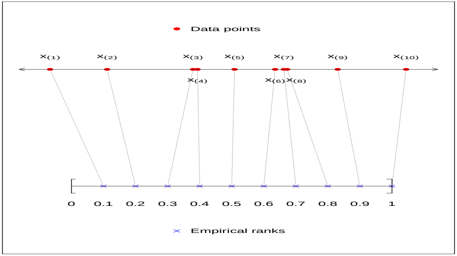

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$\widehat{R}_n$ is the **empirical OT map** from ν_n to μ_n

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 Unif$[0,1]^d$, $\mathcal{N}(0, I_d)$ distribution, deterministic quasi-Monte Carlo sequences)

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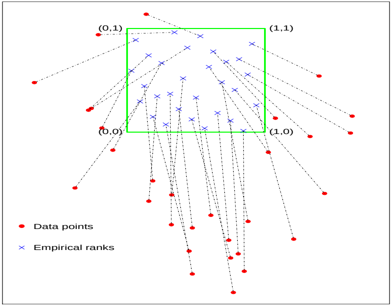

Multivariate rank function as an OT map

- $X \sim \nu$; ν is a probability measure in $\mathbb{R}^d$ (abs. cont.)
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Population rank function (a.k.a OT map) [Chernozhukov et al. (2017)]

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

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- When $d = 1$, $R(\cdot)$ is the CDF of X, when $\mu =$ Unif$([0,1])$

Properties [D. and Sen (JASA 2020); D., Bhattacharya, and Sen (2021)]

- Distribution-freeness: If ν is absolutely continuous, then

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where R is the unique OT map from ν to μ.

No moment assumptions needed on the model

Outline

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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 $\mathbb{R}^d$, $d \geq 1$
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Goal

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

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- **Question**: How to compare two consistent tests S_N and T_N?
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- **Question**: How to compare two consistent tests S_N and T_N?
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- $X_1, \ldots, X_m \overset{iid}{\sim} \mathrm{P}_{\theta_1}$ & $Y_1, \ldots, Y_n \overset{iid}{\sim} \mathrm{P}_{\theta_2}$; $N = m + n$; $\frac{m}{N} \approx \lambda \in (0,1)$
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In principle, $\mathrm{ARE}\,(S_N, T_N)$ can depend on α and β, but in many interesting cases they don't

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

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

$$\min_{\mathcal{F}} \mathrm{ARE}\,(\mathrm{RT}^2_{m,n}, \mathrm{T}^2_{m,n}) = ??$$

$$X_1, \ldots, X_m \overset{iid}{\sim} \mathrm{P}_{\theta_1} \;\&\; Y_1, \ldots, Y_n \overset{iid}{\sim} \mathrm{P}_{\theta_2}; \quad N = m + n$$

Independent coordinates case

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

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

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

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

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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

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

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

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

Model for Independent Component Analysis (ICA)

$\mathcal{F}_{\text{ICA}} = \{f_1(\cdot - \theta) : f_1 \in \mathcal{F}\}_{\theta \in \mathbb{R}^d}$ where $f_1 \in \mathcal{F}$ 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

$$X = A\, W$$

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

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Recap

- Exact distribution-free, nonparametric test, gives uniformly level α test and high efficiency compared to Hotelling T^2 test
- Provides the first comprehensive extension of classical nonparametric testing to the multivariate setting skip
- Using Gaussian reference distribution ensures $\mathrm{ARE}\,(\mathrm{RT}^2_{m,n}, \mathrm{T}^2_{m,n}) \geq 1$ for many popular subfamilies. Note that the test is agnostic to the underlying subfamily skip

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Thank you. Questions?

Multivariate two-sample goodness-of-fit test

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

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

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

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

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- **Energy test**: Reject H_0 if $\mathrm{E}_{m,n}\left(\{X_i\}_{i=1}^m, \{Y_j\}_{j=1}^n\right) > \kappa_\alpha$ (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:

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

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

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Distribution-freeness

Under H_0, distribution of $\mathrm{RE}_{m,n}$ is free of $P \equiv Q$, if P is abs. cont.

- Dist. of $\mathrm{RE}_{m,n}$ just depends on c_i's, m, n and d
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Simplification when $d = 1$

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

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

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

$$\mathbb{P}(\mathrm{RE}_{m,n} > \kappa_{\alpha}^{(m,n)}) \to 1 \qquad \text{as } \; m, n \to \infty.$$

Proposed test has asymptotic power 1, against all fixed alternatives

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

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

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

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

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

Pitman efficiency

Some observations

- Efficiency of $\mathrm{RE}_{m,n}$ w.r.t. $\mathrm{E}_{m,n}$ depends on the type I error α and power β, which makes it hard obtain efficiency lower bounds

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Rank Energy $\mathrm{RE}_{m,n}$ [D., Bhattacharya, and Sen (working paper)]

- $$\lim_{m,n\to\infty} \mathbb{P}_{\mathrm{H}_1}(\mathrm{RE}_{m,n} \text{ rejects } \mathrm{H}_0) > \alpha$$
- Only consistent, exactly dist.-free test that can distinguish H_0 & H_1

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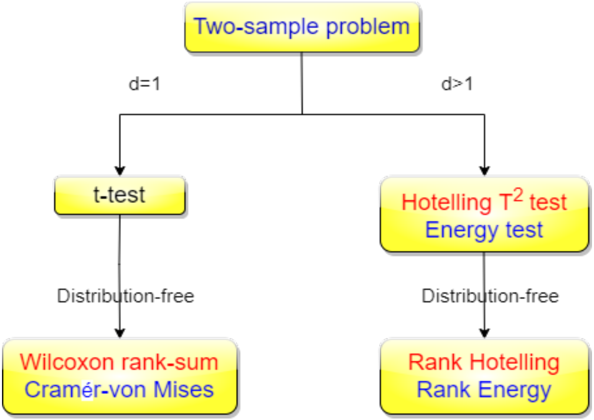
- Tuning-free, robust, computationally feasible procedures, performs particularly well under heavy-tailed data ▸▸ skip

Summary


Two-sample problem
d=1
d>1
t-test
Hotelling T2 test
Energy test
Distribution-free
Distribution-free
Wilcoxon rank-sum
Cramér-von Mises
Rank Hotelling
Rank Energy

References

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D., Bhattacharya and Sen (2021+). (working paper)

Nonparametric association/conditional association

- Suppose

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- $T_n \xrightarrow{a.s.} T(X, Y)$

Measure of Association

We answer this question in the affirmative 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

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References:

D., Ghosal, and Sen (2020). https://arxiv.org/pdf/2010.01768.pdf (RR at AoS)

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

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Gaussian mixture models and multiple testing:

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https://www.tandfonline.com/doi/full/10.1080/01621459.2021.1888739

(JASA, published online)

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Ghosh, D., Karmakar & Sen (2021). https://arxiv.org/abs/2111.15524 ⏩ skip

Rate of convergence result

$$T_0 = \operatorname*{arg\,min}_{T\#P=Q} \int \|x - T(x)\|^2 \, dP(x),$$

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

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 $Y_i = f_0(X_i) + \epsilon_i$, $i = 1, \ldots, n$, where ϵ_i's are iid $\mathcal{N}(0,1)$, 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:

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

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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,

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

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

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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 $\bar{Q}_n := T_0 \# P_n$. Then,

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

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

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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

$$T_0 \overset{???}{:=} \underset{T\#P=Q}{\arg\min} \int \|x-T(x)\|^2 \, dP(x), \quad T\#P = Q \Leftrightarrow X \sim P,\ T(X) \sim Q.$$

- Does a solution always exist?
- Is the solution unique?

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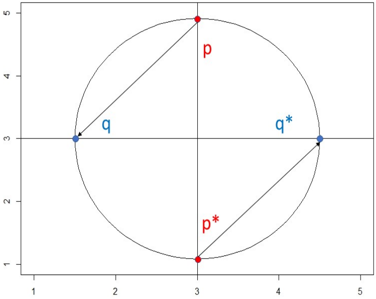
  No! Take $P = 0.5\delta_p + 0.5\delta_{p^*}$ and $Q = 0.5\delta_q + 0.5\delta_{q^*}$.



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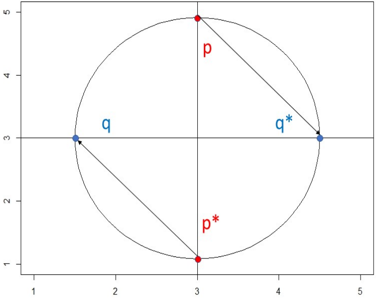

Crossmatch test (Rosenbaum 2005)

Pitman asymptotics for crossmatch test (Rosenbaum 2005)

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

$$\lim_{m,n\to\infty} \mathbb{P}_{\mathrm{H}_1}(T_{m,n} \text{ rejects } \mathrm{H}_0) = \alpha.$$

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- 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

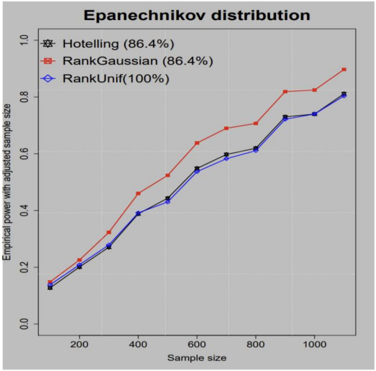

Figure: X_1, Y_1 are i.i.d. Epanechnikov with location parameters 0 and 0.1 respectively. $X_2, X_3 \sim X_1$, $Y_2, Y_3 \sim Y_1$ and $X := (X_1, X_2, X_3)$, $Y := (Y_1, Y_2, Y_3)$. Here

$$\text{eff}(\text{RankUnif}, \text{Hotelling}) = 0.864$$

and $\text{eff}(\text{RankGaussian}, \text{Hotelling}) > 1$ skip

Power plot with varying location parameter

Log-normal location problem (slightly heavy-tailed)

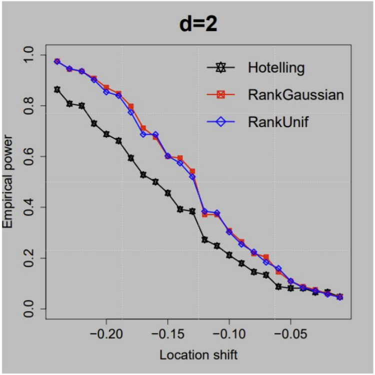

Figure: U_1, U_2 are iid standard normal, and V_1, V_2 are normal with variance 1 and varying mean. Define $X_i := \exp(U_i)$ and $Y_i := \exp(V_i)$. Set $X := (X_1, X_2)$ and $Y := (Y_1, Y_2)$ — sample size $n = 200$ skip

Power plot with varying location parameter

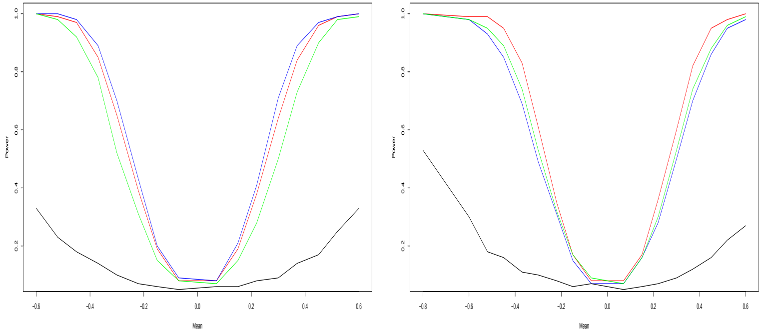

Figure: (Left panel) X_1, Y_1 are i.i.d. normal with mean 0 and μ respectively (and unit variance). $X_2, X_3 \sim X_1$, Y_2, $Y_3 \sim Y_1$ and $X := (X_1, X_2, X_3)$. Similarly define Y. ⏩ skip

(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 Gorfine (Heller et al., 2013), En - energy statistic (Székely 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 $\alpha = 0.05,\ 0.1$ 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 $\alpha = 0.05,\ 0.1$ and $n = 100, 300, 500, 700, 900,\ d = 8$.

What happens for $d = 1$?

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

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

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

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

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- $T_0(\cdot)$ is the distribution function of X, say $F(\cdot)$
- Note that increasing functions can be viewed as "derivatives" of convex functions.

- Suppose $T_0 \in C^\alpha$ (Hölder or Sobolev class), $\alpha > 1$
- The minimax rate of convergence is

$$n^{-\frac{2\alpha}{2\alpha-2+d}} + n^{-1}$$

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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)

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

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

- $T_0(X) \sim Y$, $X \sim \mu$ with density f, $Y \sim \nu$ with density g. Then change of variable formula implies

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

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

$$n^{-\frac{2(\beta-k)}{2\beta+d}}$$

- $T_0(X) \sim Y$, $X \sim \mu$ with density f, $Y \sim \nu$ with density g. Then change of variable formula implies

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

- Estimating anti-derivative of f, g related to estimating T_0

- (Caffarelli Regularity, 1992, 1996) — $T_0 \in C^\alpha$ corresponds to $f, g \in C^{\alpha-1}$, $\alpha > 1$

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

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- Modified Rank Hotelling T^2:

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

- Test is distribution-free — if $Y \stackrel{d}{=} X - \theta$ then detection boundary at $\|\theta\| \sim \sqrt{d/n}$ 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**: $F(X) \sim \text{Uniform}([0,1])$
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$$F = \underset{T: T(X) \stackrel{d}{=} U}{\arg\min} \ \mathbb{E}|X - T(X)|^2$$

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

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

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

- $X \sim \nu$; ν is a probability measure in $\mathbb{R}^d$ (abs. cont.)
- $U \sim \text{Uniform}([0,1]^d)$

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- **Data**: $X_1, \ldots, X_n$ iid ν (abs. cont.) on $\mathbb{R}^d$
- $\{c_1, \ldots, c_n\} \subset \mathbb{R}^d$ — grid of "reference" points

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

$$\hat{\mathbf{R}}_{\mathbf{n}} = \underset{\sigma \in S_n}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \|X_i - c_{\sigma(i)}\|^2 \equiv \underset{\mathbf{T}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \|X_i - \mathbf{T}(X_i)\|^2$$

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

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

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

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

Result gives the required regularity of the empirical multivariate rank map

Population version

Assume $m/(m+n) = \lambda \in (0,1)$.

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

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

$$\mathrm{R}_\lambda : \mathrm{R}_\lambda(\mathbf{Z}) \sim \mathrm{Uniform}([0,1]^d)$$

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

Pitman efficiency

- Consider $X_1, \ldots, X_n \sim \mathrm{P}_{\theta_1}$ and $Y_1, \ldots, Y_m \sim \mathrm{P}_{\theta_2}$, with $m/(m+n) = \lambda \in (0,1)$. We want to test:

$$\mathrm{H}_0 : \theta_2 - \theta_1 = 0 \qquad \text{versus} \qquad \mathrm{H}_1 : \theta_2 - \theta_1 = h(m+n)^{-1/2}.$$

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

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

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