Soft and subspace robust multivariate rank tests based on entropy regularized optimal transport

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Abstract

In this paper, we extend the recently proposed multivariate rank energy distance, based on the theory of optimal transport, for statistical testing of distributional similarity, to soft rank energy distance. Being differentiable, this in turn allows us to extend the rank energy to a subspace robust rank energy distance, dubbed Projected soft-Rank Energy distance, which can be computed via optimization over the Stiefel manifold. We show via experiments that using projected soft rank energy one can trade-off the detection power vs the false alarm via projections onto an appropriately selected low dimensional subspace. We also show the utility of the proposed tests on unsupervised change point detection in multivariate time series data. All codes are publicly available at the link provided in the experiment section.

I. INTRODUCTION

This paper is concerned with the classical two-sample hypothesis test, also known as the Goodness-of-Fit (GoF) test. Given samples $X_1, \ldots, X_m$ and $Y_1, \ldots, Y_n$, that are independent and identically distributed (i.i.d.) according to distributions $\mu$ and $\nu$, respectively, on $\mathbb{R}^d$, one wants to test following hypotheses,

$$H_0 : \mu = \nu, \text{ vs. } H_1 : \mu \neq \nu.$$ 

Two sample multivariate goodness-of-fit-test test has been studied extensively using both parametric and non-parametric methods. A brief and relevant background is provided in Section II but we refer the reader to some classical [1]–[5] and recent texts [6]–[9] for background. To be concise and retain focus on the approach undertaken in this paper, we begin by summarizing the main contributions below. To fully appreciate the contributions, the reader may directly peruse section II first and come back here.

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A. Summary of main contributions

1) We extend the recently proposed nonparametric two-sample testing proposed in [10] to a new test that exploits the recent developments in computation of optimal transport, namely entropic relaxation [11]. We show via extensive experiments that this proposed test is nearly non-parametric under the null for small values of entropic regularization parameter.

2) In contrast to [10], the proposed test provides an efficient and scalable approximation to optimal transport, always admissible, a differential function of the data and we exploit this fact towards proposing a subspace robust two-sample testing that has the benefit to trade-off power of detection and false alarms in high dimensional testing under a limited number of samples. In this context, we provide an approach that is complementary to subspace robust Wasserstein distances and tests based on that [12], [13]. This test can be efficiently computed using a Riemannian optimization over the Stiefel manifold.

3) We provide an application of the proposed test to unsupervised detection of change points in multivariate time series data and observe that the test is very sensitive to shifts in support of the signal. This is a useful property but it makes the test also very sensitive to the presence of outliers.

The rest of the paper is organized as follows. In section II we provide the context needed to appreciate the recent developments and the subsequent innovations made in this paper. In section III we outline in detail the proposed tests. In section IV we provide ample empirical evidence in support of the proposed tests and an application to unsupervised detection of change points in multivariate time series data.

II. Background and related work

Notation: Let \( \mathcal{P}(\mathbb{R}^d) \) denote the set of all probability measures on \( \mathbb{R}^d \). Unless otherwise stated we will assume that distributions \( \mu, \nu, \ldots \) are absolutely continuous. For a random variable \( X \), \( X \sim \mu \) reads that \( X \) is distributed with the distribution \( \mu \). We will use upper-case letters \( X, Y \) for univariate random-variables. The notation \( T, P \) will be reserved for maps, matrices, etc. The rest of the notation is introduced as needed.

A. Multivariate Ranks and Quantiles

Rank based distribution-free goodness of tests have been studied comprehensively in 1-D e.g Kolmogorov-Smirnov test [14], Wilcoxon signed-rank test [15], Wald-Wolfowitz runs test [16]. Lack of canonical ordering in \( d \)-dimensional space, for \( d \geq 2 \), does not guarantee the exact distribution freeness studied in [17]–[23]. Marc Hallin and authors in [24], [25] first introduced the notion of multivariate rank based on measure transportation theory that guarantees distribution freeness. However, these works were based on semi-discrete optimal transport and failed to provide distribution freeness for a fixed sample size. Nabarun in [10] proposed the notion of multivariate rank
which provides the distribution freeness for fixed sample size. In the later subsection, we will discuss rank and quantile in the 1-D case and cover the background of multivariate rank proposed in [10].

a) Ranks and Quantiles for univariate distributions: Let $X$ be a univariate random variable with c.d.f. $F: \mathbb{R} \rightarrow [0, 1]$. It is a standard result that when $F$ is continuous, the random variable $F(X) \sim U[0, 1]$ - the uniform distribution on $[0, 1]$. For any $x \in \mathbb{R}$, $F(x)$ is referred to as the rank-function. For any $0 < p < 1$, the quantile function is defined by $Q(p) = \inf\{x \in \mathbb{R} : p \leq F(x)\}$. When $F$ is continuous, the quantile function $Q = F^{-1}$.

Since there exists no natural ordering in $\mathbb{R}^d$, defining ranks and quantiles in high dimension is not straightforward. To extend the notion of rank in $\mathbb{R}^d$, theory of Optimal Transport (OT) has been used to propose meaningful and useful notions of multivariate rank and quantile functions [10]. In it’s most standard setting, given two distributions, a source distribution $\mu \in \mathcal{P}(\mathbb{R}^d)$ and a target distribution $\nu \in \mathcal{P}(\mathbb{R}^d)$, OT aims to find a map $T: \mathbb{R}^d \rightarrow \mathbb{R}^d$ that pushes $\mu$ to $\nu$ with a minimal cost. That is, given $X \sim \mu$, and $Y \sim \nu$, OT finds a map $T$ that solves for,

$$\inf_T \int \|x - T(x)\|^2d\mu(x) \text{ subject to } Y = T(X) \sim \nu$$

Note that if $T(X) \sim \nu$ when $X \sim \mu$, we write $\nu = T_\#\mu$. The key insight in using the theory of OT to multivariate ranks and quantiles, comes from noticing that in case of $d = 1$, the optimal transport map is given by $T = F_\nu^{-1} \circ F_\mu$ where $F_\mu$ and $F_\nu$ are the distribution functions for $\mu$ and $\nu$ respectively. When $\nu = U[0, 1]$, this gives the rank function $F_\mu$. In [10], the authors used McCann’s theorem [26] to extend the notion of rank for high dimensional case stated by the following theorem:

**Theorem 1 (McCann [26]):** Assume $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ be absolutely continuous measures, then there exists transport maps $R(\cdot)$ and $Q(\cdot)$, that are gradients of real-valued $d$-variate convex functions such that $R_\#\mu = \nu$, $Q_\#\nu = \mu$, $R$ and $Q$ are unique and $R \circ Q(x) = x$, $Q \circ R(y) = y$.

Based on this result, the authors in [10] give the following definitions for the rank and quantile functions in high dimensions.

**Definition 1 (Nabarun [10]):** Given absolutely continuous measure $\mu \in \mathcal{P}(\mathbb{R}^d)$ and $\nu = U[0, 1]^d$ - the uniform measure on the unit cube in $\mathbb{R}^d$, the ranks and quantile maps for $\mu$ are defined as the maps $R(\cdot)$ and $Q(\cdot)$ respectively as defined in Theorem 1

**B. Multivariate Rank from Samples**

Let $X_1, \ldots, X_n$ be i.i.d. samples drawn from $\mu \in \mathcal{P}(\mathbb{R}^d)$. Let $\mu_n$ denote the empirical measure supported on these samples. In general, there does not exist a map $R$ from $\mu_n$ to $U[0, 1]^d$ [1] On the other hand there does exist a map $Q$ from $U[0, 1]^d$ to $\mu_n$, and is a special case of the OT problem referred to as the semi-discrete optimal

\(^1\)While there does not exist a map, there does exist a plan obtained by solving the so-called Kantorovich problem, which is a relaxation of the Monge problem [25].
transport. Using the convex geometry of the problem the authors in [27] propose a randomized rank map by using
the solution to the Quantile map $Q$ obtained from the semi-discrete OT. However, it may be computationally
expensive to do so [27]. To circumvent this, the authors in [10] propose to use the following notion of empirical
multivariate rank, by mapping the samples $X_1, \cdots, X_n$ to fixed set $d$-dimensional Halton sequence [28] of size $n$,
denoted by $\mathcal{H}_{n}^{d} := \{h_1, \ldots, h_n\}$. For details on Halton sequences we refer the reader to [28]. The main point to
note is that the empirical measure $\nu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{h_i}$ converges in distribution to $U[0, 1]^d$.

Now given the empirical distribution of samples and the empirical distribution concentrated on a given set of
Halton sequences,

$$\mu_n^X = \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i} \quad \text{and} \quad \nu_n^H = \frac{1}{n} \sum_{i=1}^{n} \delta_{h_i},$$

the empirical rank function is defined as follows. First, one solves for the following discrete optimal transport
problem, also known as the 2-D assignment problem in the literature [11].

$$\hat{P}_n = \arg \min_{P \in \Pi} \sum_{i,j=1}^{n} C_{i,j} P_{i,j}, \quad (2)$$

where $C_{i,j} = \|X_i - h_j\|^2$, $\Pi = \{P : P1 = \frac{1}{n} 1^\top P = \frac{1}{n} 1^\top\}$. It is well known that the solution to this problem,
under the given set-up, is one of the scaled permutation matrices. Consequently, one obtains a map $\hat{R}_n(X_i) = h_{\sigma(i)}$,
where $\sigma(i)$ is the non-zero index in the $i$-th row of $P_n$.

Definition 2: [10] $\hat{R}_n$ as defined above is called as the empirical rank map.

C. Goodness-of-Fit (GoF) tests: Rank Energy Distance

Given two sets of i.i.d. samples $\{X_1, \ldots, X_m\} \in \mathbb{R}^d$ and $\{Y_1, \ldots, Y_n\} \in \mathbb{R}^d$ with empirical measures $\mu_n^X, \mu_n^Y$
respectively. In [10], the authors proposed a distribution-free multivariate GoF test based on the energy distance
[8] between the empirical ranks obtained for each of the sample sets, which is referred as the Rank Energy (RE)
test. Following [10], RE for GoF testing is defined as follows. Draw $m + n$ Halton sequences $h_1, \cdots, h_{m+n}$ and
compute the joint-empirical rank map $\hat{R}_{m,n}$ between the empirical measure formed by combining the two sets of
samples,

$$\mu_{m,n}^{X,Y} = \frac{1}{m+n} (m \mu_n^X + n \mu_n^Y),$$

and the empirical measure concentrated on the Halton sequences, $\nu_{m,n}^H = \frac{1}{m+n} \sum_{i=1}^{m+n} \delta_{h_i}$. The rank energy is
defined as,
\[
\text{RE}^2_{m,n} = \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} \| \hat{R}_{m,n}(X_i) - \hat{R}_{m,n}(Y_j) \| - \frac{1}{m^2} \sum_{i,j=1}^{m} \| \hat{R}_{m,n}(X_i) - \hat{R}_{m,n}(X_j) \|
\]
\[
- \frac{1}{n^2} \sum_{i,j=1}^{n} \| \hat{R}_{m,n}(Y_i) - \hat{R}_{m,n}(Y_j) \|. \tag{3}
\]

It can be shown that the \( \text{RE}^2_{m,n} \) is distribution free for all sample sizes, see [10], which follows from the fact that under the null, the empirical ranks map is uniformly distributed over the \((m+n)!\) permutations.

Based on [10], the rank energy test rejects \( H_0 \) if \( \frac{mn}{m+n} \text{RE}^2_{m,n} > \kappa_{m,n}^{\alpha} \), where \( \kappa_{m,n}^{\alpha} \) is a threshold that is picked as a function of \( m, n \) and a desired level of False Alarm (FA) level \( \alpha \).

In general, in (3), one can use a characteristic kernel \( k(\cdot, \cdot) \) [29] and via defining
\[
B = \frac{1}{mn} \sum_{i,j=1}^{m,n} k(\hat{R}_{m,n}(X_i), \hat{R}_{m,n}(Y_j)), \quad C = \frac{1}{m^2} \sum_{i,j=1}^{m} k(\hat{R}_{m,n}(X_i), \hat{R}_{m,n}(X_j)),
\]
\[
D = \frac{1}{n^2} \sum_{i,j=1}^{n} k(\hat{R}_{m,n}(Y_i), \hat{R}_{m,n}(Y_j)),
\]

one can define a kernelized rank energy via the following equation:
\[
\text{RE}^2_{m,n} = 2B - C - D. \tag{4}
\]

III. PROPOSED MULTIVARIATE RANKS AND TESTS OF GOODNESS-OF-FIT

In this work we are motivated by potential use of these tests towards generative adversarial networks (GANs), which necessitates that the \( \text{RE}_{m,n} \) be a differentiable function of data samples \( X_1, \cdots, X_m, Y_1, \cdots, Y_n \). In this context we are motivated by the use of Sinkhorn iterations for solving the discrete OT problem [30] via entropic regularization and noting that as an algorithm one can readily differentiate through the iterative steps [31].

A. Soft Rank Energy Distance

To define soft rank energy, we first need to define the notion of a soft rank. To do so we consider the Optimal Transport Plan between \( \mu_m^X \) and \( \nu_m^H \), via solving for the following entropic regularized problem [11],
\[
P^0 = \arg \min_{P \in \Pi} \sum_{i,j=1}^{m} C_{i,j} P_{i,j} - \epsilon H(P), \tag{5}
\]
where \( C_{i,j} = \| X_i - h_j \|^2 \), \( \epsilon > 0 \), \( \Pi = \{ P : P1 = \frac{1}{n} 1, 1^T P = \frac{1}{n} 1^T \} \), and \( H(P) = -\sum_{i,j} P_{i,j} \log P_{i,j} \) is the entropy functional. For \( \epsilon > 0 \), \( \hat{R}_n \) will not be a permutation matrix, see [11], and in this case we define a soft rank
map via,
\[ \hat{R}^{s,\epsilon}(X_i) = \sum_{j=1}^{m} \sum_{j=1}^{m} \frac{P_{i,j}^0}{m} h_j. \] (6)

Using this notion of rank, we define the soft rank energy statistics as follows.

\[ sRE_{m,n}^2 = \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} \| \hat{R}^{s,\epsilon}_{m,n}(X_i) - \hat{R}^{s,\epsilon}_{m,n}(Y_j) \| - \frac{1}{m^2} \sum_{i=1}^{m} \| \hat{R}^{s,\epsilon}_{m,n}(X_i) - \hat{R}^{s,\epsilon}_{m,n}(X_j) \| \]
\[ - \frac{1}{n^2} \sum_{i,j=1}^{n} \| \hat{R}^{s,\epsilon}_{m,n}(Y_i) - \hat{R}^{s,\epsilon}_{m,n}(Y_j) \|, \] (7)

where \( \hat{R}^{s,\epsilon}_{m,n} \) is the map obtained by the entropic regularized mapping between \( \mu_{m,n}^X, \nu_{m,n}^H \). One can also use the kernelized version of \( sRE_{m,n}^2 \) similar to \( RE_{m,n}^2 \) (see equation (4)).

**B. Projected Soft Rank Energy Tests**

Recently projected Wasserstein distances or subspace-robust Wasserstein distances were proposed in [12] for robustness to noise in computing the transport maps. This approach was recently exploited in [13] for two-sample testing to address the diminishing power of the OT based tests in high-dimensions by finding an appropriate low-dimensional subspace to compare the two samples. In the present context, given two empirical distributions, \( \mu_{m,n}^X, \nu_{m,n}^Y \), the projected Wasserstein-2 distance is defined as,

\[ \max_{U \in \mathbb{R}^{d \times k}} \sum_{i,j} P_{i,j} \left\| U X_i - U Y_j \right\|^2 \] (8)

Motivated by these developments, here we propose the subspace robust versions soft rank energy, namely the projected soft rank energy statistics.

We first define Projected soft Rank Energy Distance (\( PsRE_{m,n}^2 \)) as follows. Let \( \hat{R}_{m,n} \) be the empirical rank computed with projected data \( U U^T X_i, U U^T Y_j, i = 1, \ldots, m, j = 1, \ldots, n \) and fixed set of Halton sequences \( h_1, \ldots, h_{m+n} \subset [0,1]^d \) in the unit cube in \( \mathbb{R}^d \). The projected soft rank energy statistics is defined as:

\[ PsRE_{m,n}^2 = \max_{U \in \mathbb{R}^{d \times k}} \sum_{i,j} P_{i,j} \left\| U X_i - U Y_j \right\|^2 \] (9)

The \( PsRE_{m,n}^2 \) is defined in an analogous manner using Equation (7). There are several reasons to consider the projected versions. In the experiment section, we will show that in high dimension for some specific distributions
rank energy based hypothesis test loses its power for a fixed number of samples.

IV. EXPERIMENTAL RESULTS

In this section, we will compare the proposed scaled $s\text{RE}_{m,n}^2$ statistics to the scaled $\text{RE}_{m,n}^2$ based on the synthetic data. Going forward for the sake of brevity we refer scaled $s\text{RE}_{m,n}^2$ and scaled $\text{RE}_{m,n}^2$ as $\text{RE}$ and $s\text{RE}$ respectively. We will illustrate the behavior of $s\text{RE}$ statistics under the null and show experimentally that our proposed statistics can achieve distribution-freeness with a small regularizer-based OT plan. We will demonstrate how $s\text{RE}$ statistics depend on the optimal transport regularization parameter and find out which parameters achieve the notion of multivariate rank as closely as possible to $\text{RE}$ [10]. We will also observe the effect of sample dimension on $s\text{RE}$ statistics and show comparatively better results using projected soft rank energy [II-B] for some specific distributional settings in higher dimensions. Finally, we will use $s\text{RE}$ statistics in an application e.g. change point detection on some real data.

Reproducible research: All codes are available at [https://github.com/ShoaibBinMasud/soft_projected_multivariate](https://github.com/ShoaibBinMasud/soft_projected_multivariate)

rank.git

A. Synthetic data

We consider the following distributional settings to observe the behaviour of $s\text{RE}$ statistics. We draw $m$ and $n$ i.i.d. samples of $d$ dimensional vectors $X = (X_1, \ldots, X_d)$ and $Y = (Y_1, \ldots, Y_d)$ respectively for each setting and carry-out two-sample goodness of fit test based on these observations. Throughout the experiments we assume $m = n$.

(v1) $(X_1, \ldots, X_d) \overset{i.i.d.}{\sim} \text{cauchy}(0, 1)$ $(Y_1, \ldots, Y_d) \sim \text{Cauchy}(0.2, 1)$

(v2) $X_1, Y_1 \overset{i.i.d.}{\sim} \mathcal{U}[0, 1]$, $X_k = 0.25 + 0.35 \times X_{k-1} + U_k$, $Y_k = 0.25 + 0.5 \times Y_{k-1} + U_k$ for $k = 2, \ldots, d$, where $U_2, \ldots, U_d \overset{i.i.d.}{\sim} \mathcal{U}[0, 1]$

(v3) $X \sim \mathcal{N}_d(0, \Sigma_X)$ and $Y \sim \mathcal{N}_d(0, \Sigma_Y)$, where $\Sigma_X = 0.35|\cdot| |\cdot|$ and $\Sigma_Y = 0.65|\cdot| |\cdot|$ for $1 \leq i, j \leq d$

(v4) $X \sim \mathcal{N}_d(0, \Sigma_X)$ and $Y \sim \mathcal{N}_d(0, \Sigma_Y)$, where $\Sigma_X(i, i) = 1$ and $\Sigma_X(i, j) = 0.2$ for $i \neq j$ and $\Sigma_Y(i, i) = 1$ and $\Sigma_Y(i, j) = 0.5$ for $1 \leq i, j \leq d$

(v5) $V \sim \mathcal{N}_d(0, \Sigma_V)$ and $W \sim \mathcal{N}_d(0, \Sigma_W)$, where $\Sigma_V = 0.35|\cdot| |\cdot|$ and $\Sigma_W = 0.65|\cdot| |\cdot|$ for $1 \leq i, j \leq d$. Set $X_i = \exp(V_i)$ and $Y_i = \exp(V_i)$ for $i = 1, \ldots, d$

(v6) $V \sim \mathcal{N}_d(0, \Sigma_V)$ and $W \sim \mathcal{N}_d(0, \Sigma_W)$, where $\Sigma_V(i, i) = 1$ and $\Sigma_V(i, j) = 0.75$ for $i \neq j$ and $\Sigma_W(i, i) = 1$ and $\Sigma_W(i, j) = 0.5$ for $1 \leq i, j \leq d$. Set $X_i = \exp(V_i)$ and $Y_i = \exp(V_i)$ for $i = 1, \ldots, d$

(v7) $X \sim \mathcal{N}_d(\mu_X, 3\mathbf{I})$ and $Y \sim \mathcal{N}_d(\mu_Y, 3\mathbf{I})$ where $\mu_X = (0, \ldots, 0)$ and $\mu_Y = (0.25, \ldots, 0.25)$

(v8) $X_1, \ldots, X_d, V_1, \ldots, V_d \overset{i.i.d.}{\sim} \text{Gamma}(2, 0.1)$ and $W_1, \ldots, W_d = \exp(Z)$ where $Z \sim \mathcal{N}(0, 1)$. Set $Y_i = V_i W_i$ for $i = 1, \ldots, d$ and $A \sim \text{Ber}(0.8)$. 

(v9) \( Z_1, Z_2 \sim_{\text{i.i.d.}} \mathcal{N}_d(0, I) \). Let \( W = (W_1, W_2, \ldots, W_d) \sim_{\text{i.i.d.}} \mathcal{U}(10) \). Finally, set \( X := Z_1 \) and \( Y := AZ_2 + (1 - A)W \).

(v10) \( Z_1, Z_2 \sim_{\text{i.i.d.}} \mathcal{N}_d(0, I) \). Let \( W = (W_1, W_2, \ldots, W_d) \sim_{\text{i.i.d.}} \mathcal{N}(10, 0.1) \). Set \( X := Z_1 \) and \( Y := AZ_2 + (1 - A)W \).

(v11) \( X \sim \text{Laplace}(0, I_d) \) and \( Y \sim \text{Laplace}(0, I_d) \) where \( \mu = (1, 0, \ldots, 0) \)

(v12) \( X_1, \ldots, X_d \sim_{\text{i.i.d.}} \mathcal{N}(0, 1) \otimes \mathcal{N}(0, 4) \) and \( Y_1, \ldots, Y_d \sim_{\text{i.i.d.}} \mathcal{N}(0, 1) \)

Many of the distributional settings considered above are directly taken from [10], [13]. For instance (v1)-(v10) are adopted from [10]. (v11), (v12) are slightly modified version of similar settings in [32]. (v1) and (v8) are heavy-tailed Cauchy and Gamma distribution respectively with no finite first moment. In (v9) and (v10), \( X \) is a multivariate Gaussian, whereas \( Y \) is a multivariate Gaussian with a small percentage of Uniform and Gaussian noise respectively. (v3)-(v8) and (v12) are multivariate normals and log-normals. (v2) represents the auto-regressive model whereas in (v11) both \( X, Y \) are sampled from Laplace distribution.

B. Distribution of sRE statistics under the null

To illustrate the distribution of sRE statistics under the null, we choose (v1)-(v7) and (v11) distributional settings, that include a heavy-tailed Cauchy, multivariate normal, log normal and Laplace distribution. We draw 200 i.i.d. samples of 3 dimensional vectors \( X = (X_1, X_2, X_3) \sim P_X \) and \( Y = (Y_1, Y_2, Y_3) \sim P_Y \), assuming \( P_X = P_Y \). For each setting, non-normalized kernel density of sRE statistics is estimated using 1000 replicates of \( X, Y \in \mathbb{R}^{200 \times 3} \), with different regularizers, \( \epsilon = 0, 0.001, 0.01, 0.1, 1 \) (Figure 1), where \( \epsilon = 0 \) refers to RE which guarantees exact distribution-freeness [10].

![Fig. 1](image_url)

Fig. 1. The estimated kernel density of soft rank energy with different regularizer \( \epsilon = 0, 0.001, 0.01, 0.1, 1 \) under the null for \( m = n = 200 \) and \( d = 3 \). Y-axis represents non-normalized kernel density estimated value \( f(x) \).

Estimated RE (\( \epsilon = 0 \)) statistics densities appear to be similar (Figure 1(a)) for (v1)-(v7) and (v11), that proves the distribution-freeness under the null as claimed in [10]. We observe the analogous density estimates of sRE statistics with \( \epsilon = 0.001, 0.01 \) (Figure 1(b)-(c)) for all settings, which also resemblance the density pattern obtained using \( \epsilon = 0 \). As, \( \epsilon \) increases e.g. \( \epsilon = 0.1, 1 \), estimated density curves no longer follow the same shape for different distributional settings (Figure 1(d)-(e)). Since entropic schemes for optimal transport with small regularizer converges
to Monge-Kantorovich problem \cite{33}, transport plan using $\epsilon = 0.001, 0.01$ preserve the concept of multivariate rank \cite{10} to some extent. However, with larger $\epsilon$, the transport plan gets more diffused, and sRE statistics digress largely from RE statistics.

C. Effect of OT regularizer on sRE statistics

In this subsection, we observe how sRE statistics vary with respect to the optimal transport regularization parameter $\epsilon$ under alternate hypothesis. To analyze the relation, 3-dimensional, $m = n = 200$ i.i.d. samples of $X \sim P_X$, $Y \sim P_Y$ are drawn for each setting listed in IV-A assuming $P_X \neq P_Y$. We compute the average sRE statistics with different regularizers $\epsilon = 0.0001, 0.001, 0.1, 1, 5, 10$, using 500 replicates of $X \in \mathbb{R}^{m \times d}, Y \in \mathbb{R}^{n \times d}$ (see Figure 2), where $\epsilon = 0$ simply represents the RE statistics. Average sRE statistics for the distributional settings (v1)-(v8), (v11) and (v12) with $\epsilon = 0.0001, 0.001, 0.01$, are approximately equivalent to RE statistics (Figure 2(a-h,k,l)). However, when $\epsilon$ increases e.g. $\epsilon = 0.1, 1, 5, 10$, average sRE decreases rapidly. Since the optimal transport plan gets diffused with larger $\epsilon$, soft ranks obtained by multiplying the row-normalized plan with halton sequences (Equation 6) take approximately same values for the samples from different distribution, thus weaken the notion of multivariate ranks that generally assign unique values to the order statistics. For (v9) and (v10), multivariate Gaussian distributions with small fraction of uniform and Gaussian noise respectively, average sRE fluctuates with $\epsilon$ (Figure 2(k)-(l)). However, even with large regularizers $\epsilon = 0.1, 1, 5, 10$, average sRE is still comparable to the RE statistics. To be noted here, both RE and sRE are not robust to noise. Additionally, a minimal shift either in mean or covariance in one of the dimensions e.g. (v11), (v12) may yield higher RE and sRE statistics, thus rejecting the true null hypothesis and raise false alarms in many practical applications e.g. change point detection. Future research can be carried out to make hypothesis test based on sRE statistics more robust to noise and outliers.

D. sRE with respect to different sample dimensions

We investigate the concept of multivariate soft rank in higher dimension and assess the relationship between sRE statistics and the dimension, for $d > 2$. We draw $m = n = 200$ i.i.d. samples of $X \in P_X$ and $Y \sim P_Y$, $P_X \neq P_Y$, of dimension $d \in D$, where $D = \{3, 8, 20, 50, 100, 200\}$, for distributional settings (v1)-(v3), (v5), (v6), (v9), (v11) and (v12). For every combination of $m$ and $d$, average sRE statistics are computed using 500 replicates of $X, Y \in \mathbb{R}^{m \times d}$ with regularizer $\epsilon = 0.01$ (Figure 3). $\epsilon = 0.01$ is chosen since sRE statistics imitate the distribution-free behaviour under the null, provide values comparable to RE (Figures 1, 2) with less computational complexity. Average sRE statistics show positive correlation with the dimension for (v1), (v3), (v5) and (v6) (Figure 3(a, c, d, e)). We observe a similar trend for the autoregressive setting (v2) (Figure 3(b)). However, for (v9) which is a multivariate Gaussian contaminated with uniform noise, sRE statistics first decreases slightly and then increases at a much higher rate when $d > 20$ (Figure 3(f)). For (v11), we observe a sharp decrease in average sRE but it starts
Fig. 2. Average soft rank energy statistics on y-axis with different regularizers ϵ on x-axis computed over 500 replicates for each distributional setting having of \( m = n = 200 \) and \( d = 3 \).

Increasing after \( d > 20 \), though sRE statistics is still small compared to values in smaller dimension. We notice a phenomenon for (v12) alike to (v11) with an elbow at \( d = 8 \) (Figure 3[h]), yet small compared to other normal and lognormal settings e.g. (v3), (v5) and (v6) in higher dimensions. A small shift in mean and variance in one particular dimension, while preserving the same mean and variance along all the other dimensions of \( Y \) in (v11) and of \( X \) in (v12), explains such behaviour of average sRE statistics. Therefore, in high dimension, sRE based hypothesis test might consequently results into frequent rejection of true null hypothesis for similar structures e.g. (v11) and (v12).

E. Projected Soft Rank Energy

We compare the scaled PsRE\(^2\) (henceforth referred as PsRE), proposed in Section III-B to sRE for the settings (v11) and (v12). In higher dimension, for these cases, sRE based hypothesis test might not be as useful as in lower dimension since sRE statistics do not exhibit the typical positive dependency with the dimension (see Figure 3). To check whether PsRE provides more distinguishable statistics between the null and alternate hypothesis than sRE, we draw \( d = 100\)-dimensional \( m = n = 200 \) i.i.d. samples of \( X \in P_X \) and \( Y \sim P_Y \) when \( P_X = P_Y \) (null hypothesis) and \( P_X \neq P_Y \) (alternate hypothesis). First, we compute the average sRE statistics in \( d = 100 \) and then project \( X, Y \in \mathbb{R}^{m \times 100} \) to 8-dimensional subspace, \( X_{\text{proj}}, Y_{\text{proj}} \in \mathbb{R}^{m \times 8} \), using a Python manifold optimization package called as Pymanopt and compute the sRE statistics with regularizer \( \epsilon = 0.001 \), under both null and alternate...
hypothesis (Figure 4). We observe that under the null and alternate hypotheses, average $sRE$ statistics are very similar when $d = 100$ both for (v11) and (v12), which consequently leads to poor power. On the contrary, average $PsRE$ statistics are comparatively larger for both (v11), (v12) which eventually ensures greater power to GoF test with a compromise to produce few false alarms.

**F. Algorithm for Change Point Detection based on proposed sRE**

In this section, we incorporate the idea of sRE statistics in a widely studied two-sample test e.g. change point detection [34], and evaluate the performance of sRE statistics on a real multivariate time-series dataset. Following the recent works in [35], [36], we apply sRE as a test statistic to detect the change points on the dataset utilizing
a sliding window based two-sample test. Given a time series data $Z[t] \in \mathbb{R}^d$, $t = 1, \ldots, T$, consists of distinct segments $[0, \tau_1], [\tau_1 + 1, \tau_2], \ldots, [\tau_k + 1, T]$ with $\tau_1 < \tau_2 < \ldots$, coming from unknown distributions where $\tau_1, \tau_2, \ldots, \tau_k$ are referred as the change points. Unsupervised change point detection problem aims to estimate $\tau_1, \tau_2, \ldots, \tau_k$ without any prior knowledge of the underlying distribution of distinct time segments and the number change points. Given a window size $n$, we define two different time segments at time $t$ by taking samples before $t$ as $X = \{Z[t-n], Z[t-n+1], \ldots, Z[t-1]\} \in \mathbb{R}^{n \times d}$ and after $t$ as $Y = \{Z[t+n], Z[t+n-1], \ldots, Z[t+1]\} \in \mathbb{R}^{n \times d}$.

We assume both $X, Y$ are sampled from unknown distribution $\mu, \nu$ respectively. Similar to hypothesis testing set up, we reject the null hypothesis $H_0$ if $\mu \neq \nu$ and will define time $t$ as a change point.

1) Performance on real data: We applied our proposed computationally non-parametric sRE statistics based change point detection on HASC-PAC2016 dataset, which consists of over 700 three-axis accelerometer sequences of subjects performing six types of actions: stay, walk, jog, skip, stairs up and stairs down. We only have taken one longest sequence where all of the actions were present. We select the window size $n = 250$ and compute the sRE statistics with $\epsilon = 0.01$. We then convolve the sRE statistics with a low-pass filter as proposed in [35] (Figure 5).

![Figure 5](image.png)

**Fig. 5.** Sample output for HASC-PAC2016 human activity accelerometer data sequence (grey) with the filtered (solid green) and unfiltered (dashed red) sRE statistics. It appears that the our method results in frequent false alarms in support of a change point whereas HSAC does not consider that as a true change point.

Our method is able to detect all the change points that are considered as real change points in the dataset using both filtered and unfiltered sRE statistics. However, this method provides frequent false alarms. This is because sRE is very sensitive and can detect if there exists any small shift either in mean or covariance between the adjacent windows. The analysis of these properties and mitigating false alarms in presence of anomalies is an important direction of future work.
CONCLUSION AND FUTURE WORK

We have extended the concept of optimal transport-based multivariate rank to soft multivariate rank utilizing entropic regularization. Experimental results show that soft rank energy is approximately distribution-free under the null and behaves similarly to original OT-based multivariate rank energy \cite{deb2019multivariate} for small regularization parameter. The proposed soft-rank energy allows us to consider a projected version of the rank-energy tests for high-dimensional data. For several distributional settings, our proposed projected soft rank energy performs better than rank energy and soft rank energy. Future research includes analyzing the theoretical properties of the proposed tests and addressing the sensitivity of these tests to the presence of outliers in the data.

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REFERENCES

[1] P. J. Bickel, “A distribution free version of the smirnov two sample test in the p-variate case,” *The Annals of Mathematical Statistics*, vol. 40, no. 1, pp. 1–23, 1969.

[2] L. Weiss, “Two-sample tests for multivariate distributions,” *The Annals of Mathematical Statistics*, pp. 159–164, 1960.

[3] J. H. Friedman and L. C. Rafsky, “Multivariate generalizations of the wald-wolfowitz and smirnov two-sample tests,” *The Annals of Statistics*, pp. 697–717, 1979.

[4] M. F. Schilling, “Multivariate two-sample tests based on nearest neighbors,” *Journal of the American Statistical Association*, vol. 81, no. 395, pp. 799–806, 1986.

[5] L. Wasserman, *All of statistics: a concise course in statistical inference*. Springer Science & Business Media, 2013.

[6] L. Baringhaus and C. Franz, “On a new multivariate two-sample test,” *Journal of multivariate analysis*, vol. 88, no. 1, pp. 190–206, 2004.

[7] D. Sejdinovic, B. Sriperumbudur, A. Gretton, and K. Fukumizu, “Equivalence of distance-based and rkhs-based statistics in hypothesis testing,” *The Annals of Statistics*, pp. 2263–2291, 2013.

[8] G. J. Székely and M. L. Rizzo, “Energy statistics: A class of statistics based on distances,” *Journal of statistical planning and inference*, vol. 143, no. 8, pp. 1249–1272, 2013.

[9] L. Wasserman, *All of nonparametric statistics*. Springer Science & Business Media, 2006.

[10] N. Deb and B. Sen, “Multivariate rank-based distribution-free nonparametric testing using measure transportation,” *arXiv preprint arXiv:1909.08733*, 2019.

[11] G. Peyré, M. Cuturi et al., “Computational optimal transport: With applications to data science,” *Foundations and Trends® in Machine Learning*, vol. 11, no. 5-6, pp. 355–607, 2019.

[12] F.-P. Paty and M. Cuturi, “Subspace robust wasserstein distances,” in *International Conference on Machine Learning*. PMLR, 2019, pp. 5072–5081.

[13] J. Wang, R. Gao, and Y. Xie, “Two-sample test using projected wasserstein distance: Breaking the curse of dimensionality,” *arXiv preprint arXiv:2010.11970*, 2020.

[14] N. V. Smirnov, “On the estimation of the discrepancy between empirical curves of distribution for two independent samples,” *Bull. Math. Univ. Moscou*, vol. 2, no. 2, pp. 3–14, 1939.
[15] F. Wilcoxon, “Probability tables for individual comparisons by ranking methods,” *Biometrics*, vol. 3, no. 3, pp. 119–122, 1947.
[16] A. Wald and J. Wolfowitz, “On a test whether two samples are from the same population,” *The Annals of Mathematical Statistics*, vol. 11, no. 2, pp. 147–162, 1940.
[17] P. J. Bickel, “On some asymptotically nonparametric competitors of hotelling’s t² 1,” *The Annals of Mathematical Statistics*, pp. 160–173, 1965.
[18] M. L. Puri and P. K. Sen, “On a class of multivariate multisample rank-order tests,” *Sankhyā: The Indian Journal of Statistics, Series A*, pp. 353–376, 1966.
[19] P. Chaudhuri, “On a geometric notion of quantiles for multivariate data,” *Journal of the American Statistical Association*, vol. 91, no. 434, pp. 862–872, 1996.
[20] S. Ghosh, *Multivariate analysis, design of experiments, and survey sampling*. CRC Press, 1999.
[21] R. Y. Liu and K. Singh, “A quality index based on data depth and multivariate rank tests,” *Journal of the American Statistical Association*, vol. 88, no. 421, pp. 252–260, 1993.
[22] M. Hallin, D. Paindaveine *et al.*, “Rank-based optimal tests of the adequacy of an elliptic varma model,” *Annals of statistics*, vol. 32, no. 6, pp. 2642–2678, 2004.
[23] M. Hallin and D. Paindaveine, “Parametric and semiparametric inference for shape: the role of the scale functional,” *Statistics & Decisions*, vol. 24, no. 3, pp. 327–350, 2006.
[24] M. Hallin *et al.*, “On distribution and quantile functions, ranks and signs in rd,” *ECARES Working Papers*, 2017.
[25] V. Chernozhukov, A. Galichon, M. Hallin, M. Henry *et al.*, “Monge–kantorovich depth, quantiles, ranks and signs,” *Annals of Statistics*, vol. 45, no. 1, pp. 223–256, 2017.
[26] R. J. McCann *et al.*, “Existence and uniqueness of monotone measure-preserving maps,” *Duke Mathematical Journal*, vol. 80, no. 2, pp. 309–324, 1995.
[27] P. Ghosal and B. Sen, “Multivariate ranks and quantiles using optimal transportation and applications to goodness-of-fit testing,” *arXiv preprint arXiv:1905.05340*, 2019.