Entropy-regularized optimal transport on multivariate normal and $q$-normal distributions

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Distance and divergence of the probability measures play a central role in statistics, machine learning, and many other related fields. The Wasserstein distance has received much attention in recent years because of its distinctions from other distances or divergences. Although computing the Wasserstein distance is costly, entropy-regularized optimal transport was proposed to approximate the Wasserstein distance computationally efficiently. The purpose of this study is to understand the theoretical aspect of entropy-regularized optimal transport. In this paper, we focus on entropy-regularized optimal transport on multivariate normal distributions and $q$-normal distributions.

We obtain the explicit form of the entropy-regularized optimal transport cost on multivariate normal and $q$-normal distributions; this provides a perspective to understand the effect of entropy regularization, which was previously known only experimentally. Furthermore, we demonstrate how the Wasserstein distance, optimal coupling, geometric structure, and statistical efficiency are affected by entropy regularization in some experiments.

Keywords: Optimal transport; Entropy regularization

1. Introduction

Comparing probability measures is a fundamental problem in statistics and machine learning. A classical way to compare probability measures is the Kullback–Leibler divergence. Let $M$ be a measurable space and $\mu, \nu$ be the probability measure on $M$; then, the Kullback–Leibler divergence is defined as

$$\text{KL}(\mu|\nu) = \int_M d\mu \log \frac{d\mu}{d\nu}.$$

The Wasserstein distance[34], also known as the Earth Mover distance[28], is another way of comparing probability measures. It is a metric on the space of probability measures derived by the mass transportation theory of two probability measures. Informally, optimal transport theory considers an optimal transport plan between two probability measures under a cost function, and the Wasserstein distance is defined by the minimum total transport cost. A significant difference between the Wasserstein distance and the Kullback–Leibler divergence is that the former can reflect metric structure, whereas the latter cannot. The Wasserstein distance can be written as

$$W_p(\mu, \nu) := \left\{ \inf_{\pi \in \Pi(\mu, \nu)} \int_{M \times M} d(x, y)^p d\pi(x, y) \right\}^{\frac{1}{p}},$$

where $d(\cdot, \cdot)$ is a distance function on a measurable metric space $M$, and $\Pi(\mu, \nu)$ denotes the set of probability measures on $M \times M$, whose marginal measures correspond with $\mu$ and $\nu$. In recent years, the application of optimal transport and the Wasserstein distance has been studied in many fields such
as statistics, machine learning, and image processing. For example, [30] generates interpolation of various three-dimensional (3D) objects using the Wasserstein barycenter. In the field of word embedding in natural language processing, [22] embedded each word as an elliptical distribution and the Wasserstein distance was applied between the elliptical distributions. There are many studies on applications of optimal transport to deep learning, including [4][24]. Moreover, [31] analyzed the denoising autoencoder [35] with gradient flow in the Wasserstein space.

In general, however, it is computationally intensive to solve the linear problem for the Wasserstein distance and the optimal coupling of two probability measures. For such a situation, a novel numerical method, entropy regularization, was proposed by [8],

\[ C_\lambda(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^n \times \mathbb{R}^n} c(x, y)\pi(x, y)dxdy - \lambda \text{Ent}(\pi). \]

This is a relaxed formulation of the original optimal transport of a cost function \( c(\cdot, \cdot) \), in which the negative Shannon entropy \(-\text{Ent}(\cdot)\) is used as a regularizer. For a small \( \lambda \), \( C_\lambda(\mu, \nu) \) can approximate the \( p\)-th power of the Wasserstein distance between two discrete probability measures, and it can be computed efficiently by using Sinkhorn’s algorithm[29]. Moreover because of the differentiability of the entropy-regularized optimal transport and the simple structure of Sinkhorn’s algorithm, we can easily compute the gradient of the entropy-regularized optimal transport cost and optimize the parameter of a parametrized probability distribution by using numerical differentiation or automatic differentiation. Then, we can define a differentiable loss function that can be applied to various supervised learning methods [10]. Entropy-regularized optimal transport can be used to approximate not only the Wasserstein distance, but also its optimal coupling as a mapping function. [7] adopted the optimal coupling of the entropy-regularized optimal transport as a mapping function from one domain to another.

Despite the empirical success of the entropy-regularized optimal transport, its theoretical aspect is less understood. [16] studies the expected Wasserstein distance between a probability measure and its empirical version. Similarly, [20] shows the consistency of the entropy-regularized optimal transport cost between two empirical distributions. [27] shows that minimizing the entropy-regularized optimal transport cost between empirical distributions is equivalent to a type of maximum likelihood estimator. [5] considered Wasserstein generative adversarial networks with an entropy regularization. [2] constructed information geometry from the convexity of the entropy-regularized optimal transport cost.

In this study, we generalized the Wasserstein distance between two multivariate normal distributions by entropy regularization. We derived the explicit form of the entropy-regularized optimal transport cost and its optimal coupling, which can be used to analyze the effect of entropy regularization directly. In general, the nonregularized Wasserstein distance between two probability measures and its optimal coupling cannot be expressed in a closed form; however, [9] proved the explicit formula for multivariate normal distributions. Our main theorem is a generalized form of [9]. We obtain an explicit form of the entropy-regularized optimal transport between two multivariate normal distributions. Furthermore, by adopting the Tsallis entropy[33] as the entropy regularization instead of the Shannon entropy, our theorem can be generalized to \( q\)-normal distributions.

Some readers may find it strange to study the entropy-regularized optimal transport for multivariate normal distributions, where the exact (nonregularized) optimal transport has been obtained explicitly. However, we think it is worth studying from several perspectives:

- Normal distributions are the simplest and best-studied probability distributions, and thus it is useful to examine the regularization theoretically in order to infer results for other distributions. In particular, we will partly answer the questions “How much do entropy constraints affect the results?” and “What does it mean to constrain by the entropy?” for the simplest cases. Furthermore, as a first step in constructing a theory for more general probability distributions, in Section 4, we propose a generalization to multivariate \( q\)-normal distributions.
• Because normal distributions are the limit distributions in asymptotic theories using the central limit theorem, studying normal distributions is necessary for the asymptotic theory of regularized Wasserstein distances and estimators computed by them. Moreover, it was proposed to use the entropy-regularized Wasserstein distance to compute a lower bound of the generalization error for a variational autoencoder [5]. The study of the asymptotic behavior of such bounds is one of the expected applications of our results.

• Though this has not yet been proved theoretically, we suspect that entropy regularization is efficient not only for computational reasons, such as the use of the Sinkhorn algorithm, but also in the sense of efficiency in statistical inference. Such a phenomenon can be found in some existing studies, including [3]. Such statistical efficiency is confirmed by some experiments in Section 6.

The remainder of this paper is organized as follows. First, we review some definitions of optimal transport and entropy-regularized optimal transport in Section 2. Then, in Section 3, we provide an explicit form of the entropy-regularized optimal transport cost and its optimal coupling between two multivariate normal distributions. We also extend this result to $q$-normal distributions for Tsallis entropy regularization in Section 4. In Section 5, we study the entropy-regularized Kantorovich estimator, which is defined by the entropy-regularized optimal transport. We analyze how entropy regularization affects the optimal result experimentally in certain sections.

2. Preliminary

In this section, we review some definitions of optimal transport and entropy-regularized optimal transport. These definitions are referred to in [26][34]. In this section, we use a tuple $(M, \Sigma)$ for a set $M$ and $\sigma$-algebra on $M$ and $P(X)$ for the set of all probability measures on a measurable space $X$.

**Definition 2.1 (Pushforward measure).** Given measurable spaces $(M_1, \Sigma_1)$ and $(M_2, \Sigma_2)$, a measure $\mu : \Sigma_1 \to [0, +\infty]$, and a measurable mapping $\varphi : M_1 \to M_2$, the pushforward measure of $\mu$ by $\varphi$ is defined by

$$\forall B \in \Sigma_2, \varphi_# \mu(B) := \mu(\varphi^{-1}(B)).$$

**Definition 2.2 (Optimal transport map).** Consider a measurable space $(M, \Sigma)$ and let $c : M \times M \to \mathbb{R}_+$ denote a cost function. Given $\mu, \nu \in P(M)$, we call $\varphi : M \to M$ the optimal transport map if $\varphi$ realizes the infimum of

$$\inf_{\varphi :\#\mu=\nu} \int_M c(x, \varphi(x)) d\mu(x).$$

This problem was originally formalized by [21]. However, the optimal transport map does not always exist. Then, Kantorovich considered a relaxation of this problem in [14].

**Definition 2.3 (Coupling).** Given $\mu, \nu \in P(M)$, the coupling of $\mu$ and $\nu$ is a probability measure on $M \times M$ that satisfies

$$\forall A \in \Sigma, \pi(A \times M) = \mu(A), \quad \pi(M \times A) = \nu(A).$$
**Definition 2.4 (Kantorovich problem).** The Kantorovich problem is defined as finding a coupling $\pi$ of $\mu$ and $\nu$ that realizes the infimum of
\[
\int_{M \times M} c(x,y) d\pi(x,y).
\]

Hereafter, let $\Pi(\mu, \nu)$ be the set of all couplings of $\mu$ and $\nu$. When we adopt a distance function as the cost function, we can define the Wasserstein distance.

**Definition 2.5 (Wasserstein distance).** Given $p \geq 1$, a measurable metric space $(M, \Sigma, d)$ and $\mu, \nu \in \mathcal{P}(M)$ with a finite $p$-th moment, the $p$-Wasserstein distance between $\mu$ and $\nu$ is defined as
\[
W_p(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \left( \int_{M \times M} d(x,y)^p d\pi(x,y) \right)^{\frac{1}{p}}.
\]

Now, we review the definition of entropy-regularized optimal transport on $\mathbb{R}^n$.

**Definition 2.6 (entropy-regularized optimal transport).** Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$, $\lambda > 0$, and let $\pi(x,y)$ be the density function of the coupling of $\mu$ and $\nu$, whose reference measure is the Lebesgue measure. We define the entropy-regularized optimal transport cost as
\[
C_\lambda(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^n \times \mathbb{R}^n} c(x,y)\pi(x,y) dxdy - \lambda \text{Ent}(\pi),
\]
where $\text{Ent}(\cdot)$ denotes the Shannon entropy of a probability measure:
\[
\text{Ent}(\pi) = -\int_{\mathbb{R}^n \times \mathbb{R}^n} \pi(x,y) \log \pi(x,y) dxdy.
\]

There is another variation in entropy-regularized optimal transport defined by the relative entropy instead of the Shannon entropy:
\[
\tilde{C}_\lambda(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^n \times \mathbb{R}^n} c(x,y)\pi(x,y) dxdy + \lambda \text{KL}(\pi|d\mu \otimes d\nu).
\]

This is definable even when $\Pi(\mu, \nu)$ includes a coupling that is not absolutely continuous with respect to the Lebesgue measure. We note that when both $\mu$ and $\nu$ are absolutely continuous, the infimum is attained by the same $\pi$ for $C_\lambda$ and $\tilde{C}_\lambda$, and it depends only on $\mu$ and $\nu$. In the following part of the paper, we assume the absolute continuity of $\mu, \nu$, and $\pi$ with respect to the Lebesgue measure for well-defined entropy-regularization.

### 3. Entropy-regularized optimal transport between multivariate normal distributions

In this section, we provide a rigorous solution of entropy-regularized optimal transport between two multivariate normal distributions. Throughout this section, we adopt the squared Euclidean distance $\|x - y\|^2$ as the cost function. To prove our theorem, we start by expressing $C_\lambda$ using mean vectors and covariance matrices. The following lemma is a known result; for example, see [9].
Lemma 3.1. Let $X \sim P, Y \sim Q$ be two random variables on $\mathbb{R}^n$ with means $\mu_1, \mu_2$ and covariance matrices $\Sigma_1, \Sigma_2$, respectively. If $\pi(x, y)$ is a coupling of $P$ and $Q$, we have

$$\int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|^2 \pi(x, y) dxdy = \|\mu_1 - \mu_2\|^2 + \text{tr} \{\Sigma_1 + \Sigma_2 - 2\text{Cov}(X, Y)\}. \quad (1)$$

Proof. Without loss of generality, we can assume $X$ and $Y$ are centralized, because

$$\int \|(x - \mu_1) - (y - \mu_2)\|^2 \pi(x, y) dxdy = \int \|x - y\|^2 \pi(x, y) dxdy - \|\mu_1 - \mu_2\|^2.$$

Therefore, we have

$$\int \|x - y\|^2 \pi(x, y) dxdy = E[\|X - Y\|^2] = E[\text{tr}\{(X - Y)(X - Y)^T\}]$$

$$= \text{tr} \{\Sigma_1 + \Sigma_2 - 2\text{Cov}(X, Y)\}.$$

By adding $\|\mu_1 - \mu_2\|^2$, we obtain (1). \qed

Lemma 3.1 shows that $\int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|^2 \pi(x, y) dxdy$ can be parameterized by the covariance matrices $\Sigma_1, \Sigma_2, \text{Cov}(X, Y)$. Because $\Sigma_1$ and $\Sigma_2$ are fixed, the infinite-dimensional optimization of the coupling $\pi$ is a finite-dimensional optimization of covariance matrix $\text{Cov}(X, Y)$.

We prepare the following lemma to prove Theorem 3.3.

Lemma 3.2. Under a fixed mean and covariance matrix, the probability measure that maximizes the entropy is a multivariate normal distribution.

Lemma 3.2 is a particular case of the principle of maximum entropy [12], and the proof can be found in [17] Theorem 3.1.

Theorem 3.3. Let $P \sim \mathcal{N}(\mu_1, \Sigma_1), Q \sim \mathcal{N}(\mu_2, \Sigma_2)$ be two multivariate normal distributions. The optimal coupling $\pi$ of $P$ and $Q$ of the entropy-regularized optimal transport

$$C_\lambda(P, Q) = \inf_{\pi \in \Pi(P, Q)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|^2 \pi(x, y) dxdy - 4\lambda \text{Ent}(\pi). \quad (*)$$

is expressed as

$$\pi \sim \mathcal{N}^\star \left( \left( \mu_1, \mu_2 \right), \left( \Sigma_1 \Sigma_\lambda \Sigma_1 \right) \right)$$

where

$$\Sigma_\lambda := \Sigma_1^{1/2} (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2} \Sigma_1^{-1/2} - \lambda I.$$

Furthermore, $C_\lambda(P, Q)$ can be written as

$$C_\lambda(P, Q) = \|\mu_1 - \mu_2\|^2 + \text{tr}(\Sigma_1 + \Sigma_2 - 2(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2})$$

$$- 2\lambda \log |(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2} - \lambda I| - 2\lambda n \log(2\pi \lambda) - 4\lambda n \log(2\pi) - 2\lambda n \quad (2)$$
and the relative entropy version can be written as
\[
\tilde{C}_\lambda(P, Q) = C_\lambda(P, Q) + 2\lambda \log |\Sigma_1||\Sigma_2| + 4\lambda n\{\log(2\pi) + 1\}.
\]

We note that we use the regularization parameter $4\lambda$ in (\*) for the sake of simplicity.

**Proof.** Although the first half of the proof can be derived directly from Lemma 3.2, we provide a proof of this theorem by Lagrange calculus, which will be used later for the extension to $q$-normal distributions. Now, we define an optimization problem that is equivalent to the entropy-regularized optimal transport as follows:

\[
\begin{align*}
\text{minimize} & \quad \int \|x - y\|^2 \rho(x, y) dx dy - 4\lambda \text{Ent}(\rho) \\
\text{subject to} & \quad \int \rho(x, y) dx = q(y) \quad \forall \quad y \in \mathbb{R}^n, \\
& \quad \int \rho(x, y) dy = p(x) \quad \forall \quad x \in \mathbb{R}^n.
\end{align*}
\]

(3)

Here, $p(x)$ and $q(y)$ are probability density functions of $P$ and $Q$, respectively. Let $\alpha(x), \beta(y)$ be Lagrange multipliers that correspond to the above two constraints. The Lagrangian function of (3) is defined as

\[
L(\pi, \alpha, \beta) := \int \|x - y\|^2 \rho(x, y) dx dy + 4\lambda \int \rho(x, y) \log \rho(x, y) dx dy \\
- \int \alpha(x) \rho(x, y) dx dy + \int \alpha(x) p(x) dx \\
- \int \beta(y) \rho(x, y) dy dy + \int \beta(y) q(y) dy.
\]

(4)

Taking the functional derivative of (4) with respect to $\pi$, we obtain

\[
\delta L(\pi, \alpha, \beta) = \int \left(\|x - y\|^2 + 4\lambda \log \rho(x, y) - \alpha(x) - \beta(y)\right) \delta \rho(x, y) dx dy.
\]

By the fundamental lemma of calculus of variations, we have

\[
\pi(x, y) \propto \exp \left(\alpha(x) + \beta(y) - \frac{\|x - y\|^2}{4\lambda}\right).
\]

(5)

Here, $\alpha(x), \beta(y)$ are determined from the constraints (3). We can assume that $\rho$ is a 2n-variate normal distribution, because for a fixed covariance matrix $\text{Cov}(X, Y)$, $-\text{Ent}(\rho)$ takes the infimum when the coupling $\rho$ is a multivariate normal distribution by Lemma 3.2. Therefore, we can express $\rho$ by using $z = (x^T, y^T)^T$ and a covariance matrix $\Sigma := \text{Cov}(X, Y)$ as

\[
\rho(x, y) \propto \exp \left\{-\frac{1}{2} z^T \left(\Sigma_1 \Sigma_2^T \Sigma_2\right)^{-1} z\right\}.
\]
Putting
\[
\begin{pmatrix}
\hat{\Sigma}_1 & \hat{\Sigma} \\
\hat{\Sigma}^T & \hat{\Sigma}_2
\end{pmatrix} = \left(\Sigma_1 \Sigma \Sigma^T \Sigma_2\right)^{-1},
\]
we write
\[
-\frac{1}{2} z^T \left(\Sigma_1 \Sigma \Sigma^T \Sigma_2\right)^{-1} z = -\frac{1}{2} \left(x^T y^T\right) \left(\hat{\Sigma}_1 \hat{\Sigma} \hat{\Sigma}^T \hat{\Sigma}_2\right) \begin{pmatrix} x \\ y \end{pmatrix}
= -\frac{1}{2} x^T \hat{\Sigma}_1 x - \frac{1}{2} y^T \hat{\Sigma}_2 y - x^T \hat{\Sigma}_y.
\tag{6}
\]
According to block matrix inversion formula [25], \(\hat{\Sigma} = -\Sigma_1^{-1} \Sigma A^{-1}\) holds, where \(A := \Sigma_2 - \Sigma^T \Sigma_1^{-1} \Sigma\) is positive definite. Then, comparing the term \(x^T y\) between (5) and (6), we obtain \(\Sigma_1^{-1} \Sigma A^{-1} = \frac{1}{2} \lambda I\) and
\[
2\lambda \Sigma_1^{-1} \Sigma = A = \Sigma_2 - \Sigma^T \Sigma_1^{-1} \Sigma.
\]
Here, \(\Sigma_1^{-1} \Sigma = \Sigma^T \Sigma_1^{-1}\) holds, because \(A\) is a symmetric matrix and thus we obtain
\[
\lambda \Sigma_1^{-1} \Sigma + \lambda \Sigma^T \Sigma_1^{-1} = \Sigma_2 - \Sigma^T \Sigma_1^{-1} \Sigma.
\]
Completing the square of the above equation, we obtain
\[
(\Sigma_1^{-1/2} (\Sigma + \lambda I) \Sigma_1^{1/2})^T (\Sigma_1^{-1/2} (\Sigma + \lambda I) \Sigma_1^{1/2}) = \Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I \tag{7}
\]
Let \(Q\) be an orthogonal matrix; then, (7) can be solved as
\[
\Sigma_1^{-1/2} (\Sigma + \lambda I) \Sigma_1^{1/2} = Q (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2}.
\]
We rearrange the above equation as follows:
\[
\Sigma_1^{1/2} (\Sigma_1^{-1} \Sigma) \Sigma_1^{1/2} + \lambda I = Q (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2}.
\]
Because the left terms and \((\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2}\) are all symmetric positive definite, we can conclude that \(Q\) is the identity matrix by the uniqueness of the polar decomposition. Finally, we obtain
\[
\Sigma = \Sigma_1^{1/2} (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2} \Sigma_1^{-1/2} - \lambda I =: \Sigma_{\lambda}.
\]
We obtain (2) by the direct calculation of \(C_\lambda\) using Lemma 3.1 with this \(\Sigma_{\lambda}\). \qed

Finally, we show how entropy regularization behaves in two simple experiments. We calculate the entropy-regularized optimal transport cost \(\mathcal{N} \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix} , \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \right)\) and \(\mathcal{N} \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix} , \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix} \right)\) in the original version and relative entropy version in Figure 1. We separate the entropy-regularized optimal transport cost into the transport cost term and regularization term and display both of them. The left panel shows the original version. The transport cost is always positive and the entropy regularization term can take both signs in general; then, the sign and total cost depend on their balance. The right panel shows the relative entropy version, which always takes a non-negative value and monotonically increases. We note that the transport cost as a function of \(\lambda\) is bounded, whereas the entropy regularization is not. Then, the larger the regularization parameter \(\lambda\), the greater the influence of entropy regularization over the total cost.
Theorem 3.3 shows that the optimal coupling of two normal distributions is also a multivariate normal distribution. It is reasonable that as $\lambda \downarrow 0$, $\Sigma_\lambda$ converges to $\Sigma_1/2(\Sigma_1/2^2\Sigma_1^{1/2})^{1/2}\Sigma_1^{-1/2}$, which is equal to the original optimal coupling of non-regularized optimal transport and as $\lambda \rightarrow \infty$, $\Sigma_\lambda$ converges to $0$.

This is a special case of the following corollary. The larger $\lambda$ becomes, the less correlated the optimal coupling is. We visualized this behavior by computing the optimal couplings of two one-dimensional normal distributions in Figure 2.

**Corollary 3.3.1.** Let $\nu_{\lambda,1} \leq \nu_{\lambda,2} \leq \ldots \leq \nu_{\lambda,n}$ be the eigenvalues of $\Sigma_\lambda$; then, $\nu_{\lambda,i}$ monotonically decreases with $\lambda$ for any $i \in \{1, 2, \ldots, n\}$.

**Proof.** Because $\Sigma_1^{-1/2}\Sigma_\lambda\Sigma_1^{1/2} = (\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2} + \lambda^2I)^{1/2} - \lambda I$ has the same eigenvalues as $\Sigma_\lambda$, if we let $\{\nu_{0,i}\}$ be the eigenvalues of $\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2}$, $\nu_{\lambda,i} = \sqrt{\nu_{0,i} + \lambda^2} - \lambda$, which is a monotonically decreasing function of the regularization parameter $\lambda$. 

It is known that a specific Riemannian metric can be defined in the space of multivariate normal distributions, which induces the Wasserstein distance [32]. To understand the effect of entropy regularization, we illustrate how entropy regularization deforms this geometric structure in Figure 3. Here, we generate various multivariate normal distributions $\{N(0, \Sigma_{r,\theta})\}$, where $\Sigma_{r,\theta}$ is defined as

$$\Sigma_{r,\theta} = \begin{pmatrix} \cos \theta - \sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}^T \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{r} \end{pmatrix} \begin{pmatrix} \cos \theta - \sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$

For $r$ and $\theta$ evenly spaced over intervals $[0.1, 1]$ and $[0, \pi/2]$, respectively, we obtain $10 \times 10$ multivariate normal distributions, and each pairwise distance is computed by $\tilde{C}_\lambda$. Finally, we apply multidimensional scaling to project them into a plane (see Figure 3). We can see entropy regularization deforming the geometric structure of the space of multivariate normal distributions. The deformation for distributions close to the isotopic normal distribution is more sensitive to the change in $\lambda$. 

**Figure 1.** Graph of the entropy-regularized optimal transport cost between $N\left((0,0),\left(\begin{array}{c}1 \\ 0\end{array}\right)\right)$ and $N\left((0,0),\left(\begin{array}{c}2 \\ -1\end{array}\right)\right)$ with respect to $\lambda$ from 0 to 10.
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**Figure 2.** Contours of density functions of the entropy-regularized optimal coupling of \( \mathcal{N}(0, 1) \) and \( \mathcal{N}(5, 2) \) in three different parameters \( \lambda = 0.1, 1, 10 \). All of the optimal couplings are two-variate normal distributions.

**Figure 3.** Multidimensional scaling of multivariate normal distributions. The pairwise dissimilarities are given by the square root of the entropy-regularized optimal transport cost \( \tilde{C}_\lambda \) for three different regularization parameters \( \lambda = 0, 0.01, 0.05 \). Each ellipse in the figure represents a contour of the density function \( \{ \mathcal{N}(0, \Sigma_{\tau, \theta}) \} \).

The following corollary states that if we allow orthogonal transformations of two multivariate normal distributions with fixed covariance matrices, then the minimum and maximum of \( C_\lambda \) are attained when \( \Sigma_1 \) and \( \Sigma_2 \) are diagonalizable by the same orthogonal matrix or, equivalently, when the ellipsoidal contours of the two density functions are aligned with the same orthogonal axes.

**Corollary 3.3.2.** With the same settings as in Theorem 3.3, fix \( \mu_1, \mu_2, \Sigma_1, \) and all eigenvalues of \( \Sigma_2 \). When \( \Sigma_1 \) is diagonalized as \( \Sigma_1 = \Gamma \Lambda_1^\downarrow \Gamma^\top \), where \( \Lambda_1^\downarrow \) is the diagonal matrix of the eigenvalues of \( \Sigma_1 \) in descending order and \( \Gamma \) is an orthogonal matrix,

(i) \( C_\lambda(P, Q) \) is minimized by \( \Sigma_2 = \Gamma \Lambda_2^\downarrow \Gamma \), and

(ii) \( C_\lambda(P, Q) \) is maximized by \( \Sigma_2 = \Gamma \Lambda_2^\uparrow \Gamma \).
where $\Lambda_1^\downarrow$ and $\Lambda_2^\uparrow$ are the diagonal matrices of the eigenvalues of $\Sigma_2$ in descending and ascending order, respectively. Therefore, neither the minimizer nor the maximizer depends on the choice of $\lambda$.

**Proof.** Because $\mu_1, \mu_2, \Sigma_1$, and all eigenvalues of $\Sigma_2$ are fixed,

$$C_\lambda(P, Q) = -2\text{tr}\left( (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2} \right) - \frac{\lambda}{2} \log |(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \lambda^2 I)^{1/2} - \lambda I| + \text{(constant)}$$

$$= \sum_{i=1}^{n} -2(\nu_i + \lambda^2)^{1/2} - \frac{\lambda}{2} \log \{(\nu_i + \lambda^2)^{1/2} - \lambda\} + \text{(constant)}$$

$$= \sum_{i=1}^{n} g_\lambda(\log(\nu_i)) + \text{(constant)}$$

where $\nu_1 \leq \cdots \leq \nu_n$ are the eigenvalues of $\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2}$ and

$$g_\lambda(x) := -2(e^x + \lambda^2)^{1/2} - \frac{\lambda}{2} \log \{e^x + \lambda^2\}.$$ Note that $g_\lambda(x)$ is a concave function, because

$$g_\lambda''(x) = -\frac{e^x(4e^x + 7\lambda^2)}{8(e^x + \lambda^2)^{3/2}} < 0.$$ Let $\nu_i^{\downarrow\downarrow} \leq \cdots \leq \nu_i^{\downarrow\uparrow}$ and $\nu_i^{\uparrow\downarrow} \leq \cdots \leq \nu_i^{\uparrow\uparrow}$ be the eigenvalues of $\Lambda_1^\downarrow \Lambda_2^\downarrow$ and $\Lambda_1^\uparrow \Lambda_2^\uparrow$, respectively. By Exercise 6.5.3 of citeposi or Theorem 6.13 and Corollary 6.14 of citehiai2014,

$$(\log(\nu_i^{\downarrow\downarrow})) \prec (\log(\nu_i)) \prec (\log(\nu_i^{\downarrow\uparrow})),$$

Here, for $(a_i), (b_i) \in \mathbb{R}^n$ such that $a_1 \geq \cdots \geq a_n$ and $b_1 \geq \cdots \geq b_n$, $(a_i) \prec (b_i)$ means

$$\sum_{i=1}^{k} a_i \leq \sum_{i=1}^{k} b_i \text{ for } k = 1, \ldots, n - 1, \text{ and } \sum_{i=1}^{n} a_i = \sum_{i=1}^{n} b_i$$

and $(a_i)$ is said to be majorized by $(b_i)$. Because $g_\lambda(x)$ is concave,

$$g_\lambda(\log(\nu_i^{\downarrow\downarrow})) \prec^w g_\lambda(\log(\nu_i)) \prec^w g_\lambda(\log(\nu_i^{\downarrow\uparrow})),$$

where $\prec^w$ represents weak supermajorization, i.e., $(a_i) \prec^w (b_i)$ means

$$\sum_{i=k}^{n} a_i \geq \sum_{i=k}^{n} b_i \text{ for } k = 1, \ldots, n$$

(see Theorem 5.A.1 of [19], for example). Therefore,

$$\sum_{i=1}^{n} g_\lambda(\log(\nu_i^{\downarrow\downarrow})) \geq \sum_{i=1}^{n} g_\lambda(\log(\nu_i)) \geq \sum_{i=1}^{n} g_\lambda(\log(\nu_i^{\downarrow\uparrow})).$$
As in case (i) (or (ii)), the eigenvalues of $\Sigma_1^{-1/2}\Sigma_2\Sigma_1^{-1/2}$ correspond to the eigenvalues of $\Lambda_1\Lambda_2^T$ (or $\Lambda_1\Lambda_2^T$, respectively), the corollary follows.

Note that a special case of Corollary 3.3.2 for the ordinary Wasserstein metric ($\lambda = 0$) has been studied in the context of fidelity and the Bures distance in quantum information theory. See Lemma 3 of [18]. Their proof is not directly applicable to our generalized result; thus, we used another approach to prove it.

4. Extension to Tsallis entropy regularization

In this section, we consider a generalization of entropy-regularized optimal transport. We now focus on the Tsallis entropy[33], which is a generalization of the Shannon entropy and appears in nonequilibrium statistical mechanics. We show that the optimal coupling of Tsallis entropy-regularized optimal transport between two $q$-normal distributions is also a $q$-normal distribution. We start by recalling the definition of the $q$-exponential function and $q$-logarithmic function based on [33].

Definition 4.1. Let $q$ be a real parameter and let $u > 0$. The $q$-logarithmic function is defined as

$$\log_q(u) := \begin{cases} \frac{1}{1-q}(u^{1-q} - 1) & \text{if } q \neq 1, \\ \log(u) & \text{if } q = 1 \end{cases}$$

and the $q$-exponential function is defined as

$$\exp_q(u) := \begin{cases} [1 + (1-q)u]^{\frac{1}{1-q}} & \text{if } q \neq 1, \\ \exp(u) & \text{if } q = 1 \end{cases}$$

Definition 4.2. Let $q < 1$ or $1 < q < 1 + \frac{2}{n}$; an $n$-variate $q$-normal distribution is defined by two parameters: $\mu \in \mathbb{R}^n$ and a positive definite matrix $\Sigma$, and its density function is

$$f(x) := \frac{1}{C_q(\Sigma)} \exp_q \left( -(x - \mu)^T \Sigma^{-1} (x - \mu) \right),$$

where $C_q(\Sigma)$ is a normalizing constant. $\mu$ and $\Sigma$ are called the location vector and scale matrix, respectively.

In the following, we write the multivariate $q$-normal distribution $N_q(\mu, \Sigma)$. We note the property of the $q$-normal distribution changes in accordance with $q$. The $q$-normal distribution has an unbounded support for $1 < q < \frac{2}{n}$ and a bounded support for $q < 1$. The second moment exists for $q < 1 + \frac{2}{n+2}$, and the covariance becomes $\frac{1}{2+2(n+2)(1-q)} \Sigma$. We remark that each $n$-variate $\left(1 + \frac{2}{\nu+n}\right)$-normal distribution is equivalent to an $n$-variate $t$-distribution with $\nu$ degrees of freedom,

$$\frac{\Gamma[(\nu+n)/2]}{\Gamma(\nu/2)\nu^{n/2}\pi^{n/2}} \sqrt{1 + \frac{1}{\nu}(x - \mu)^T \Sigma^{-1} (x - \mu)}^{-(\nu+n)/2},$$

for $1 < q < 1 + \frac{2}{n+2}$ and an $n$-variate normal distribution for $q \downarrow 1$. 
**Definition 4.3.** Let $p$ be a probability density function. The Tsallis entropy is defined as

$$S_q(p) := \int p(x) \log_q \frac{1}{p(x)} dx = \frac{1}{q-1} \left( 1 - \int p(x)^q dx \right).$$

Then, the Tsallis entropy-regularized optimal transport is defined as

$$\minimize \int \|x - y\|^2 \pi(x, y) dxdy - 2\lambda S_q(\pi)$$
subject to

$$\int \pi(x, y) dx = q(y) \text{ for } \forall y \in \mathbb{R}^n,$$

$$\int \pi(x, y) dy = p(x) \text{ for } \forall x \in \mathbb{R}^n.$$ (8)

The following lemma is a generalization of the maximum entropy principle for the Shannon entropy shown in [6] Section 2.

**Lemma 4.4.** Let $P$ be a centered $n$-dimensional probability measure with a fixed covariance matrix $\Sigma$; the maximizer of the Renyi $\alpha$-entropy

$$\frac{1}{1 - \alpha} \log \int f(x)^\alpha dx$$
under the constraint is $N_{2-\alpha}(0, ((n + 2)\alpha - n)\Sigma)$ for $\frac{n}{n+2} < \alpha < 1$.

We note that the maximizers of the Renyi $\alpha$-entropy and the Tsallis entropy with $q = \alpha$ coincide; thus, the above lemma also holds for the Tsallis entropy. This is mentioned, for example, in [23], Chapter 9.

To prove Theorem 4.6, we use the following property of multivariate $t$-distributions, which is summarized in [15] Chapter 1.

**Lemma 4.5.** Let $X$ be a random vector following an $n$-variate $t$-distribution with degree of freedom $\nu$. Considering a partition of the mean vector $\mu$ and scale matrix $\Sigma$, such as

$$X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}, \quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix},$$ (9)

$X_1$ follows a $p$-variate $t$-distribution with degree of freedom $\nu$, mean vector $\mu_1$, and scale matrix $\Sigma_{11}$, where $p$ is the dimension of $X_1$.

Recalling the correspondence of the parameter of multivariate $q$-normal distribution and the degree of freedom of the multivariate $t$-distribution $q = 1 + \frac{2}{n+2}$, we can obtain the following corollary.

**Corollary 4.5.1.** Let $X$ be a random vector following an $n$-variate $q$-normal distribution for $1 < q < 1 + \frac{2}{n+2}$. Consider a partition of the mean vector $\mu$ and scale matrix $\Sigma$ in the same way as in (9). Then, $X_1$ follows a $p$-variate $\left(1 + \frac{2(1-q)}{2-(n-p)(q-1)}\right)$-normal distribution with mean vector $\mu_1$ and scale matrix $\Sigma_{11}$, where $p$ is the dimension of $X_1$. 
Theorem 4.6. Let \( P \sim N_q(\mu_1, \Sigma_1), Q \sim N_q(\mu_2, \Sigma_2) \) be \( n \)-variate \( q \)-normal distributions for \( 1 < q < 1 + \frac{2}{n+2} \) and \( \tilde{q} = -\frac{2(q-1)}{2-2n(q-1)} \); consider the Tsallis entropy-regularized optimal transport

\[
C_\lambda(P, Q) = \inf_{\pi \in \Pi(P, Q)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|^2 \pi(x, y) dxdy - 2\lambda S_{1+\tilde{q}}(\pi).
\]

Then, there exists a unique \( \tilde{\lambda} = \tilde{\lambda}(q, \Sigma_1, \Sigma_2, \lambda) \in \mathbb{R}_+ \) such that the optimal coupling \( \pi \) of the entropy-regularized optimal transport is expressed as

\[
\pi \sim N_{1-\tilde{q}} \left( \left( \begin{array}{c} \mu_1 \\ \mu_2 \end{array} \right), \left( \begin{array}{cc} \Sigma_1 & \Sigma_\tilde{\lambda} \\
\Sigma_\tilde{\lambda}^T & \Sigma_2 \end{array} \right) \right),
\]

where

\[
\Sigma_\tilde{\lambda} := \Sigma_1^{1/2} (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \tilde{\lambda}^2 I)^{1/2} \Sigma_1^{-1/2} - \tilde{\lambda} I.
\]

Proof. The proof proceeds in a similar way as in Theorem 3.3. Let \( \alpha \in L(P) \) and \( \beta \in L(Q) \) be the Lagrangian multipliers. Then, the Lagrangian function \( L(\pi, \alpha, \beta) \) of (8) is defined as

\[
L(\pi, \alpha, \beta) := \int \|x - y\|^2 \pi(x, y) dxdy - 2\lambda \left\{ \frac{1}{\tilde{q}} \left( 1 - \int \pi(x, y)^{1+\tilde{q}} dxdy \right) \right\} \\
- \int \alpha(x) \pi(x, y) dxdy + \int \alpha(x) p(x) dx \\
- \int \beta(y) \pi(x, y) dxdy + \int \beta(y) q(y) dy
\]

and the extremum of the Tsallis entropy-regularized optimal transport is obtained by the functional derivative with respect to \( \pi \),

\[
\pi(x, y) = \left( \frac{\tilde{q}}{2(\tilde{q} + 1)\lambda} \left( -\alpha(x) - \beta(y) + \|x - y\|^2 \right) \right)^{\frac{1}{\tilde{q}}}. 
\]

Here \( \alpha \) and \( \beta \) are quadratic polynomials by Lemma 4.4. To separate the normalizing constant, we introduce a constant \( c \in \mathbb{R}_+ \), and \( \pi \) can be written as

\[
\pi(x, y) = c^{\frac{1}{\tilde{q}}} \left( \tilde{\alpha}(x) + \tilde{\beta}(y) + \frac{\tilde{q}}{2c(\tilde{q} + 1)\lambda} \|x - y\|^2 \right)^{\frac{1}{\tilde{q}}},
\]

with quadratic functions \( \tilde{\alpha}(x) \) and \( \tilde{\beta}(y) \).

Let \( \tilde{\lambda} = \frac{c(\tilde{q} + 1)\lambda}{\tilde{q}} > 0 \). Then, by the same argument as in the proof of Theorem 3.3 and using Corollary 4.5.1, we obtain the scale matrix of \( \pi \) as

\[
\Sigma = \left( \begin{array}{cc} \Sigma_1 & \Sigma_\tilde{\lambda} \\
\Sigma_\tilde{\lambda}^T & \Sigma_2 \end{array} \right),
\]

where

\[
\Sigma_\tilde{\lambda} := \Sigma_1^{1/2} (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} + \tilde{\lambda}^2 I)^{1/2} \Sigma_1^{-1/2} - \tilde{\lambda} I.
\]
Let $z = (x^T, y^T)^T$ and $K_{\tilde{q}} = \int (1 + z^T z)^{\frac{1}{2}} dz$; $\pi$ can be written as

$$\pi(x, y) = \frac{1}{K_{\tilde{q}|\Sigma|}} (1 + z^T \Sigma^{-1} z)^{\frac{1}{2}}.$$  

The constant $c$ is determined by

$$\frac{1}{K_{\tilde{q}|\Sigma|}} = c^{\frac{1}{2}}. \quad (10)$$

We will show that the above equation has a unique solution. Let $\{\tau\}_{i=1}^n$ be the eigenvalues of $(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2})^{1/2}$; $|\Sigma|$ can be expressed as $\prod_{i=1}^{2n} 2\tilde{\lambda}(\sqrt{\tau_i^2 + \tilde{\lambda}^2} - \tilde{\lambda})$. We consider

$$f(c) = \log(c^{\frac{1}{2}} K_{\tilde{q}|\Sigma|})$$

$$= \frac{1}{q} \log c + \sum_{i=1}^{2n} \log(\sqrt{\tau_i^2 + \tilde{\lambda}^2} - \tilde{\lambda}) + 2n \log(2\tilde{\lambda}) + \log K_{\tilde{q}}.$$

Because $\tilde{q} < 0$, $f(c)$ is a monotonic decreasing function and $\lim_{c\downarrow 0} f(c) = \infty$, $\lim_{c\to\infty} f(c) = -\infty$, (10) has a unique positive solution and $\tilde{\lambda}$ is determined uniquely. \qed

5. Entropy-regularized Kantorovich estimator

Many estimators are defined by minimizing the divergence or distance $\rho$ between probability measures, that is, $\arg\min_\mu \rho(\mu, \nu)$ for a fixed $\nu$. When $\rho$ is the Kullback–Leibler divergence, the estimator corresponds to the maximum likelihood estimator. When $\rho$ is the Wasserstein distance, the following estimator is called the minimum Kantorovich estimator, according to [26]. In this section, we consider a probability measure $Q^*$ that minimizes $C_\lambda(P, Q)$ for a fixed $P$ over $\mathcal{P}_2(\mathbb{R}^n)$, the set of all probability measures on $\mathbb{R}^n$ with finite second moment that are absolutely continuous with respect to the Lebesgue measure. In other words, we define the entropy-regularized Kantorovich estimator $\arg\min_{Q \in \mathcal{P}_2(\mathbb{R}^n)} C_\lambda(P, Q)$. The entropy-regularized Kantorovich estimator for discrete probability measures was studied in [3] Theorem 2. We obtain the entropy-regularized Kantorovich estimator for continuous probability measures in the following theorem:

**Theorem 5.1.** For a fixed $P \in \mathcal{P}_2(\mathbb{R}^n)$,

$$Q^* = \arg\min_{Q \in \mathcal{P}_2(\mathbb{R}^n)} C_\lambda(P, Q)$$

exists and its density function can be written as

$$dQ^* = dP * \phi_\lambda,$$

where $\phi_\lambda(x)$ is a density function of $N(0, \frac{1}{2} I)$, and $*$ denotes the convolution operator.
Lemma 5.2. The dual problem of entropy-regularized optimal transport can be written as

\[ A_\lambda(P, Q) = \sup_{\alpha \in L_1(P)} \int \alpha(x)p(x)dx + \int \beta(y)q(y)dy \]

\[ - \lambda \int \exp \left\{ \frac{\alpha(x) + \beta(y) - \|x - y\|^2}{\lambda} \right\} dxdy. \tag{11} \]

Moreover, \( A_\lambda(P, Q) = C_\lambda(P, Q) \) holds.

Proof. Recalling (4),

\[ \inf_{\pi \in \Pi(P, Q)} \sup_{\alpha \in L_1(P)} \int \alpha(x)p(x)dx + \int \beta(y)q(y)dy \]

\[ \sup_{\beta \in L_1(Q)} \inf_{\pi \in \Pi(P, Q)} L(\pi, \alpha, \beta) \]

holds by the strong duality. In the above equality, \( \inf_{\pi \in \Pi(P, Q)} L(\pi, \alpha, \beta) \) is achieved by

\[ \pi^*(x, y) \propto \exp \left\{ \frac{\alpha(x) + \beta(y) - \|x - y\|^2}{\lambda} \right\}. \]

Then, we can obtain

\[ L(\pi^*, \alpha, \beta) = \int \alpha(x)p(x)dx + \int \beta(y)q(y)dy - \lambda \int \exp \left\{ \frac{\alpha(x) + \beta(y) - \|x - y\|^2}{\lambda} \right\} dxdy. \tag{13} \]

Finally, we obtain (11) by substituting (13) into (12).

Now, we prove Theorem 5.1.

Proof. Let \( Q^* \) be the minimizer of \( \min_Q C_\lambda(P, Q) \). Applying Lemma 5.2, there exist \( \alpha^* \in L_1(P) \) and \( \beta^* \in L_1(Q^*) \) such that

\[ C_\lambda(P, Q^*) = A_\lambda(P, Q^*) = \int \alpha^*(x)p(x)dx + \int \beta^*(y)q^*(y)dy \]

\[ - \lambda \int \exp \left\{ \frac{\alpha^*(x) + \beta^*(y) - \|x - y\|^2}{\lambda} \right\} dxdy. \]

Now, \( A_\lambda(P, Q^*) \) is the minimum value of \( A_\lambda \), such that the variation \( \delta A_\lambda(P, Q^*) \) is always zero. Then,

\[ \delta A_\lambda(P, Q^*) = \int \beta^*(y)\delta q^*(y)dy = 0 \Rightarrow \beta^* \equiv 0 \]

holds and the optimal coupling of \( P, Q \) can be written as

\[ \pi^*(x, y) = \exp \left\{ \frac{\alpha^*(x) + \beta^*(y)}{\lambda} - \frac{\|x - y\|^2}{\lambda} \right\} \]

\[ = \exp \left\{ \frac{\alpha^*(x)}{\lambda} \right\} \exp \left\{ - \frac{\|x - y\|^2}{\lambda} \right\}. \]
Moreover, we can obtain a closed form of $\alpha^*(x)$ as follows from the equation $\int \pi(x,y)dy = p(x)$

$$\frac{\alpha^*(x)}{\lambda} = \log p(x) - \log \int \exp \left\{-\frac{\|x-y\|^2}{\lambda}\right\} dy = \log p(x) - \frac{n}{2} \log(\pi \lambda).$$

Then, by calculating the marginal distribution of $\pi(x,y)$ with respect to $x$, we can obtain

$$q^*(y) = \int \frac{1}{(\pi \lambda)^{n/2}} \exp \left\{-\frac{\|x-y\|^2}{\lambda}\right\} p(x)dx = (p * \phi_\lambda)(y). \tag{14}$$

Therefore, we conclude that a probability measure $Q$ that minimizes $C_\lambda(P,Q)$ is expressed as (14). \hfill \Box

It should be noted that when $P$ in Theorem 5.1 are multivariate normal distributions, $Q^*$ and $P$ are simultaneously diagonalizable by a direct consequence of the theorem. This is consistent with the result of Corollary 3.3.2(1) for minimization when all eigenvalues are fixed.

We can determine that the entropy-regularized Kantorovich estimator is a measure that convolved with an isotropic multivariate normal distribution scaled by the regularization parameter $\lambda$. This is similar to the idea of prior distributions in the context of Bayesian inference. Applying Theorem 5.1, the entropy-regularized Kantorovich estimator of the multivariate normal distribution $\mathcal{N}(\mu, \Sigma)$ is $\mathcal{N}(\mu, \Sigma + \frac{\lambda}{2} I)$. Figure 4 shows estimated multivariate normal distributions visualized by ellipses defined by $\{x : x^T \Sigma^{-1} x = 1.386\}$, where $\Sigma^{-1}$ is its precision matrix and 1.386 is the median of the chi-squared distribution with two degrees of freedom. We compare the results for the regularization parameters $\lambda = 0.01, 0.1, 1, 10, 100$. As $\lambda$ increases, the entropy-regularized Kantrovich estimator becomes more isotropic and the variance becomes much larger than the original distribution.

6. Numerical experiments

In this section, we introduce experiments that show the statistical efficiency of entropy regularization in Gaussian settings. We consider two different setups.
6.1. Estimation of covariance matrices

We provide a covariance estimation method based on entropy-regularized optimal transport. Let \( P = \mathcal{N}(\mu, \Sigma) \) be an \( n \)-variate normal distribution. We define an entropy-regularized Kantorovich estimator \( \hat{P}_\lambda \), that is,

\[
\hat{P}_\lambda = \arg \min_Q C_\lambda(P, Q).
\]

We generate some samples from \( \mathcal{N}(\mu, \Sigma) \) and estimate the mean and covariance matrix. We compare the maximum likelihood estimator \( \hat{P}_{\text{MLE}} = \mathcal{N}(\hat{\mu}_{\text{MLE}}, \hat{\Sigma}_{\text{MLE}}) \) and \( \hat{P}_\lambda \) with respect to the prediction error

\[
\text{KL}(P, \hat{P}_{\text{MLE}}), \quad \text{KL}(P, \hat{P}_\lambda).
\]

In our experiment, the dimension \( n \) is set to 30 and the sample size set to 60. The experiment proceeds as follows.

1. Obtain a random sample of size 60 from \( \mathcal{N}(0, \Sigma) \) and its sample covariance matrix \( \hat{\Sigma} \).
2. Obtain the entropy-regularized minimum Kantorovich estimator of \( \hat{\Sigma} \).
3. Compute the prediction error between \( \Sigma \) and the barycenter obtained in step 3.
4. Repeat the above steps 1000 times and obtain a confidence interval of the prediction error.

Table 1 shows the confidence interval of the prediction error of the minimum Kantorovich estimator. We can see that the prediction error is smaller than the maximum likelihood estimator under adequately small \( \lambda \).

6.2. Wasserstein barycenter

A barycenter with respect to the Wasserstein distance is definable\[1\] and is widely used for image interpolation and 3D object interpolation tasks with entropy regularization \[3,30\].

**Definition 6.1.** Let \( \{Q_i\}_{i=1}^m \) be a set of probability measures in \( \mathcal{P}(\mathbb{R}^n) \). The barycenter with respect to \( C_\lambda \) is defined as

\[
\arg \min_{P \in \mathcal{P}(\mathbb{R}^n)} \sum_{i=1}^m C_\lambda(P, Q_i).
\]

Now, we restrict \( P \) and \( \{Q_i\}_{i=1}^n \) to be multivariate normal distributions and apply our theorem to illustrate the effect of entropy regularization.

The experiment proceeds as follows.

1. Obtain a random sample of size 60 from \( \mathcal{N}(0, \Sigma) \) and its sample covariance matrix \( \hat{\Sigma} \).
2. Repeat step 1 three times and obtain \( \{\hat{\Sigma}_i\}_{i=1}^3 \).
3. Obtain the barycenter of \( \{\hat{\Sigma}_i\}_{i=1}^3 \).
4. Compute the prediction error between \( \Sigma \) and the barycenter obtained in step 3.
5. Repeat the above steps 100 times and obtain a confidence interval of the prediction error.

We show the results for several values of the regularization parameter \( \lambda \) in Table 2. We can see the same behavior of the prediction error as in Table 1.
6.3. Gradient descent on $\text{Sym}_+(n)$

We use a gradient descent method to compute the barycenter. Applying the gradient descent method to the loss function defined by the Wasserstein distance was proposed in [22]. This idea is extendable to entropy-regularized optimal transport. The detailed algorithm is shown below. Because $C_\lambda(P,Q)$ is a function of a positive definite matrix, we used a manifold gradient descent algorithm on the manifold of positive definite matrices.

We review the manifold gradient descent algorithm used in our numerical experiment. Let $\text{Sym}_+(n)$ be the manifold of $n$-dimensional positive definite matrices. We require a formula for a gradient operator and the inner product of $\text{Sym}_+(n)$ in the gradient descent algorithm. In this paper, we use the following inner product from citeposi Chapter 6. For a fixed $X \in \text{int}(\text{Sym}_+(n))$, we define an inner product of $\text{Sym}_+(n)$ as

$$g_X(Y,Z) = \text{tr} \left( YX^{-1}ZX^{-1} \right), \; Y, Z \in \text{Sym}_+(n),$$  \hspace{1cm} (15)

(15) is the best choice in terms of the convergence speed according to [13]. Let $f : \text{Sym}_+(n) \to \mathbb{R}$ be a differential matrix function. Then, the induced gradient of $f$ under (15) is

$$\text{grad} \; f(X) = X \left( \frac{\partial f(X)}{\partial X} \right) X.$$

We consider the updating step after obtaining the gradient of $f$. $\text{grad} \; f(X)$ is an element of the tangent space, and we have to project it to $\text{Sym}_+(n)$. This projection map is called a retraction. It is known that the Riemannian metric $g_X$ leads to the following retraction:

$$\exp_X x = X \exp(X^{-1}x),$$

where $\exp$ is the matrix exponential. Then, the corresponding gradient descent method becomes as shown in Algorithm 1.

Algorithm 1 Gradient descent on the manifold of positive definite matrices

```
Input: f(X)
initilize X
while not convergence do
  $\eta$ : step size
  grad ← $X \left( \frac{\partial f(X)}{\partial X} \right) X$
  $X \leftarrow \exp_X (\eta \text{grad}) = X \exp(\eta X^{-1} \text{grad})$
end while
Output: X
```

Algorithm 2 Newton–Schulz method

```
Input: A ∈ \text{Sym}_+(n), \epsilon > 0
Y ← \frac{A}{(1+\epsilon\|A\|)} \; , \; Z ← I
while not convergence do
  T ← (3I - ZY)/2
  Y ← YT \; ; \; Z ← TZ
end while
Output: $\sqrt{(1+\epsilon\|A\|)}Y$
```

6.4. Approximate the matrix square root

To compute the gradient of the square root of a matrix in the objective function, we approximate it using the Newton–Schulz method[11], which can be implemented by matrix operations as shown in Algorithm 2. It is amenable to automatic differentiation, such that we can easily apply the gradient descent method to our algorithm. We can determine that the prediction error of $\hat{P}_\lambda$ is significantly smaller than $\hat{P}_{\text{MLE}}$ when the value of the regularization parameter $\lambda$ is adequately selected.

7. Conclusion

In this paper, our main theorem shows the entropy-regularized optimal transport cost between two multivariate normal distributions and the explicit form of the optimal coupling. Then, using this explicit
Table 1. Average prediction error of MLE and entropy-regularized Kantorovich estimator with 95% confidential interval

| $\lambda$  | KL($P, \hat{P}_W$)     |
|------------|------------------------|
| 0 (MLE)    | 10.69 ± 0.112          |
| 0.01       | 8.973 ± 0.087          |
| 0.1        | 4.180 ± 0.033          |
| 0.5        | 3.093 ± 0.010          |
| 1.0        | 5.075 ± 0.009          |

Table 2. Average prediction error of the entropy-regularized barycenter with 95% confidential interval

| $\lambda$  | KL($P, \hat{P}_W$)     |
|------------|------------------------|
| 0.001      | 4.875 ± 0.035          |
| 0.01       | 4.887 ± 0.036          |
| 0.025      | 5.710 ± 0.536          |
| 0.05       | 7.570 ± 0.772          |

form, we demonstrate experimentally how entropy regularization affects the Wasserstein distance, the optimal coupling, and the geometric structure of multivariate normal distributions.

Furthermore, we propose the Tsallis entropy-regularized optimal transport and expand our main theorem to multivariate $q$-normal distributions. We also derive the entropy-regularized Kantorovich estimator of a probability measure, which is the convolution of a multivariate normal distribution and its own density function. Our experiments show that the entropy-regularized Kantorovich estimator of the covariance matrix and the Wasserstein barycenter of multivariate normal distributions outperforms the maximum likelihood estimator in the prediction error for adequately selected $\lambda$.

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