From Optimal Transport to Discrepancy

Sebastian Neumayer* Gabriele Steidl*

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Abstract

A common way to quantify the „distance” between measures is via their discrepancy, also known as maximum mean discrepancy (MMD). Discrepancies are related to Sinkhorn divergences $S_\varepsilon$ with appropriate cost functions as $\varepsilon \to \infty$. In the opposite direction, if $\varepsilon \to 0$, Sinkhorn divergences approach another important distance between measures, namely the Wasserstein distance or more generally optimal transport „distance”. In this chapter, we investigate the limiting process for arbitrary measures on compact sets and Lipschitz continuous cost functions. In particular, we are interested in the behavior of the corresponding optimal potentials $\hat{\varphi}_\varepsilon$, $\hat{\psi}_\varepsilon$ and $\hat{\varphi}_K$ appearing in the dual formulation of the Sinkhorn divergences and discrepancies, respectively. While part of the results are known, we provide rigorous proofs for some relations which we have not found in this generality in the literature. Finally, we demonstrate the limiting process by numerical examples and show the behavior of the distances when used for the approximation of measures by point measures in a process called dithering.

1. Introduction

The approximation of probability measures based on their discrepancies is a well examined problem in approximation and complexity theory [29, 34, 38]. Discrepancies appear in a wide range of applications, e.g., in the derivation of quadrature rules [38], the construction of designs [14], image dithering and representation [10] [25] [42] [46], see also Fig. 1 generative adversarial networks [13] and multivariate statistical testing [18] [26] [27]. In the last two applications they are also called kernel based maximum mean discrepancies (MMDs).

On the other hand, optimal transport (OT) „distances” and in particular Wasserstein distances became very popular for tackling various problems in imaging sciences, graphics or machine learning [13]. There exists a large amount of papers both on the theory and applications of OT, for image dithering with Wasserstein distances see, e.g., [7] [23] [30].

Recently, regularized versions of OT for a more efficient numerical treatment, known as Sinkhorn divergences [12], were used as replacement of OT. For appropriately related transport cost functions and discrepancy kernels, the Sinkhorn divergences interpolate between the OT distance if the parameter goes to zero and the discrepancy if it goes to infinity [19]. In this chapter, the convergence behavior is examined for general measures on compact sets.

*Department of Mathematics, Technische Universität Kaiserslautern, Paul-Ehrlich-Str. 31, D-67663 Kaiserslautern, Germany, \{name\}@mathematik.uni-kl.de.

1Department of Mathematics, Technische Universität Kaiserslautern, Paul-Ehrlich-Str. 31, D-67663 Kaiserslautern, Germany, \{name\}@mathematik.uni-kl.de.
sets. Since cost functions applied in practice are mainly Lipschitz, we restrict our attention to such costs. This simplifies some proofs, since the theorem of Arzela-Ascoli can be utilized. To make the paper self-contained, we provide most of the proofs although some of them are not novel and the corresponding papers are cited in the context. For estimating approximation rates when approximating measures by those of certain subsets, see, e.g., [8, 16, 20, 38], the dual form of the discrepancy, respectively of the (regularized) Wasserstein distance, plays an important role. Therefore, we are interested in the properties of the dual optimal potentials for varying regularization parameters. In Proposition 5.8 we prove that the optimal dual potentials converge uniformly to certain functions as $\varepsilon \to \infty$. Then, in Corollary 6.2 we see that the normalized difference of these limiting functions coincides with the optimal potential in the dual form of the discrepancy if the cost function and the kernel are appropriately related. This behavior is underlined by a numerical example.

This chapter is organized as follows: Section 2 recalls basic results on measures, on the Kullback-Leibler (KL) divergence and from Convex Analysis. In Section 3 we introduce discrepancies, in particular their dual formulation. Since they rely on positive definite kernels, we have a closer look at positive definite and conditionally positive definite kernels. Optimal transport and in particular Wasserstein distances are considered in Section 4. In Section 5 we investigate the limiting processes for the KL regularized OT distances, when the regularization parameter goes to zero or infinity. Some results in Proposition 5.3 are novel in this generality, Proposition 5.8 seems to be new as well. Remark 5.2 highlights why the KL divergence should be preferred as regularizer instead of the (neg)-entropy when dealing with non discrete measures. KL regularized OT does not fulfill $\text{OT}_\varepsilon(\mu, \mu) = 0$, which motivates the definition of the Sinkhorn divergence $S_\varepsilon$ in Section 6. Further, we prove $\Gamma$-convergence to the discrepancy as $\varepsilon \to \infty$ if the cost function of the Sinkhorn divergence
is adapted to the kernel defining the discrepancy. Section 2.1 underlines the results on the limiting process by numerical example. Further, we provide an example on the dithering of the Gaussian when Sinkhorn divergences with respect to different regularization parameters ε are involved. Finally, conclusions and directions of future research are given in Section 8.

2. Preliminaries

**Measures** Let $X$ be a compact Polish space (separable, complete metric space) with metric $d_X$. By $B(X)$ we denote the Borel σ-algebra on $X$ and by $M(X)$ the linear space of all finite signed Borel measures on $X$, i.e., the space of all $µ: B(X) → R$ satisfying $µ(X) < ∞$ and for any sequence $\{B_k\}_{k ∈ N} ⊂ B(X)$ of pairwise disjoint sets the relation

$$µ(\bigcup_{k=1}^{∞} B_k) = \sum_{k=1}^{∞} µ(B_k).$$

In the following, the subset of non-negative measures is denoted by $M^+(X)$. The support of a measure $µ$ is defined as the closed set

$$supp(µ) := \{x ∈ X : B ⊂ X open, x ∈ B ⇒ µ(B) > 0\}.$$

The total variation measure of $µ ∈ M(X)$ is defined by

$$|µ|(B) := \sup \left\{ \sum_{k=1}^{∞} |µ(B_k)| : \bigcup_{k=1}^{∞} B_k = B, B_k pairwise disjoint \right\}.$$

With the norm $∥µ∥_M = |µ|(X)$ the space $M(X)$ becomes a Banach space. By $C(X)$ we denote the Banach space of continuous real-valued functions on $X$ equipped with the norm $∥φ∥_{C(X)} := \max_{x ∈ X} |φ(x)|$. The space $M(X)$ can be identified via Riesz’ representation theorem with the dual space of $C(X)$ and the weak-* topology on $M(X)$ gives rise to the weak convergence of measures, i.e., a sequence $\{µ_k\}_{k ∈ N} ⊂ M(X)$ converges weakly to $µ$ and we write $µ_k ⇀ µ$, if

$$\lim_{k → ∞} \int_X φ dµ_k = \int_X φ dµ \quad for all φ ∈ C(X).$$

For a non-negative, finite measure $µ$ and $p ∈ [1, ∞)$, let $L_p(X, µ)$ be the Banach space (of equivalence classes) of complex-valued functions with norm

$$∥f∥_{L_p(X, µ)} = \left( ∫_X |f|^p dµ \right)^{\frac{1}{p}} < ∞.$$

A measure $ν ∈ M(X)$ is absolutely continuous with respect to $µ$ and we write $ν ≪ µ$ if for every $A ∈ B(X)$ with $µ(A) = 0$ we have $ν(A) = 0$. If $µ, ν ∈ M^+(X)$ satisfy $ν ≪ µ$, then the Radon-Nikodym derivative $σ_µ ∈ L_1(X, ν)$ (also denoted by $\frac{dν}{dµ}$) exists and $ν = σ_µ dµ$. Further, $µ, ν ∈ M(X)$ are mutually singular and we write $µ ⊥ ν$ if two disjoint sets $X_µ, X_ν ∈ B(X)$ exist such that $X = X_µ \cup X_ν$ and for every $A ∈ B(X)$ we have $µ(A) = µ(A \cap X_µ)$ and $ν(A) = ν(A \cap X_ν)$. For any $µ, ν ∈ M^+(X)$, there exists a unique Lebesgue decomposition of $µ$ with respect to $ν$ given by $µ = σ_µ ν + µ⊥$, where $σ_1 ∈ L_1(X, ν)$ and $µ⊥ ⊥ ν$. 

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By $\mathcal{P}(\mathbb{X})$ we denote the set of Borel probability measures on $\mathbb{X}$, i.e., non-negative Borel measures with $\mu(\mathbb{X}) = 1$. This set is weakly compact, i.e., compact with respect to the weak-$*$ topology. Note that there is an ambiguity in the notation since the above usual weak-$*$ convergence is called weak convergence in stochastics. In Section 4 we introduce a metric on $\mathcal{P}(\mathbb{X})$ such that it becomes a Polish space.

**Convex Analysis** The following can be found, e.g., in [3]. Let $V$ be a real Banach space with dual $V^*$, i.e., the space of real-valued continuous linear functionals on $V$. We use the notation $\langle v, x \rangle = v(x)$, $v \in V^*$, $x \in V$. For $F: V \to (-\infty, +\infty]$, the domain of $F$ is given by $\text{dom} F := \{ x \in V : F(x) \in \mathbb{R} \}$. If $\text{dom} F \neq \emptyset$, then $F$ is called proper. The subdifferential of $F: V \to (-\infty, +\infty]$ at a point $x_0 \in \text{dom} F$ is defined as

$$\partial F(x_0) := \{ v \in V^* : F(x) \geq F(x_0) + \langle v, x - x_0 \rangle \},$$

and $\partial F(x_0) = \emptyset$ if $x_0 \notin \text{dom} F$. The Fenchel (convex) conjugate $F^*: V^* \to (-\infty, +\infty]$ is given by

$$F^*(v) = \sup_{x \in V} \{ \langle v, x \rangle - F(x) \}.$$

If $F \to ( -\infty, +\infty]$ is convex and lower semi-continuous (lsc) at $x \in \text{dom} F$, then

$$v \in \partial F(x) \iff x \in \partial F^*(v). \quad (1)$$

By $\Gamma(V)$ we denote the set of proper, convex, lsc functions mapping from $V$ to $(-\infty, +\infty]$. Let $W$ be another real Banach space. Then, for $F \in \Gamma(V)$, $G \in \Gamma(W)$ and a linear, bounded operator $A: V \to W$ with the property that there exists $x \in \text{dom} F$ such that $G$ is continuous at $Ax$, the following Fenchel-Rockafellar duality relation is fulfilled

$$\sup_{x \in V} \{ -F(-x) - G(Ax) \} = \inf_{w \in W} \{ F^*(A^*w) + G^*(w) \}, \quad (2)$$

see [17] Thm. 4.1, p. 61], where we consider

$$\sup_{x \in V} \{ -F(-x) - G(Ax) \} = - \inf_{x \in V} \{ F(-x) + G(Ax) \}$$

as primal problem with respect to the notation in [17]. If the optimal (primal) solution $\hat{x}$ exists, it is related to any optimal (dual) solution $\hat{w}$ by

$$A\hat{x} \in \partial G^*(\hat{w}), \quad (3)$$

see [17] Prop. 4.1].

**Kullback-Leibler divergence** A function $f: [0, +\infty) \to [0, +\infty]$ is called entropy function, if it is convex, lsc and $\text{dom} f \cap (0, +\infty) \neq \emptyset$. The corresponding recession constant is given by $f'_\infty = \lim_{x \to \infty} f'(x)$. For every $\mu, \nu \in \mathcal{M}^+(\mathbb{X})$ with Lebesgue decomposition $\mu = \sigma \mu + \mu^\perp$, the $f$-divergence is defined as

$$D_f(\mu, \nu) = \int_{\mathbb{X}} f \circ \sigma \, d\nu + f'_\infty \mu^\perp(\mathbb{X}). \quad (4)$$
It fulfills $D_f(\mu, \nu) \geq 0$ for all $\mu, \nu \in \mathcal{M}^+(X)$ with equality if and only if $\mu = \nu$, and is in general neither symmetric nor satisfies a triangle inequality. The associated mapping $D_f: \mathcal{M}^+(X) \times \mathcal{M}^+(X) \to [0, +\infty]$ is jointly convex and weakly lsc, see [32, Cor. 2.9]. The $f$-divergence can be written in the dual form

$$D_f(\mu, \nu) = \sup_{\varphi \in C(X)} \int_X \varphi \, d\mu - \int_X f^* \circ \varphi \, d\mu,$$

see [32, Rem. 2.10]. Hence, $D_f(\cdot, \nu)$ is the convex conjugate of $H: C(X) \to \mathbb{R}$ given by $H(\varphi) := \int_X f^* \circ \varphi \, d\nu$. If $f^*$ is differentiable, we directly deduce from (1) that

$$\varphi \in \partial_\mu D_f(\mu, \nu) \iff \mu = \nabla H(\varphi) \iff \mu = \nabla f^* \circ \varphi \nu. \quad (5)$$

In the following, we focus on the Shannon-Boltzmann entropy function and its convex conjugate given by

$$f(x) = x \log(x) - x + 1 \quad \text{and} \quad f^*(x) = \exp(x) - 1$$

with the agreement $0 \log 0 = 0$. The corresponding $f$-divergence is the Kullback-Leibler divergence $KL: \mathcal{M}^+(X) \times \mathcal{M}^+(X) \to [0, +\infty]$. For $\mu, \nu \in \mathcal{M}^+(X)$ with existing Radon-Nikodym derivative $\sigma = \frac{d\mu}{d\nu}$ of $\mu$ with respect to $\nu$, formula (4) can be written as

$$KL(\mu, \nu) := \int_X \log(\sigma) \, d\mu + \nu(X) - \mu(X). \quad (6)$$

If the above Radon-Nikodym derivative does not exist, (4) implies $KL(\mu, \nu) = +\infty$. For $\mu, \nu \in \mathcal{P}(X)$ the last two summands in (6) cancel each other. In particular, we have for discrete measures $\mu = \sum_{j=1}^n \mu_j \delta_{x_j}$ and $\nu = \sum_{j=1}^n \nu_j \delta_{x_j}$ with $\mu_j, \nu_j \geq 0$ and $\sum_{j=1}^n \mu_j = \sum_{j=1}^n \nu_j = 1$ that

$$KL(\mu, \nu) = \sum_{j=1}^n \log \left( \frac{\mu_j}{\nu_j} \right) \mu_j.$$

Further, the KL divergence is strictly convex with respect to the first variable. Due to the convex conjugate pairing

$$H(\varphi) = \int_X \exp(\varphi) - 1 \, d\nu \quad \text{and} \quad H^*(\mu) = KL(\mu, \nu), \quad (7)$$

the derivative relation (5) simplifies to

$$\varphi \in \partial_\mu KL(\mu, \nu) \iff \mu = e^\varphi \nu \iff \varphi = \log \left( \frac{d\mu}{d\nu} \right). \quad (8)$$

Finally, note that the KL divergence and the total variation norm $\| \cdot \|_M$ are related by the Pinsker inequality $\|\mu - \nu\|^2_M \leq KL(\mu, \nu)$. 

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3. Discrepancies

In this section, we introduce the notation of discrepancies and have a closer look at (conditionally) positive definite kernels. In particular, we emphasize how conditionally positive definite kernels can be modified to positive definite ones.

Let $\sigma_X \in \mathcal{M}(X)$ be non-negative with $\text{supp}(\sigma_X) = X$. The given definition of discrepancies is based on symmetric, positive definite, continuous kernels. There is a close relation to general discrepancies related to measures in $\mathcal{B}(X)$, see [38]. Recall that a symmetric function $K : X \times X \to \mathbb{R}$ is positive definite if for any finite number $n \in \mathbb{N}$ of points $x_j \in X$, $j = 1, \ldots, n$, the relation

$$
\sum_{i,j=1}^{n} a_i a_j K(x_i, x_j) \geq 0
$$

is satisfied for all $(a_j)_{j=1}^{n} \in \mathbb{R}^n$ and strictly positive definite if strict inequality holds for all $(a_j)_{j=1}^{n} \neq 0$. Assuming that $K \in C(X \times X)$ is symmetric, positive definite, we know by Mercer’s theorem [11, 35, 45] that there exists an orthonormal basis $\{\phi_k : k \in \mathbb{N}\}$ of $L^2(X, \sigma_X)$ and non-negative coefficients $\{\alpha_k\}_{k \in \mathbb{N}} \in \ell_1$ such that $K$ has the Fourier expansion

$$
K(x, y) = \sum_{k=0}^{\infty} \alpha_k \phi_k(x) \overline{\phi_k(y)}
$$

with absolute and uniform convergence of the right-hand side. If $\alpha_k > 0$ for some $k \in \mathbb{N}_0$, the corresponding function $\phi_k$ is continuous. Every function $f \in L^2(X, \sigma_X)$ has a Fourier expansion

$$
f = \sum_{k=0}^{\infty} \hat{f}_k \phi_k, \quad \hat{f}_k := \int_X f \phi_k \, d\sigma_X.
$$

Moreover, for $k \in \mathbb{N}_0$ with $\alpha_k > 0$, the Fourier coefficients of $\mu \in \mathcal{P}(X)$ are well-defined by

$$
\hat{\mu}_k := \int_X \phi_k \, d\mu.
$$

The kernel $K$ gives rise to a reproducing kernel Hilbert space (RKHS). More precisely, the function space

$$
H_K(X) := \left\{ f \in L^2(X, \sigma_X) : \sum_{k=0}^{\infty} \alpha_k^{-1} |\hat{f}_k|^2 < \infty \right\}
$$

equipped with the inner product and the corresponding norm

$$
\langle f, g \rangle_{H_K(X)} = \sum_{k=0}^{\infty} \alpha_k^{-1} \hat{f}_k \overline{\hat{g}_k}, \quad \|f\|_{H_K(X)} = \langle f, f \rangle_{H_K(X)}^{\frac{1}{2}}
$$

forms a Hilbert space with reproducing kernel, i.e.,

$$
K(x, \cdot) \in H_K(X) \quad \text{for all } x \in X
$$

$$
f(x) = \langle f, K(x, \cdot) \rangle_{H_K(X)} \quad \text{for all } f \in H_K(X), \ x \in X.
$$

Note that $f \in H_K(X)$ implies $\hat{f}_k = 0$ if $\alpha_k = 0$, in which case we make the convention $\alpha_k^{-1} \hat{f}_k = 0$ in [%10]. Indeed, $H_K(X)$ is the closure of the linear span of $\{K(x_j, \cdot) : x_j \in X\}$.
with respect to the norm \[10\]. The space \(H_K(X)\) is continuously embedded in \(C(X)\) and hence point evaluations in \(H_K(X)\) are continuous. Since the series in \[9\] converges uniformly and the functions \(\phi_k\) are continuous, the function

\[
\|K(x, \cdot)\|_{H_K(X)} = \left\| \sum_{k=0}^{\infty} \alpha_k \phi_k(x) \bar{\phi}_k(\cdot) \right\|_{H_K(X)} = \left( \sum_{k=0}^{\infty} \alpha_k |\phi_k(x)|^2 \right)^{\frac{1}{2}}
\]

is also continuous so that we have \(\int_X \|K(x, \cdot)\|_{H_K(X)} \, d\mu(x) < \infty\). By the definition of Bochner integrals, see \[28\], Prop. 1.3.1, we have for any \(\mu\),

\[
\text{Bochner integrals, see } [28, \text{Prop. 1.3.1}], \text{ we have for any } \mu \in \mathcal{P}(X) \text{ that }
\]

\[
\int_X K(x, \cdot) \, d\mu(x) \in H_K(X).
\]  

(12)

For \(\mu, \nu \in \mathcal{M}(X)\), the discrepancy \(D_K(\mu, \nu)\) is defined as norm of the linear linear operator \(T : H_K \to \mathbb{R}\) with \(\varphi \mapsto \int_X \varphi \, d\xi\),

\[
D_K(\mu, \nu) = \max_{\|\varphi\|_{H_K(X)} \leq 1} \int_X \varphi \, d\xi,
\]  

(13)

where \(\xi := \mu - \nu\), see [22] [38]. If \(\mu_n \rightharpoonup \mu\) and \(\nu_n \rightharpoonup \nu\) as \(n \to \infty\), then also \(\mu_n \otimes \nu_n \rightharpoonup \mu \otimes \nu\). Therefore, the continuity of \(K\) implies that \(\lim_{n \to \infty} D_K(\mu_n, \nu_n) = D_K(\mu, \nu)\). Since

\[
\int_X \varphi \, d\xi = \int_X \langle \varphi, K(x, \cdot) \rangle_{H_K(X)} \, d\xi(x) = \left\langle \varphi, \int_X K(x, \cdot) \, d\xi(x) \right\rangle_{H_K(X)},
\]

we obtain by Schwarz’ inequality that the optimal dual potential (up to the sign) is given by

\[
\hat{\varphi}_K = \frac{\int_X K(x, \cdot) \, d\xi(x)}{\| \int_X K(x, \cdot) \, d\xi(x) \|_{H_K(X)}} = \frac{\int_X K(x, \cdot) \, d\mu(x) - \int_X K(x, \cdot) \, d\nu(x)}{\| K(x, \cdot) \, d\mu(x) - \int_X K(x, \cdot) \, d\nu(x) \|_{H_K(X)}}.
\]  

(14)

In the following, it is always clear from the context if the Fourier transform of the function or the optimal dual function is meant. Further, Riesz’ representation theorem implies

\[
D_K(\mu, \nu) = \max_{\|\varphi\|_{H_K(X)} \leq 1} \int_X \varphi \, d\xi = \left\| \int_X K(x, \cdot) \, d\xi(x) \right\|_{H_K(X)},
\]

so that we conclude by Fubini’s theorem and \[11\] that

\[
D_K^2(\mu, \nu) = \left\| \int_X K(x, \cdot) \, d\xi(x) \right\|^2_{H_K(X)} = \int_{X^2} K \, d(\xi \otimes \xi) = \int_{X^2} K \, d(\mu \otimes \mu) + \int_{X^2} K \, d(\nu \otimes \nu) - 2 \int_{X^2} K \, d(\mu \otimes \nu).
\]  

(15)

By \[9\], we finally get

\[
D_K^2(\mu, \nu) = \sum_{k=0}^{\infty} \alpha_k |\hat{\mu}_k - \hat{\nu}_k|^2,
\]  

(16)

where the summation runs over all \(k \in \mathbb{N}_0\) with \(\alpha_k > 0\).
Kernels. In this paragraph, we want to have a closer look at appropriate kernels. Recall that for symmetric, positive definite kernels $K_i \in C(\mathbb{X} \times \mathbb{X})$, $i = 1, 2$ and $\alpha > 0$, the kernels $\alpha K_1$, $K_1 + K_2$, $K_1 \cdot K_2$ and $\exp(K_1)$ are again positive definite, see [44, Lem. 4.5 - 4.6].

In particular, so-called radial kernels of the form

$$K(x, y) := h(\text{dist}_{\mathbb{X}}(x, y)),$$

where $h: [0, +\infty) \to \mathbb{R}$, are of interest. In the following, the discussion is restricted to compact sets $\mathbb{X}$ in $\mathbb{R}^d$ and the Euclidean distance $\text{dist}_{\mathbb{X}}(x, y) = \|x - y\|$. Many results on positive definite functions on $\mathbb{R}^d$ go back to Schoenberg [43] and Micchelli [36]. For a good overview, we refer to [49], where some of the following statements can be found. Clearly, restricting positive definite kernels on $\mathbb{R}^d$ to compact subsets $\mathbb{X}$ results in positive definite kernels on $\mathbb{X}$. The radial kernels related to the Gaussian, which are quite popular in MMDs, and the inverse multiquadric

$$h(r) = e^{-r^2/c^2} \quad \text{and} \quad h(r) = (c^2 + r^2)^{-p}, \quad c, p > 0,$$

are known to be strictly positive definite on $\mathbb{R}^d$ for every $d \in \mathbb{N}$. Further, the following compactly supported functions $h$ give rise to positive definite functions in $\mathbb{R}^d$:

$$h(r) = (1 - r)^p, \quad p \geq \left\lfloor \frac{d}{2} \right\rfloor + 1,$$

where $[a]$ denotes the largest integer which is not larger than $a \in \mathbb{R}$ and $a_+ := \max(a, 0)$. In connection with Wasserstein distances we are interested in (negative) powers of distances $K(x, y) = \|x - y\|^p$, $p > 0$, related to the functions $h(r) = r^p$. Unfortunately, all these functions are not positive definite! By [17], we know that $\tilde{K}(x, y) = 1 - \|x - y\|$ is positive definite in one dimension $d = 1$. A more general result for the Euclidean distance is given in the following proposition.

**Proposition 3.1.** Let $K(x, y) = -\|x - y\|$. For every compact set $\mathbb{X} \subset \mathbb{R}^d$, there exists a constant $C > 0$ such that the function

$$\tilde{K}(x, y) := C - \|x - y\|$$

is positive definite on $\mathbb{X}$. Further, for $\mu, \nu \in \mathcal{P}(\mathbb{X})$, it holds

$$\mathcal{D}_K^2(\mu, \nu) = \mathcal{D}_{\tilde{K}}^2(\mu, \nu) \quad \text{and} \quad \hat{\phi}_K = \hat{\phi}_{\tilde{K}}.$$

**Proof.** In [24, Cor. 2.15] it was shown that $\tilde{K}$ is positive definite. The rest follows in a straightforward way from [15] and [14] regarding that $\mu$ and $\nu$ are probability measures. \hfill $\square$

Some interesting functions such as negative powers of Euclidean distances or the smoothed distance function $\sqrt{c^2 + \|x - y\|^2}$, $0 < c \ll 1$, are conditionally positive definite. Let $\Pi_{m-1}(\mathbb{R}^d)$ denote the ($d+m-1$)-dimensional space of polynomials on $\mathbb{R}^d$ of absolute degree (sum of exponents) $\leq m - 1$. A function $K: \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ is conditionally positive definite of order $m$ if for all points $x_1, \ldots, x_n \in \mathbb{R}^d$, $n \in \mathbb{N}$, the relation

$$\sum_{i,j=1}^{n} a_i a_j K(x_i, x_j) \geq 0$$

holds for all choices of $a_i \in \mathbb{R}$, $i = 1, \ldots, n$.
Lemma 3.2. Let \( m \) be a positive definite \( m \) \( \sum_{i=1}^{n} a_i P(x_i) = 0 \) for all \( P \in \Pi_{m-1}(\mathbb{R}^d) \).

If strong inequality holds in (18) except for \( a_i = 0 \) for all \( i = 1, \ldots, n \), then \( K \) is called strictly conditionally positive definite of order \( m \). In particular, for \( m = 1 \), the condition (18) relaxes to \( \sum_{i=1}^{n} a_i = 0 \).

The radial kernels related to the following functions are strictly conditionally positive definite of order \( m \) on \( \mathbb{R}^d \):

\[
\begin{align*}
    h(r) &= (-1)^{[\gamma]}(c^2 + r^2)^p, \quad p > 0, p \notin \mathbb{N}, m = [p], \\
    h(r) &= (-1)^{[p/2]}p^p, \quad p > 0, p \notin 2\mathbb{N}, m = [p/2], \\
    h(r) &= (-1)^{k+1}r^{2k} \log(r), \quad k \in \mathbb{N}, m = k + 1,
\end{align*}
\]

where \([a]\) denotes the smallest integer which is not smaller than \( a \in \mathbb{R} \). The first group of functions are called multiquadric and the last group is known as thin plate splines. In connection with Wasserstein distances, the second group of functions is of interest.

By the following lemma, it is easy to turn conditionally positive definite functions into positive definite ones. However, only for conditionally positive definite functions of order \( m = 1 \), the discrepancy remains the same.

**Lemma 3.2.** Let \( \Xi := \{u_k : k = 1, \ldots, N\} \) with \( N := (d+m-1) \) be a set of points such that \( P(u_k) = 0 \) for all \( k = 1, \ldots, N, P \in \Pi_{m-1}(\mathbb{R}^d) \), is only fulfilled for the zero polynomial. Denote by \( \{P_k : k = 1, \ldots, N\} \) the set of Lagrangian basis polynomials with respect to \( \Xi \), i.e., \( P_k(u_j) = \delta_{jk} \). Let \( K \in \mathcal{C}(\Xi \times \Xi) \) be a symmetric conditionally positive definite kernel of order \( m \).

i) Then

\[
\tilde{K}(x, y) = K(x, y) - \sum_{j=1}^{N} P_j(x)K(u_j, y) - \sum_{k=1}^{N} P_k(y)K(x, u_k) + \sum_{j,k=1}^{N} P_j(x)P_k(y)K(u_j, u_k)
\]

is a positive definite kernel.

ii) In particular, we have for \( m = 1, \mu, \nu \in \mathcal{P}(\Xi) \) and any fixed \( u \in \Xi \) that

\[
\tilde{K}(x, y) = K(x, y) - K(u, y) - K(x, u) + K(u, u)
\]

and

\[
\phi^2_K(\mu, \nu) = \phi^2_K(\mu, \nu),
\]

\[
\phi_K = \frac{\int_\Xi K(x, \cdot) \, d\mu(x) - \int_\Xi K(x, \cdot) \, d\nu(x) + c_\nu - c_\mu}{\| \int_\Xi K(x, \cdot) \, d\mu(x) - \int_\Xi K(x, \cdot) \, d\nu(x) + c_\nu - c_\mu \|_{H_K(\Xi)}},
\]

where

\[
c_\mu := \int_\Xi K(x, u) \, d\mu(x) \quad \text{and} \quad c_\nu := \int_\Xi K(x, u) \, d\nu(x).
\]
Proof. Part i) follows by straightforward computation, see also [49, Thm. 10.18]. Concerning Part ii), since $\mu$ and $\nu$ are probability measures, we obtain using (20) that

$$\mathcal{D}_K^2(\mu, \nu) = \int_{\mathcal{X}^2} \tilde{K} \, d(\mu \otimes \mu) + \int_{\mathcal{X}^2} \tilde{K} \, d(\nu \otimes \nu) - 2 \int_{\mathcal{X}^2} \tilde{K} \, d(\mu \otimes \nu)$$

$$+ c_\mu + c_\nu - 2c_\nu + c_\mu + c_\nu - 2c_\mu$$

$$= \int_{\mathcal{X}^2} K \, d(\mu \otimes \mu) + \int_{\mathcal{X}^2} K \, d(\nu \otimes \nu) - 2 \int_{\mathcal{X}^2} K \, d(\mu \otimes \nu) + c_{\mu} + c_{\nu} - 2c_{\nu} + c_{\mu} + c_{\nu} - 2c_{\mu}$$

$$= \mathcal{D}_K^2(\mu, \nu).$$

For the optimal dual potential in (14) related to $\mathcal{D}_K$ we have

$$\hat{\phi}_K = \frac{\int_{\mathcal{X}} \tilde{K}(x, \cdot) \, d\mu(x) - \int_{\mathcal{X}} \tilde{K}(x, \cdot) \, d\nu(x)}{\| \int_{\mathcal{X}} K(x, \cdot) \, d\mu(x) - \int_{\mathcal{X}} K(x, \cdot) \, d\nu(x) \|_{H_K(\mathcal{X})}}$$

$$= \frac{\int_{\mathcal{X}} K(x, \cdot) \, d\mu(x) - \int_{\mathcal{X}} K(x, \cdot) \, d\nu(x) + c_\nu - c_\mu}{\| \int_{\mathcal{X}} K(x, \cdot) \, d\mu(x) - \int_{\mathcal{X}} K(x, \cdot) \, d\nu(x) + c_\nu - c_\mu \|_{H_K(\mathcal{X})}}.$$

\qed

4. Optimal Transport and Wasserstein Distances

The following discussion about optimal transport is based on [1, 13, 41], where many aspects simplify due to the compactness of $\mathcal{X}$ and the assumption that the cost $c$ is Lipschitz continuous. Let $\mu, \nu \in \mathcal{P}(\mathcal{X})$ and $c \in C(\mathcal{X} \times \mathcal{X})$ be a non-negative, symmetric and Lipschitz continuous function. Then, the Kantorovich problem of optimal transport (OT) reads

$$\text{OT}(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X}^2} c \, d\pi,$$

(21)

where $\Pi(\mu, \nu)$ denotes the set of all joint probability measures $\pi$ on $\mathcal{X}^2$ with marginals $\mu$ and $\nu$. In our setting, the OT functional $\pi \mapsto \int_{\mathcal{X}^2} c \, d\pi$ is continuous, and every such minimizer $\hat{\pi}$ is called optimal transport plan. In general, we can not expect the optimal transport plan to be unique. However, if $\mathcal{X}$ is a compact subset of a separable Hilbert space, $c(x, y) = \|x - y\|_H^p$, $p \in (1, \infty)$, and either $\mu$ or $\nu$ is regular, then (21) has a unique solution.

The $c$-transform $\varphi^c \in C(\mathcal{X})$ of $\varphi \in C(\mathcal{X})$ is defined as

$$\varphi^c(y) = \min_{x \in \mathcal{X}} \{ c(x, y) - \varphi(x) \}.$$

Note that $\varphi^c$ has the same Lipschitz constant as $c$. A function $\varphi^c \in C(\mathcal{X})$ is called $c$-concave if it is the $c$-transform of some function $\varphi \in C(\mathcal{X})$.

The dual formulation of the OT problem (21) reads

$$\text{OT}(\mu, \nu) = \max_{(\varphi, \psi) \in C(\mathcal{X})^2} \int_{\mathcal{X}} \varphi \, d\mu + \int_{\mathcal{X}} \psi \, d\nu.$$

(22)

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Any maximizing pair is of the form \((\varphi, \psi) = (\hat{\varphi}, \hat{\psi})\) for some \(c\)-concave function \(\hat{\varphi}\) and fulfills 
\[
\hat{\varphi}(x) + \hat{\varphi}^c(y) = c(x, y) \text{ in } \text{supp}(\hat{\pi}),
\]
where \(\hat{\pi}\) is any optimal transport plan. The function \(\hat{\varphi}\) is called (Kantorovich) potential for the couple \((\mu, \nu)\). If \((\hat{\varphi}, \hat{\psi})\) is an optimal pair, clearly also \((\hat{\varphi} - C, \hat{\psi} + C)\) with \(C \in \mathbb{R}\) is optimal and manipulations outside of \(\text{supp}(\mu)\) and \(\text{supp}(\nu)\) do not change the functional value. But even if we exclude such manipulations, the optimal dual potentials are in general not unique as Example 4.1 shows.

**Example 4.1.** Choose \(X = [0, 1], c(x, y) = |x - y|\), \(\mu = \delta_{0/2} + \delta_{1/2}\) and \(\mu = \delta_{0/1} + \frac{1}{2}\delta_{0.9}/2\). Then, \(\text{OT}(\mu, \nu) = 0.1\) with the unique optimal transport plan \(\hat{\pi} = \frac{1}{2}\delta_{0.0.1} + \frac{1}{2}\delta_{0.1.9}\). Optimal dual potentials are given by

\[
\hat{\varphi}_1(x) = \begin{cases} 
0.1 - x & \text{for } x \in [0, 0.1], \\
x - 0.9 & \text{for } x \in [0.9, 1], \\
0 & \text{else},
\end{cases}
\quad \text{and} \quad
\hat{\varphi}_2(x) = \begin{cases} 
0.2 - x & \text{for } x \in [0, 0.2], \\
x - 0.9 & \text{for } x \in [0.9, 1], \\
0 & \text{else}.
\end{cases}
\]

Clearly, these potentials do not differ only by a constant.

**Remark 4.2.** Note that the space \(C(X)^2\) in the dual problem could also be replaced with \(C(\text{supp}(\mu)) \times C(\text{supp}(\nu))\). Using the Tietze extension theorem, any feasible point of the restricted problem can be extended to a feasible point of the original problem and hence the problems coincide. If the problem is restricted, all other concepts have to be adapted accordingly.

For \(p \in [1, \infty)\), the \(p\)-Wasserstein distance \(W_p\) between \(\mu, \nu \in \mathcal{P}(X)\) is defined by

\[
W_p(\mu, \nu) := \left( \min_{\pi \in \Pi(\mu, \nu)} \int_X \text{dist}(x, y)^p d\pi(x, y) \right)^{\frac{1}{p}}.
\]

It is a metric on \(\mathcal{P}(X)\) which metrizes the weak topology. Indeed, due to compactness of \(X\), we have that \(\mu_k \rightharpoonup \mu\) if and only if \(\lim_{k \to \infty} W_p(\mu_k, \mu) = 0\). Further, it holds that \(\mu_k \to \mu\) and \(\nu_k \to \nu\) implies \(W_p(\mu, \nu) \leq \liminf_{k \to \infty} W_p(\mu_k, \nu_k)\).

For \(1 \leq p \leq q < \infty\) it holds \(W_p \leq W_q\). The distance \(W_1\) is also called Kantorovich-Rubinstein distance or Earth’s mover distance. Here, it holds \(\varphi^c = -\varphi\) and the dual problem reads

\[
W_1(\mu, \nu) = \max_{|\varphi|_{\text{Lip}(X)} \leq 1} \int_X \varphi d\xi, \quad \xi := \mu - \nu,
\]

where the maximum is taken over all Lipschitz continuous functions with Lipschitz constant bounded by 1. This looks similar to the discrepancy \([13]\), but the space of test functions is larger for \(W_1\).

The distance \(W_1\) is related to \(W_p\) by

\[
W_1(\mu, \nu) \leq W_p(\mu, \nu) \leq C W_1(\mu, \nu)^{\frac{1}{p}}
\]

with a constant \(0 \leq C < \infty\) depending on \(\text{diam}(X)\) and \(p\).

Finally, we like to mention that the linearized 2-Wasserstein distance is closely related to the \(H^{-1}\) weighted homogeneous Sobolev norm \([18]\) and appears in the Benamou-Brenier formula of \(W_2\) \([2]\). Non-asymptotic comparisons between the \(W_2\) distance and the \(H^{-1}\) norm controlling \(W_2(\mu, \nu)\) by \(\|\mu - \nu\|_{H^{-1}(X)}\) were given in \([30]\).
5. Regularized Optimal Transport

In this section, we give a self-contained introduction to continuous regularized optimal transport. For $\mu, \nu \in \mathcal{P}(X)$ and $\varepsilon > 0$, regularized OT is defined as

$$\text{OT}_\varepsilon(\mu, \nu) := \min_{\pi \in \Pi(\mu, \nu)} \left\{ \int_{X^2} c \, d\pi + \varepsilon \text{KL}(\pi, \mu \otimes \nu) \right\}. \quad (23)$$

Compared to the original OT problem, we will see in the numerical part that $\text{OT}_\varepsilon$ can be efficiently solved numerically, see also [13]. Moreover, $\text{OT}_\varepsilon$ has the following properties.

**Lemma 5.1.**

i) There exists a unique minimizer $\hat{\pi}_\varepsilon \in \mathcal{P}(X)$ of (23) with finite value.

ii) The function $\text{OT}_\varepsilon$ is weakly continuous and differentiable.

iii) For any $\mu, \nu \in \mathcal{P}(X)$ and $\varepsilon_1, \varepsilon_2 \in [0, \infty]$ with $\varepsilon_1 \leq \varepsilon_2$ it holds

$$\text{OT}_{\varepsilon_1}(\mu, \nu) \leq \text{OT}_{\varepsilon_2}(\mu, \nu).$$

**Proof.**

i): First, note that $\mu \otimes \nu$ is a feasible point and hence the infimum is finite. Existence of minimizers follows since the functional is weakly lsc and $\Pi(\mu, \nu) \subset \mathcal{P}(X^2)$ is weakly compact. Uniqueness follows since $\text{KL}(\cdot, \mu \otimes \nu)$ is strictly convex.

ii): The proof uses the dual formulation in Proposition 5.4, see [19, Prop. 2].

iii): Let $\hat{\pi}_{\varepsilon_2}$ be the minimizer for $\text{OT}_{\varepsilon_2}(\mu, \nu)$. Then, it holds

$$\text{OT}_{\varepsilon_2}(\mu, \nu) = \int_{X^2} c \, d\hat{\pi}_{\varepsilon_2} + \varepsilon_2 \text{KL}(\hat{\pi}_{\varepsilon_2}, \mu \otimes \nu) \geq \int_{X^2} c \, d\hat{\pi}_{\varepsilon_2} + \varepsilon_1 \text{KL}(\hat{\pi}_{\varepsilon_2}, \mu \otimes \nu) \geq \text{OT}_{\varepsilon_1}(\mu, \nu).$$

Note that in special cases, e.g., for absolutely continuous measures, see [6, 31], it is possible to show convergence of the optimal solutions $\hat{\pi}_\varepsilon$ to an optimal solution of $\text{OT}(\mu, \nu)$ as $\varepsilon \to 0$. However, we are not aware of a fully general result. An extension of entropy regularization to unbalanced OT is discussed in [9].

Originally, entropic regularization was proposed in [12] for discrete probability measures with the negative entropy $E$, see also [39],

$$\widetilde{\text{OT}}_\varepsilon(\mu, \nu) := \min_{\pi \in \Pi(\mu, \nu)} \left\{ \int_{X^2} c \, d\pi + \varepsilon E(\pi) \right\}, \quad E(\pi) := \sum_{i,j=1}^n \log(p_{ij})p_{ij} = \text{KL}(\pi, \lambda \otimes \lambda),$$

where $\lambda$ denotes the counting measure. For $\pi \in \Pi(\mu, \nu)$ it is easy to check that

$$E(\pi) = \text{KL}(\pi, \mu \otimes \nu) + \sum_{i,j=1}^n \log(\mu_i \nu_j) \mu_i \nu_j = \text{KL}(\pi, \mu \otimes \nu) + \text{KL}(\mu \otimes \nu, \lambda \otimes \lambda),$$

so that $\text{OT}_\varepsilon(\mu, \nu) = \widetilde{\text{OT}}_\varepsilon(\mu, \nu)$, i.e., the actual regularizer choice does not matter. For non discrete measures, special care is necessary as the following remark shows.
Remark 5.2. \((\text{KL}(\pi, \mu \otimes \nu) \text{ versus } E(\pi) \text{ regularization})\) Since the entropy is only defined for measures with densities, we consider compact sets \(X \subset \mathbb{R}^d\) equipped with the normalized Lebesgue measure \(\lambda\) and \(\mu, \nu \ll \lambda\) with densities \(\sigma_\mu, \sigma_\nu \in L_1(X)\). For \(\pi \ll \lambda \otimes \lambda\) with density \(\sigma_\pi\) the entropy is defined by

\[
E(\pi) = \int_{X^2} \log(\sigma_\pi) \sigma_\pi \, d(\lambda \otimes \lambda) = \text{KL}(\pi, \lambda \otimes \lambda).
\]

Note that for any \(\pi \in \Pi(\mu, \nu)\) we have

\[
\pi \ll \mu \otimes \nu \iff \pi \ll \lambda \otimes \lambda,
\]

where the right implication is straightforward and the left one can be seen as follows: If \(\pi \ll \lambda \otimes \lambda\) with density \(\sigma_\pi \in L_1(X \times X)\), then it holds \(0 = \int_{\{z \in X : \sigma_\mu(z) = 0\}} \int_X \sigma_\pi(x, y) \, dy \, dx\) and consequently \(\sigma_\pi(x, y) = 0\) a.e. on \(\{z \in X : \sigma_\mu(z) = 0\} \times X\) (one can choose any representative of \(\sigma_\mu\)). The same reasoning can be applied for \(X \times \{z \in X : \sigma_\nu(z) = 0\}\). Thus,

\[
\pi = \sigma_\pi(\lambda \otimes \lambda) = \frac{\sigma_\pi(x, y)}{\sigma_\mu(x) \sigma_\nu(y)} (\mu \otimes \nu),
\]

where the quotient is defined as zero if \(\sigma_\mu\) or \(\sigma_\nu\) vanish. Consequently, the left implication also holds true.

If \(\text{KL}(\mu \otimes \nu, \lambda \otimes \lambda) < \infty\), we conclude for any \(\pi \ll \lambda \otimes \lambda\) with \(\pi \in \Pi(\mu, \nu)\) that the following expressions are well-defined

\[
\begin{align*}
\text{KL}(\pi, \lambda \otimes \lambda) - \text{KL}(\mu \otimes \nu, \lambda \otimes \lambda) & = \int_{X^2} \log(\sigma_\pi) \, d\pi - \int_{X^2} \log(\frac{d(\mu \otimes \nu)}{d(\lambda \otimes \lambda)}) \, d(\mu \otimes \nu) \\
& = \text{KL}(\pi, \mu \otimes \nu) + \int_{X^2} \log(\sigma_\mu(x) \sigma_\nu(y)) \, d\pi(x, y) - \int_{X^2} \log(\sigma_\mu(x) \sigma_\nu(y)) \, d\mu(x) \, d\nu(y) \\
& = \text{KL}(\pi, \mu \otimes \nu).
\end{align*}
\]

Consequently, in this case we also have \(\overline{\text{OT}}_\varepsilon(\mu, \nu) = \text{OT}_\varepsilon(\mu, \nu)\). The crux is the condition \(\text{KL}(\mu \otimes \nu, \lambda \otimes \lambda) < \infty\), which is equivalent to \(\mu, \nu\) having finite entropy, i.e., \(\sigma_\mu, \sigma_\nu\) are in a so-called Orlicz space \(L \log L\) [37]. The authors in [10] considered the entropy as regularization (with continuous cost function) and pointed out that \(\overline{\text{OT}}_\varepsilon(\mu, \nu)\) admits a (finite) minimizer exactly in this case. However, we have seen that we can avoid this existence trouble if we regularize with \(\text{KL}(\pi, \mu \otimes \nu)\) instead, which therefore seems to be a more natural choice.

Another possibility is to use quadratic regularization instead, see [33] for more details. In connection with discrepancies, we are especially interested in the limiting case \(\varepsilon \to \infty\). The next proposition is basically known, see [13, 19]. However, we have not found it in this generality in the literature.

**Proposition 5.3.**

i) It holds \(\lim_{\varepsilon \to \infty} \text{OT}_\varepsilon(\mu, \nu) = \text{OT}_\infty(\mu, \nu)\), where

\[
\text{OT}_\infty(\mu, \nu) \colon= \int_{X^2} c \, d(\mu \otimes \nu).
\]
Proposition 5.4. The (pre-)dual problem of $\text{OT}_\varepsilon(\mu, \nu)$ is given by

\[
\text{OT}_\varepsilon(\mu, \nu) = \sup_{(\varphi, \psi) \in C(X)^2} \left\{ \int_X \varphi \, d\mu + \int_X \psi \, d\nu - \varepsilon \int_{X^2} \exp\left(\frac{\varphi(x) + \psi(y) - c(x, y)}{\varepsilon}\right) - 1 \, d(\mu \otimes \nu) \right\}. \tag{24}
\]

If optimal dual solutions $\hat{\varphi}_\varepsilon$ and $\hat{\psi}_\varepsilon$ exist, they are related to the optimal transport plan $\hat{\pi}_\varepsilon$ by

\[
\hat{\pi}_\varepsilon = \exp\left(\frac{\hat{\varphi}_\varepsilon(x) + \hat{\psi}_\varepsilon(y) - c(x, y)}{\varepsilon}\right) \mu \otimes \nu. \tag{25}
\]

Proof. We consider $F \in \Gamma(C(X)^2)$, $G \in \Gamma(C(X)^2)$ with convex conjugates $F^* \in \Gamma(M(X)^2)$, $G^* \in \Gamma(M(X)^2)$ and the linear bounded operator $A: C(X)^2 \rightarrow C(X^2)$ with adjoint operator $A^*: M(X)^2 \rightarrow M(X)^2$ defined by

\[
F(\varphi, \psi) = \int_X \varphi \, d\mu + \int_X \psi \, d\nu,
\]

\[
G(\varphi) = \varepsilon \int_{X^2} \exp\left(\frac{\varphi - c}{\varepsilon}\right) - 1 \, d(\mu \otimes \nu),
\]

\[
A(\varphi, \psi)(x, y) = \varphi(x) + \psi(y).
\]

Then (24) has the form of the left-hand side in (2). Incorporating (7), we get

\[
G^*(\pi) = \int_X c \, d\pi + \varepsilon \text{KL} (\pi, \mu \otimes \nu).
\]

Using the indicator function $\iota_C$ defined by $\iota_C(x) := 0$ for $x \in C$ and $\iota_C(x) := +\infty$ otherwise, we have

\[
F^*(A^* \pi) = \sup_{(\varphi, \psi) \in C(X)^2} \langle A^* \pi, (\varphi, \psi) \rangle - \int_X \varphi \, d\mu - \int_X \psi \, d\nu
\]

\[
= \sup_{(\varphi, \psi) \in C(X)^2} \langle C, (\varphi(x) + \psi(y)) \rangle - \int_X \varphi \, d\mu - \int_X \psi \, d\nu
\]

\[
= \iota_C(\mu \chi)(\pi).
\]
Now, the duality relation follows from (24).

If the optimal solution $(\hat{\varphi}_\varepsilon, \hat{\psi}_\varepsilon)$ exists, we can apply (3) and (8) to obtain

$$\hat{\varphi}_\varepsilon(x) + \hat{\psi}_\varepsilon(y) = c + \log \left( \frac{d\hat{\pi}_\varepsilon}{d(\mu \otimes \nu)} \right)$$

which yields (25).

\[\square\]

**Remark 5.5.** Using the Tietze extension theorem, we could also replace the space $C(\mathbb{X})^2$ by $C(\text{supp}(\mu)) \times C(\text{supp}(\nu))$.

Note that the last term in (24) is a smoothed version of the constraint $\varphi(x) + \psi(y) \leq c(x, y)$ appearing in (22). Clearly, the values of $\varphi$ and $\psi$ are only relevant on supp$(\mu)$ and supp$(\nu)$, respectively. Further, for any $\varphi, \psi \in C(\mathbb{X})$ and $C \in \mathbb{R}$, the potentials $\varphi + C, \psi - C$ realize the same value in (24).

For fixed $\varphi$ or $\psi$, the corresponding maximizing potentials in (24) are given by

$$\hat{\psi}_{\varphi, \varepsilon} = T_{\mu, \varepsilon}(\varphi) \text{ on supp}(\nu) \quad \text{and} \quad \hat{\varphi}_{\psi, \varepsilon} = T_{\nu, \varepsilon}(\psi) \text{ on supp}(\mu),$$

respectively. Here, $T_{\mu, \varepsilon} : C(\mathbb{X}) \to C(\mathbb{X})$ is defined as

$$T_{\mu, \varepsilon}(\varphi)(x) := -\varepsilon \log \left( \int_{\mathbb{X}} \exp\left( \frac{\varphi(y) - c(x, y)}{\varepsilon} \right) d\mu(y) \right).$$

Therefore, any pair of optimal potentials $\hat{\varphi}_\varepsilon$ and $\hat{\psi}_\varepsilon$ must satisfy

$$\hat{\psi}_\varepsilon = T_{\mu, \varepsilon}(\hat{\varphi}_\varepsilon) \text{ on supp}(\nu), \quad \hat{\varphi}_\varepsilon = T_{\nu, \varepsilon}(\hat{\psi}_\varepsilon) \text{ on supp}(\mu).$$

For every $\varphi \in C(\mathbb{X})$ and $C \in \mathbb{R}$, it holds $T_{\mu, \varepsilon}(\varphi + C) = T_{\mu, \varepsilon}(\varphi) + C$. Hence, $T_{\mu, \varepsilon}$ can be also interpreted as an operator on the quotient space $C(\mathbb{X})/\mathbb{R}$, where $f_1, f_2 \in C(\mathbb{X})$ are equivalent if they differ by a real constant. This space can equipped with the oscillation norm $\|f\|_{0, \infty} := \frac{1}{2}(\max f - \min f)$ and for $f \in C(\mathbb{X})/\mathbb{R}$ there exists a representative $\tilde{f} \in C(\mathbb{X})$ with $\|f\|_{0, \infty} = \|\tilde{f}\|_{\infty}$. Finally, it is also possible to restrict the domain of $T_{\mu, \varepsilon}$ to $C(\text{supp}(\mu))$ and $C(\text{supp}(\mu))/\mathbb{R}$, respectively. This interpretation is useful for showing convergence of the Sinkhorn algorithm. In the next lemma, we collect a few properties of $T_{\mu, \varepsilon}$, see also [20 47].

**Lemma 5.6.** i) For any measure $\mu \in P(\mathbb{X}), \varepsilon > 0$ and $\varphi \in C(\mathbb{X})$, the function $T_{\mu, \varepsilon}(\varphi) \in C(\mathbb{X})$ has the same Lipschitz constant as $c$ and satisfies

$$T_{\mu, \varepsilon}(\varphi)(x) \in \left[ \min_{y \in \text{supp}(\mu)} c(x, y) - \varphi(y), \max_{y \in \text{supp}(\mu)} c(x, y) - \varphi(y) \right].$$

ii) For fixed $\mu \in P(\mathbb{X})$, the operator $T_{\mu, \varepsilon} : C(\text{supp}(\mu)) \to C(\mathbb{X})$ is 1-Lipschitz and the operator $T_{\mu, \varepsilon} : C(\text{supp}(\mu))/\mathbb{R} \to C(\mathbb{X})/\mathbb{R}$ is contractive.

**Proof.** i): For $x_1, x_2 \in \mathbb{X}$ (possibly changing the naming of the variables) we obtain

$$\left| T_{\mu, \varepsilon}(\varphi)(x_1) - T_{\mu, \varepsilon}(\varphi)(x_2) \right|$$

$$= \varepsilon \log \int_{\mathbb{X}} \exp\left( \frac{\varphi(y) - c(x_2, y)}{\varepsilon} \right) d\mu(y) - \log \int_{\mathbb{X}} \exp\left( \frac{\varphi(y) - c(x_1, y)}{\varepsilon} \right) d\mu(y)$$

$$= \varepsilon \log \left( \int_{\mathbb{X}} \exp\left( \frac{\varphi(y) - c(x_2, y)}{\varepsilon} \right) d\mu(y) \right) / \left( \int_{\mathbb{X}} \exp\left( \frac{\varphi(y) - c(x_1, y)}{\varepsilon} \right) d\mu(y) \right).$$
Incorporating the Lipschitz continuity of \( c \), we get
\[
\exp\left(\frac{c(x_1, y) - c(x_2, y)}{\varepsilon}\right) \leq \exp\left(\frac{|c(x_1, y) - c(x_2, y)|}{\varepsilon}\right) \leq \exp\left(\frac{L}{\varepsilon}|x_1 - x_2|\right),
\]
so that
\[
\int_X \exp\left(\frac{\varphi(y) - c(x_2, y)}{\varepsilon}\right) d\mu(y) \leq \exp\left(\frac{L}{\varepsilon}|x_1 - x_2|\right) \int_X \exp\left(\frac{\varphi(y) - c(x_1, y)}{\varepsilon}\right) d\mu(y).
\]
Thus, \( T_{\mu, \varepsilon}(\varphi) \) is Lipschitz continuous
\[
|T_{\mu, \varepsilon}(\varphi)(x) - T_{\mu, \varepsilon}(\varphi)(y)| \leq \varepsilon \log\left(\exp\left(\frac{L}{\varepsilon}|x_1 - x_2|\right)\right) = L|x_1 - x_2|.
\]
Finally, (27) follows directly from (26) since \( \mu \) is a probability measure.

ii): Similar as before, we obtain for any \( x \in X \) and \( \varphi_1, \varphi_2 \in C(\text{supp}(\mu)) \) that
\[
|T_{\mu, \varepsilon}(\varphi_1)(x) - T_{\mu, \varepsilon}(\varphi_2)(x)| = \varepsilon \log \left( \int_X \exp\left(\frac{\varphi_1(y) - c(x, y)}{\varepsilon}\right) d\mu(y) / \int_X \exp\left(\frac{\varphi_2(y) - c(x, y)}{\varepsilon}\right) d\mu(y) \right).
\]
For any \( y \in X \) we get
\[
\exp\left(\frac{\varphi_1(y) - c(x, y)}{\varepsilon}\right) \leq \exp\left(\|\varphi_1 - \varphi_2\|_\infty\right) \exp\left(\frac{\varphi_2(y) - c(x, y)}{\varepsilon}\right),
\]
and strict inequality holds on a set of positive measure if \( \varphi_1 - \varphi_2 \) is not constant. In this case, we obtain
\[
|T_{\mu, \varepsilon}(\varphi_1)(x) - T_{\mu, \varepsilon}(\varphi_2)(x)| < \|\varphi_1 - \varphi_2\|_\infty
\]
and the first part of the statements follows. Using equivalence classes and \( \|\cdot\|_\infty \) instead, this directly implies for \( \varphi_1 \neq \varphi_2 \) that
\[
\|T_{\mu, \varepsilon}(\varphi_1) - T_{\mu, \varepsilon}(\varphi_2)\|_{0, \infty} < \|\varphi_1 - \varphi_2\|_{0, \infty}.
\]

Now, we are able to prove the existence of an optimal solution \( (\hat{\varphi}_\varepsilon, \hat{\psi}_\varepsilon) \).

**Proposition 5.7.** The optimal potentials \( \hat{\varphi}_\varepsilon, \hat{\psi}_\varepsilon \in C(X) \) exist and are unique on \( \text{supp}(\mu) \) and \( \text{supp}(\nu) \), respectively (up to the additive constant).

**Proof.** Let \( \varphi_n, \psi_n \in C(X) \) be maximizing sequences of (24). Using the operator \( T_{\mu, \varepsilon} \), these can be replaced by
\[
\tilde{\psi}_n = T_{\mu, \varepsilon}(\varphi_n) \quad \text{and} \quad \tilde{\varphi}_n = T_{\nu, \varepsilon} \circ T_{\mu, \varepsilon}(\varphi_n),
\]
which are Lipschitz continuous with the same constant as \( c \) by Lemma [5.6 i] and therefore uniformly equicontinuous. Next, we can choose some \( x_0 \in \text{supp}(\mu) \) and w.l.o.g. assume \( \psi_n(x_0) = 0 \). Due to the uniform Lipschitz continuity, the potentials \( \tilde{\psi}_n \) are uniformly bounded and by (27) the same holds true for \( \tilde{\varphi}_n \). Now, the theorem of Arzela-Ascoli implies that both sequences contain convergent subsequences. Since the functional in (24) is continuous, we can readily infer the existence of optimal potentials \( \hat{\varphi}_\varepsilon, \hat{\psi}_\varepsilon \in C(X) \). Due to the uniqueness of \( \hat{\varphi}_\varepsilon, [25] \) implies that \( \hat{\varphi}_\varepsilon|_{\text{supp}(\mu)} \) and \( \hat{\psi}_\varepsilon|_{\text{supp}(\nu)} \) are uniquely determined up to an additive constant. \( \square \)
Combining the optimality condition (26) and (24), we directly obtain for any pair of optimal solutions

\[ OT_\varepsilon(\mu, \nu) = \int_X \hat{\varphi}_\varepsilon \, d\mu + \int_X \hat{\psi}_\varepsilon \, d\nu. \]  

(28)

Adding, e.g., the additional constraint

\[ \int_X \varphi \, d\mu = \frac{1}{2} OT_\infty(\mu, \nu), \]  

(29)

the restricted optimal potentials \( \hat{\varphi}_\varepsilon |_{\text{supp}(\mu)} \) and \( \hat{\psi}_\varepsilon |_{\text{supp}(\nu)} \) are unique. The next proposition investigates the limits of the potentials as \( \varepsilon \to 0 \) and \( \varepsilon \to \infty \).

**Proposition 5.8.**  

i) Under the constraint (29), the restricted potentials \( \hat{\varphi}_\varepsilon |_{\text{supp}(\mu)} \) and \( \hat{\psi}_\varepsilon |_{\text{supp}(\nu)} \) converge uniformly for \( \varepsilon \to \infty \) to

\[ \hat{\varphi}_\infty(x) = \int_X c(x, y) \, d\nu(y) - \frac{1}{2} OT_\infty(\mu, \nu), \]

\[ \hat{\psi}_\infty(y) = \int_X c(x, y) \, d\mu(x) - \frac{1}{2} OT_\infty(\mu, \nu), \]

respectively.

ii) For \( \varepsilon \to 0 \) every accumulation point of \( (\hat{\varphi}_\varepsilon |_{\text{supp}(\mu)}), \hat{\psi}_\varepsilon |_{\text{supp}(\nu)} ) \) can be extended to an optimal dual pair for \( OT(\mu, \nu) \) satisfying (29). In particular, \( \lim_{\varepsilon \to 0} OT_\varepsilon(\mu, \nu) = OT(\mu, \nu) \).

**Proof.** i): Since \( \mathcal{X} \) is bounded, the Lipschitz continuity of the potentials together with (29) implies that all \( \hat{\varphi}_\varepsilon \) are uniformly bounded on \( \text{supp}(\mu) \). Then, we conclude for \( y \in \text{supp}(\nu) \) using l'Hôpital’s rule, dominated convergence and (29) that

\[
\lim_{\varepsilon \to \infty} \hat{\psi}_\varepsilon(y) = \lim_{\varepsilon \to \infty} \frac{\int_X (\hat{\varphi}_\varepsilon(x) - c(x, y)) \exp\left(\frac{\hat{\varphi}_\varepsilon(x) - c(x, y)}{\varepsilon}\right) \, d\mu(x)}{\int_X \exp\left(\frac{\hat{\varphi}_\varepsilon(x) - c(x, y)}{\varepsilon}\right) \, d\mu(x)} \\
= \lim_{\varepsilon \to \infty} \int_X c(x, y) \exp\left(\frac{\hat{\varphi}_\varepsilon(x) - c(x, y)}{\varepsilon}\right) - \hat{\varphi}_\varepsilon(x) \exp\left(\frac{\hat{\varphi}_\varepsilon(x) - c(x, y)}{\varepsilon}\right) \, d\mu(x) \\
= \int_X c(x, y) \, d\mu(x) - \lim_{\varepsilon \to \infty} \int_X \hat{\varphi}_\varepsilon(x) \left( \exp\left(\frac{\hat{\varphi}_\varepsilon(x) - c(x, y)}{\varepsilon}\right) - 1 \right) + \hat{\varphi}_\varepsilon(x) \, d\mu(x) \\
= \int_X c(x, y) \, d\mu(x) - \frac{1}{2} OT_\infty(\mu, \nu).
\]

Again, a similar reasoning, incorporating (27), can be applied for \( \hat{\varphi}_\varepsilon \). Finally, note that pointwise convergence of uniformly Lipschitz continuous functions on compact sets implies uniform convergence.

ii): By continuity of the integral, we can directly infer that (29) is satisfied for any accumulation point. Note that for any fixed \( \varphi \in C(\mathcal{X}) \), \( x \in \mathcal{X} \) and \( \varepsilon \to 0 \) it holds

\[ T_{\mu, \varepsilon}(\varphi)(x) \to \min_{y \in \text{supp}(\mu)} c(x, y) - \varphi(y), \]
see [19, Prop. 9], which by uniform Lipschitz continuity of $T_{\mu,\varepsilon}(\hat{\phi})$ directly implies the convergence in $C(\mathbb{X})$. Let $\{(\hat{\phi}_{\varepsilon,j}, \hat{\psi}_{\varepsilon,j})\}_j$ be a subsequence converging to $(\hat{\phi}_0, \hat{\psi}_0) \in C(\text{supp}(\mu)) \times C(\text{supp}(\nu))$. Then, we have

$$\hat{\psi}_0 = \lim_{j \to \infty} \hat{\psi}_{\varepsilon,j} = \lim_{j \to \infty} T_{\mu,\varepsilon,j}(\hat{\phi}_{\varepsilon,j}) = \lim_{j \to \infty} \left( T_{\mu,\varepsilon,j}(\hat{\phi}_{\varepsilon,j}) - T_{\mu,\varepsilon,j}(\hat{\phi}_0) + T_{\mu,\varepsilon,j}(\hat{\phi}_0) \right).$$

By Lemma [5.6 ii] it holds

$$\|T_{\mu,\varepsilon,j}(\hat{\phi}_{\varepsilon,j}) - T_{\mu,\varepsilon,j}(\hat{\phi}_0)\|_\infty \leq \|\hat{\phi}_{\varepsilon,j} - \hat{\phi}_0\|_\infty$$

and we conclude

$$\hat{\psi}_0 = \lim_{j \to \infty} T_{\mu,\varepsilon,j}(\hat{\phi}_0) = \min_{y \in \text{supp}(\mu)} c(\cdot, y) - \hat{\phi}_0(y).$$

Similarly, we get

$$\hat{\phi}_0 = \min_{y \in \text{supp}(\nu)} c(\cdot, y) - \hat{\psi}_0(y).$$

Thus, $(\hat{\phi}_0, \hat{\psi}_0)$ can be extended to a feasible point in $C(\mathbb{X})^2$ of (22) by Remark 4.2.

Due to continuity of (28) and since $\text{OT}_\varepsilon$ is monotone in $\varepsilon$, this implies

$$\lim_{j \to \infty} \text{OT}_\varepsilon(j, \mu, \nu) = \int_\mathbb{X} \hat{\phi}_0 \, d\mu + \int_\mathbb{X} \hat{\psi}_0 \, d\nu \leq \text{OT}(\mu, \nu) \leq \lim_{j \to \infty} \text{OT}_\varepsilon(j, \mu, \nu).$$

Hence, the extended potentials are optimal for (22). Since the subsequence choice was arbitrary, this also shows Proposition 5.3 ii).

So far we cannot show the convergence of the potentials for $\varepsilon \to 0$. Essentially, our approach would require that all $T_{\mu,\varepsilon}$ are contractive with a uniform constant $\beta < 1$, which is not the case. However, we observed convergence in our numerical examples.

### 6. Sinkhorn Divergence

The regularized OT functional $\text{OT}_\varepsilon$ is biased, which motivates the introduction of the **Sinkhorn divergence**

$$S_\varepsilon(\mu, \nu) = \text{OT}_\varepsilon(\mu, \nu) - \frac{1}{2} \text{OT}_\varepsilon(\mu, \mu) - \frac{1}{2} \text{OT}_\varepsilon(\nu, \nu).$$

Indeed, it was shown that $S_\varepsilon$ is non-negative, bi-convex and metrizes the convergence in law under mild assumptions [19]. Clearly, we have $S_0 = \text{OT}$. By (14) and Proposition 5.8 we obtain the following corollary.

**Corollary 6.1.** Assume that $K \in C(\mathbb{X} \times \mathbb{X})$ is symmetric and positive definite. Set $c(x, y) := -K(x, y)$. Then, it holds $S_\infty(\mu, \nu) = \mathcal{D}_K(\mu, \nu)$ and the optimal dual potential $\hat{\phi}_K$ realizing $\mathcal{D}_K(\mu, \nu)$ is related to the uniform limits $\hat{\phi}_\infty, \hat{\psi}_\infty$ of $\hat{\phi}_\varepsilon, \hat{\psi}_\varepsilon$ in $\text{OT}_\varepsilon(\mu, \nu)$ with constraint (29) by

$$\hat{\phi}_K = \frac{\hat{\phi}_\infty - \hat{\psi}_\infty}{\|\hat{\phi}_\infty - \hat{\psi}_\infty\|_{H_K(\mathbb{X})}}.$$
Note that \([12]\) already implies that for the above cost function it holds \(\hat{\varphi}_\infty, \hat{\psi}_\infty \in H_K(X)\). By Corollary 6.1, we have for \(c(x,y) := -K(x,y)\) that \(S_\infty(\mu, \nu) = \partial K(\mu, \nu)\) if \(K \in C(X \times X)\) is symmetric, positive definite. For the cost function \(c(x,y) = \|x - y\|^p\) of the classical \(p\)-Wasserstein distance, we have already seen in Section 3 that \(K(x,y) = -c(x,y)\) is not positive definite. However, at least for \(p = 1\) the Kernel is conditionally positive definite of order 1 and can be tuned by Proposition [5,1] to a positive definite kernel by adding a constant which neither changes the value of the discrepancy nor of the optimal dual potential. More generally, we have the following corollary.

**Corollary 6.2.** Let \(K \in C(X \times X)\) be symmetric, conditionally positive definite of order 1, and let \(\tilde{K}\) be the corresponding positive definite kernel in \([19]\). Then we have for \(c = -\tilde{K}\) that

\[
S_\infty(\mu, \nu) = \partial K(\mu, \nu)
\]

and for the optimal dual potentials

\[
\hat{\varphi}_\infty(x) = \int_X -K(x,y) \nu(y) + \frac{1}{2} \int_{X^2} K d(\mu \otimes \nu) + K(x, \xi) + \frac{1}{2} (c_\nu - c_\mu - K(\xi, \xi))
\]

\[
\hat{\psi}_\infty(y) = \int_X -K(x,y) \mu(x) + \frac{1}{2} \int_{X^2} K d(\mu \otimes \nu) + K(\xi, y) + \frac{1}{2} (c_\mu - c_\nu - K(\xi, \xi))
\]

with some fixed \(\xi \in X\) and \(c_\mu, c_\nu\) defined as in \([20]\).

**Proof.** By Corollary 6.1 and Lemma 3.2 we obtain

\[
S_\infty(\mu, \nu) = \partial K(\mu, \nu) = \partial K(\mu, \nu).
\]

The second claim follows by Proposition 5.8.

In the following, we want to characterize the convergence of the functional \(S_\varepsilon(\cdot, \nu)\) in the limiting cases \(\varepsilon \to 0\) and \(\varepsilon \to \infty\) for fixed \(\nu \in \mathcal{P}(X)\). Recall that a sequence \(\{F_n\}_{n \in \mathbb{N}}\) of functionals \(F_n : \mathcal{P}(X) \to (-\infty, +\infty]\) is said to \(\Gamma\)-converge to \(F : \mathcal{P}(X) \to (-\infty, +\infty]\) if the following two conditions are fulfilled for every \(\mu \in \mathcal{P}(X)\), see [4]:

i) \(F(\mu) \leq \liminf_{n \to \infty} F_n(\mu_n)\) whenever \(\mu_n \to \mu\),

ii) there is a sequence \(\{\mu_n\}_{n \in \mathbb{N}}\) with \(\mu_n \to \mu\) and \(\limsup_{n \to \infty} F_n(\mu_n) \leq F(\mu)\).

The importance of \(\Gamma\)-convergence relies in the fact that every cluster point of minimizers of \(\{F_n\}_{n \in \mathbb{N}}\) is a minimizer of \(F\).

**Proposition 6.3.** It holds \(S_\varepsilon(\cdot, \nu) \xrightarrow{\Gamma} S_\infty(\cdot, \nu)\) as \(\varepsilon \to \infty\) and \(S_\varepsilon(\cdot, \nu) \xrightarrow{\Gamma} \text{OT}(\cdot, \nu)\) as \(\varepsilon \to 0\).

**Proof.** 1. In both cases the \(\limsup\)-inequality follows from Proposition 5.3 by choosing for some fixed \(\mu \in \mathcal{P}(X)\) the constant sequence \(\mu_n = \mu, n \in \mathbb{N}\).

2. Concerning the \(\liminf\)-inequality, we first treat the case \(\varepsilon \to \infty\). Let \(\mu_n \to \mu\) and \(\varepsilon_n \to \infty\). Since \(\text{OT}_{\varepsilon}(\mu, \nu)\) is increasing with \(\varepsilon\), it holds for every fixed \(m \in \mathbb{N}\) that

\[
\liminf_{n \to \infty} S_{\varepsilon_n}(\mu_n, \nu) = \liminf_{n \to \infty} \left(\text{OT}_{\varepsilon_n}(\mu_n, \nu) - \frac{1}{2} \text{OT}_{\varepsilon_n}(\mu_n, \mu_n) - \frac{1}{2} \text{OT}_{\varepsilon_n}(\nu, \nu)\right)
\]

\[
\geq \liminf_{n \to \infty} \left(\text{OT}_{m}(\mu_n, \nu) - \frac{1}{2} \text{OT}_{\infty}(\mu_n, \mu_n) - \frac{1}{2} \text{OT}_{\infty}(\nu, \nu)\right).
\]
Due to the weak continuity of $OT_m$ and $OT_\infty$, we obtain

$$\liminf_{n \to \infty} S_{\varepsilon_n}(\mu_n, \nu) \geq OT_m(\mu, \nu) - \frac{1}{2} OT_\infty(\mu, \mu) - \frac{1}{2} OT_\infty(\nu, \nu).$$

Letting $m \to \infty$, Proposition 5.3 implies the lim inf-inequality.

Next, we consider $\varepsilon \to 0$. Let $\mu_n \rightharpoonup \mu$ and $\varepsilon_n \to 0$. With similar arguments as above we obtain for any fixed $m \in \mathbb{N}$ that

$$\liminf_{n \to \infty} S_{\varepsilon_n}(\mu_n, \nu) \geq \liminf_{n \to \infty} (OT(\mu_n, \nu) - \frac{1}{2} OT_m(\mu_n, \mu_n)) - \frac{1}{2} OT_m(\nu, \nu)$$

and weak continuity of $OT_m$ and $OT$ implies

$$\liminf_{n \to \infty} S_{\varepsilon_n}(\mu_n, \nu) \geq OT(\nu, \mu) - \frac{1}{2} OT_m(\mu, \mu) - \frac{1}{2} OT_m(\nu, \nu).$$

Using again Proposition 5.3, we verify the lim inf-inequality.

7. Numerical approach and examples

In this section, we discuss the Sinkhorn algorithm for computing $OT_\varepsilon$ based on the (pre)-dual form (24) and show some numerical examples. As pointed out in Remark 5.5, we can restrict the potentials and the update operator (26) to $\text{supp}(\mu)$ and $\text{supp}(\nu)$, respectively. In particular, this restriction results in a discrete problem if both input measures are atomic. For a fixed starting iterate $\psi(0)$, the Sinkhorn algorithm iterates are defined as

$$\varphi^{(i+1)} = T_{\nu,\varepsilon}(\psi^{(i)}),$$
$$\psi^{(i+1)} = T_{\mu,\varepsilon}(\varphi^{(i+1)}).$$

Equivalently, we could rewrite the scheme with just one potential and the following update $\psi^{(i+1)} = T_{\mu,\varepsilon} \circ T_{\nu,\varepsilon}(\psi^{(i)})$. According to Proposition 5.6, the operator $T_{\mu,\varepsilon} \circ T_{\nu,\varepsilon}$ is contractive and hence the Banach fixed point theorem implies that the algorithm converges linearly. Note that it suffices to enforce the additional constraint (29) after the Sinkhorn scheme by adding an appropriately chosen constant. Then, the value of $OT_\varepsilon(\mu, \nu)$ can be computed from the optimal potentials using (28). Here, we do not want to go into more detail on implementation issues, since this is not the main scope of this chapter. The numerical examples only serve as an illustration of the theoretical results. All computations in this section are performed using GEOMLOSS, a publicly available PyTorch implementation for regularized optimal transport. Implementation details can be found in Feydy et al. [19] and in the corresponding Github repository.

**Demonstration of convergence results.** In the following, we present a numerical toy example for illustrating the convergence results from the previous sections. First, we want to verify the interpolation behavior of $S_\varepsilon(\mu, \nu)$ between $OT(\mu, \nu)$ and $\mathcal{D}_K(\mu, \nu)$. We choose $X = [0, 1]$, $c(x, y) = |x - y|$ and the probability measures $\mu$ and $\nu$ depicted in Fig. 2. The resulting energies $S_\varepsilon(\mu, \nu)$ in the log-scale are plotted in the same figure.

We observe that the values converge as shown in Proposition 5.3 and that the change mainly happens in the interval $[10^{-2}, 10^1]$. Additionally, the numerical results indicate
(a) Measure ϱ
(b) Measure ν
(c) Values $S_\epsilon(\rho, \nu)$ for increasing $\epsilon$

Figure 2: Energy values between $S_0$ and $S_\infty$ for two given measures on $[0, 1]$ and cost function $c(x, y) = |x - y|$. Every blue dot corresponds to the position and the weight of a Dirac measure.

(a) $\sup \sup \text{supp}(\rho) |\hat{\varphi}_\epsilon - \hat{\varphi}_\infty|$ for increasing values of $\epsilon$
(b) $\sup \sup \text{supp}(\nu) |\hat{\psi}_\epsilon - \hat{\psi}_\infty|$ for increasing values of $\epsilon$
(c) $\hat{\varphi}_{1e^{-4}} + \hat{\psi}_{1e^{-4}}$

Figure 3: Numerical verification of Prop. 5.8 and of $\hat{\psi}_\epsilon \approx -\hat{\varphi}_\epsilon$ for small $\epsilon$.

$S_{\epsilon_1}(\rho, \nu) \leq S_{\epsilon_2}(\rho, \nu)$ for $\epsilon_1 > \epsilon_2$, which is the opposite behavior as for OT, where the energies increase, see Lemma 5.1 iii). So far we are not aware of any theoretical result in this direction for $S_\epsilon(\rho, \nu)$.

Next, we investigate the behavior of the corresponding optimal potentials $\hat{\varphi}_\epsilon$ and $\hat{\psi}_\epsilon$ in (24). The convergence of the potentials as shown in Proposition 5.8 iii) is numerically verified in Fig. 3. Further, the corresponding potentials $\hat{\varphi}_\epsilon$ are depicted in Fig. 4 and the differences $\hat{\varphi}_\epsilon - \hat{\psi}_\epsilon$ are depicted in Fig. 5. According to Corollary 6.1, this difference is related to the optimal potential $\hat{\varphi}_K$ in the dual formulation of the related discrepancy. The shape of the potentials ranges from something almost linear for small $\epsilon$ to something more quadratic for large $\epsilon$. Again, we observe that the changes mainly happen for $\epsilon$ in the interval $[10^{-2}, 10^1]$ and that numerical instabilities start to occur for $\epsilon > 10^3$. For small values of $\epsilon$, we actually observe numerical convergence and that the relation $\hat{\psi}_\epsilon \approx -\hat{\varphi}_\epsilon$ holds true, see Fig. 3c. This fits the theoretical findings for $W_1(\rho, \nu)$ in Section 4.

Dithering results. Now, we want to take a short glimpse at a more involved problem. In the following, we investigate the influence of using $S_\epsilon$ with different values $\epsilon$ as approximation quality measure in dithering. For this purpose, we choose $X = [-1, 1]^2$, $c(x, y) = |x - y|$ and $\mu = C \exp(-9\|x\|^2/2)(\lambda \otimes \lambda)$, where $C \in \mathbb{R}$ is a normalizing constant. In order to deal with a fully discrete problem, $\mu$ is approximated by an atomic measure with $90 \times 90$ spikes.
(a) $\hat{\varphi}_{0.02}$
(b) $\hat{\varphi}_{0.08}$
(c) $\hat{\varphi}_{0.32}$
(d) $\hat{\varphi}_{1.28}$
(e) $\hat{\varphi}_{8.92}$
(f) $\hat{\varphi}_{\infty}$

Figure 4: Optimal potentials $\hat{\varphi}_{\varepsilon}$ in $\text{OT}_\varepsilon(\mu, \nu)$ for increasing values of $\varepsilon$.

on a regular grid. Then, we approximate $\mu$ with a measure $\nu \in \mathcal{P}_{\text{emp}}^{400}(X)$ (empirical measure with 400 spikes) in terms of the following objective function

$$
\min_{\nu \in \mathcal{P}_{\text{emp}}^{400}(X)} S_\varepsilon(\mu, \nu).
$$

(30)

For solving this problem, we can equivalently minimize over the positions of the equally weighted Dirac spikes in $\nu$. Hence, we need the gradient of $S_\varepsilon$ with respect to these positions. If $\varepsilon = \infty$, this gradient is given by an analytic expression. Otherwise, we can apply automatic differentiation tools to the Sinkhorn algorithm in order to compute a numerical gradient, see [19] for more details. Here, it is important to ensure high enough numerical precision and to perform enough Sinkhorn iterations. In any case, the gradient serves as input for the L-BFGS-B (Quasi-Newton) method in which the Hessian is approximated in a memory efficient way [5]. The numerical results are depicted in Fig. 6 where all examples are iterated to a very high numerical precision. Numerically, we nicely observe the convergence of $S_\varepsilon(\mu, \hat{\nu})$ in the limits $\varepsilon \to 0$ and $\varepsilon \to \infty$ as implied from the $\Gamma$-convergence result in Proposition 6.3. Visually, the result using Fourier methods is most appealing. Differences could be caused by the different numerical approaches. In particular, the minimization of (30) is quite challenging and our applied approach is pretty straightforward without including any special knowledge about the problem. Noteworthy, the Fourier method uses a truncation of $S_{\infty}^2 = \mathcal{D}_K^2$ in the Fourier domain, see (16), namely

$$
\sum_{k=0}^{N} \alpha_k |\hat{\mu}_k - \hat{\nu}_k|^2, \quad N := 128
$$

as target functional, see [25]. The value of $S_{\infty}$ for the Fourier method is slightly larger than the result using optimization of $S_{\infty}$ directly. Since the computational cost increases as $\varepsilon$
Figure 5: Difference $\hat{\phi}_\varepsilon - \hat{\psi}_\varepsilon$ of optimal potentials in $\text{OT}_\varepsilon(\mu, \nu)$ for increasing $\varepsilon$, where the normalized function $\hat{\phi}_\infty - \hat{\psi}_\infty$ coincides with the optimal dual potential $\hat{\phi}_K$ in the discrepancy by Corollary 6.2.

gets smaller, we suggest to choose $\varepsilon \approx 1$ or to directly stick with discrepancies. This also avoids that the approximation rates suffer from the so-called curse of dimensionality.

Finally, note that we sampled $\mu$ with a lot more points than we used for the dithering. If not enough points are used, we would observe clustering of the dithered measure around the positions of $\mu$. One possibility to avoid such a behavior for $S_\varepsilon$ could be to use the semi-discrete approach described in [21], avoiding any sampling of the measure $\mu$. In the Fourier based approach, this issue was less pronounced.

8. Conclusions

In this chapter, we examined the behavior of the Sinkhorn divergences $S_\varepsilon$ as $\varepsilon \to \infty$ and $\varepsilon \to 0$, with focus on the first case which leads to discrepancies for appropriate cost functions and kernels. We considered a quite general scenario of measures involving, e.g., convex combinations of measures with densities and point measures (spikes). Besides application questions, some open theoretical problem are left. While $\text{OT}_\varepsilon$ is monotone increasing in $\varepsilon$ for any cost function $c$, we observed numerically for $c(x, y) = \|x - y\|$ that $S_\varepsilon$ is monotone decreasing. Further, in Proposition 5.8 ii), we were not able to show convergence of the whole sequence of optimal potentials $\{(\hat{\phi}_\varepsilon, \hat{\psi}_\varepsilon)\}_\varepsilon$ so far.

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Figure 6: Optimal approximations $\hat{\nu}$ and corresponding energies $S_\varepsilon(\mu, \hat{\nu})$ for increasing $\varepsilon$.

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**A. Basic Theorems**

We frequently apply the theorem of Arzela-Ascoli. By definition, a sequence $\{f_n\}_{n \in \mathbb{N}}$ of continuous functions on $X$ is *uniformly bounded*, if there exists a constant $M \geq 0$ independent of $n$ and $x$ such that for all $f_n$ and all $x \in X$ it holds $|f_n(x)| \leq M$. The sequence is said to be *uniformly equicontinuous* if, for every $\varepsilon > 0$, there exists a $\delta > 0$ such that for all functions $f_n$

$$|f_n(x) - f_n(y)| < \varepsilon$$

whenever $d_X(x, y) < \delta$.

**Theorem A.1.** (Arzela-Ascoli) Let $\{f_n\}_{n \in \mathbb{N}}$ be a uniformly bounded, uniformly equicontinuous sequence of continuous functions on $X$. Then, the sequence has a uniformly convergent subsequence.

For the dual problems, we want to extend continuous functions from $A \subset X$, to the whole space, which is possible by the following theorem. In the standard version, the theorem
comes without the bounds, but they can be included directly since \( \min \) and \( \max \) of two continuous functions are again continuous functions.

**Theorem A.2.** (Tietze Extension Theorem) Let a closed subset \( A \subset X \) and a continuous function \( f : A \to \mathbb{R} \) be given. If \( g, h \in C(X) \) are such that \( g \leq h \) and \( g(x) \leq f(x) \leq h(x) \) for all \( x \in A \), then there exists a continuous function \( F : X \to \mathbb{R} \) such that \( F(x) = f(x) \) for all \( x \in A \) and \( g(x) \leq F(x) \leq h(x) \) for all \( x \in X \).

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