Wasserstein Steepest Descent Flows of Discrepancies with Riesz Kernels

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Abstract

The aim of this paper is twofold. Based on the geometric Wasserstein tangent space, we first introduce Wasserstein steepest descent flows. These are locally absolutely continuous curves in the Wasserstein space whose tangent vectors point into a steepest descent direction of a given functional. This allows the use of Euler forward schemes instead of Jordan–Kinderlehrer–Otto schemes. For $\lambda$-convex functionals, we show that Wasserstein steepest descent flows are an equivalent characterization of Wasserstein gradient flows. The second aim is to study Wasserstein flows of the maximum mean discrepancy with respect to certain Riesz kernels. The crucial part is hereby the treatment of the interaction energy. Although it is not $\lambda$-convex along generalized geodesics, we give analytic expressions for Wasserstein steepest descent flows of the interaction energy starting at Dirac measures. In contrast to smooth kernels, the particle may explode, i.e., a Dirac measure becomes a non-Dirac one. The computation of steepest descent flows amounts to finding equilibrium measures with external fields, which nicely links Wasserstein flows of interaction energies with potential theory. Finally, we provide numerical simulations of Wasserstein steepest descent flows of discrepancies.

1 Introduction

Wasserstein gradient flows have received much attention both from the theoretic and application point of view for many years. For a good overview on the theory, we refer to the books of Ambrosio, Gigli and Savaré [2] and Santambrogio [44]. The theory of gradient flows on probability distributions provides a framework for analyzing and constructing particle-based methods by connecting the optimization of functionals with dynamical systems based on differential geometric ideas. A pioneering example is given by the overdamped Langevin equation, where the associated Fokker–Planck equation is just the gradient flow of the

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Figure 1: Halftoning of an image. Gray values are considered as values of a probability density function of a measure which is approximated by an empirical measure such that the discrepancy between both measures becomes small. The halftoned image shows the position of the point measures.

Kullback–Leibler functional $F(\mu) = KL(\mu, \nu)$ in the Wasserstein geometry [29,37–39]. Recently similar ideas have been worked out, replacing either the functional or the underlying geometry, and were also adopted as information flows in deep learning approaches, see for instance [3,21,26,32,33,36,41,50,51] among the huge amount of papers.

Our interest in Wasserstein flows arises from the approximation of probability measures by empirical measures when halftoning images. In [18,20,24], the gray values of an image are considered as values of a probability density function $\rho$ of a measure $\nu$, and the aim consists in approximating this measure by those empirical measure $\mu = \frac{1}{M} \sum_{i=1}^{M} \delta_{x_i}$, $x_i \in \mathbb{R}^2$, which minimizes the (maximum mean) discrepancy with the negative distance kernel $K(x,y) = -\|x - y\|$, i.e., the functional

$$F(\mu) = D^2_{-\|\cdot\|}(\mu, \nu) = \sum_{i=1}^{M} \int_{\mathbb{R}^2} \|x_i - y\| \rho(y) \, dy - \frac{1}{2M} \sum_{i,j=1}^{M} \|x_i - x_j\| + c. \quad (1)$$

The attraction term ensures that the points $x_i$ are pushed to areas where the density is high, while the repulsion term avoids point clustering. For an illustration see Figure 1. The discrepancy with negative distance kernel is also known as energy distance [46,48]. Note that halftoning with the kernel $K(x,y) = -\|x - y\|^{-1}$ was addressed under the name electrostatic halftoning in the initial paper [45], see also [49]. The halftoning functional (1) is a special instance of discrepancy functionals

$$F(\mu) = D^2_{K}(\mu, \nu) = -\int_{\mathbb{R}^{2d}} K(x,y) \nu(y) \, d\nu(x) + \frac{1}{2} \int_{\mathbb{R}^{2d}} K(x,y) \, d\mu(x) \, d\mu(y) + c,$$

potential energy interaction energy
defined for conditionally positive definite kernels \( K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) and arbitrary probability measures \( \mu, \nu \) on \( \mathbb{R}^d \), where the first term is the potential energy of \( \mu \) with respect to the potential of \( \nu \) and the second term is known as interaction energy of \( \mu \). The restriction to empirical measures \( \mu = \frac{1}{M} \sum_{i=1}^{M} \delta_{x_i} \) leads to the consideration of particle gradient flows of \( F(x_1, \ldots, x_M) := D^2_K(\frac{1}{M} \sum_{i=1}^{M} \delta_{x_i}, \nu) \) in \( \mathbb{R}^d \). In [3], it has been established that for smooth kernels \( K \) these particle flows are indeed Wasserstein gradient flows. In other words, Wasserstein gradient flows starting at an empirical measure remain empirical measures and coincide with usual gradient descent flows in \( \mathbb{R}^d \). The situation changes for non-smooth kernels like the negative distance kernel applied in (1). Here it is known that, for the interaction energy, the Wasserstein gradient flow starting at an empirical measures cannot remain empirical, see [5]. This implies that for the negative distance kernel, particle gradient flows of the discrepancy functional cannot be Wasserstein gradient flows. In one dimension, this can be readily seen by the isometric embedding of the Wasserstein space \( \mathcal{P}_2(\mathbb{R}) \) into the Hilbert space \( L_2((0,1)) \), see [9, 12, 27]. In dimensions \( d \geq 2 \), the geometry of the Wasserstein space is more complicated, and it is not obvious to answer if (sub)gradients of the above functionals exist at any measure, in particular at measures which are not absolutely continuous. To study such cases, we recall the concept of the geometric tangent space of \( \mathcal{P}_2(\mathbb{R}^d) \) which generalizes tangent vector fields to tangent velocity plans [2, 22]. Based on this, we introduce the notion of the direction of steepest descent, which leads us to a pointwise notion of the Wasserstein flows, which we call Wasserstein steepest descent flows. For functionals, which are \( \lambda \)-convex along generalized geodesics, we show that a curve is a Wasserstein gradient flow if and only if it is a Wasserstein steepest descent flows. If Wasserstein gradient and steepest descent flows coincide in a more general setting, remains an open question. Unfortunately, for the Riesz kernel \( K(x, y) = -\|x - y\|^r \), \( r \in (0, 2) \), neither the interaction energy nor the discrepancy functional are \( \lambda \)-convex along generalized geodesics in dimensions \( d \geq 2 \). It is not trivial to check if these functionals are regular such that the theory in [2, Thm 11.3.2] applies to this scenario. For the interaction energy, we provide analytic solutions for Wasserstein steepest descent flows starting at Dirac measures, which completes the findings for \( d = 1 \) in [9] and for \( d \geq 2 \) in [13, 16, 25]. In particular, the direction of steepest descent at \( \delta_0 \) relates to the well studied optimization problem of equilibrium measures with external field in potential theory [31, 43]. For the discrepancy functional, we determine steepest descent directions for Riesz kernels with \( r \in [1, 2) \) and show numerical simulations of Wasserstein steepest descent flows starting at Dirac measures for target Dirac measures in two and three dimensions. For a simulation of such flows with neural networks we refer to [1, 28].

**Outline of the paper** We start by providing preliminaries on Wasserstein spaces as geodesic spaces in Section 2. Basic facts on Wasserstein gradient flows, in particular, on the existence and uniqueness of Wasserstein proxies and on the convergence of the MMS to Wasserstein gradient flows are recalled in Section 3. Then, in Section 4, we introduce
Wasserstein steepest descent flows which rely on the concept of the geometric Wasserstein tangent space. We show for locally Lipschitz continuous functions which are $\lambda$-convex along generalized geodesics, that there exists a unique Wasserstein steepest descent flow which coincides with the Wasserstein gradient flow. Then we turn to special functionals arising from discrepancies defined with respect to Riesz kernels in Section 6. Discrepancy functionals are, up to a constant, the sum of an interaction energy and a potential energy. In Section 7, we investigate Wasserstein steepest descent flows of the interaction energy starting at Dirac measures. This leads to the task of solving a constrained optimization problem related to a penalized one which has to be solved when computing Wasserstein proxies. We provide an analytic formula for the Wasserstein steepest descent flow. Finally, in Section 8, we present numerically computed particle gradient flows for the whole discrepancy functional, which are in good agreement with our findings for small time intervals.

2 Preliminaries

**Wasserstein Space**  Let $\mathcal{M}(\mathbb{R}^d)$ denote the space of $\sigma$-additive signed Borel measures, $\mathcal{P}(\mathbb{R}^d)$ the set of all Borel probability measures, and $\mathcal{P}_2(\mathbb{R}^d)$ its subset of measures with finite second moments, i.e.

$$\mathcal{P}_2(\mathbb{R}^d) := \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} \|x\|^2_2 \, d\mu(x) < \infty \right\}.$$ 

The set $\mathcal{P}_2^r(\mathbb{R}^d)$ of absolutely continuous probability measures with respect to the Lebesgue measure is a dense subset of $\mathcal{P}_2(\mathbb{R}^d)$. For $\mu \in \mathcal{M}(\mathbb{R}^d)$ and measurable $T : \mathbb{R}^d \to \mathbb{R}^n$, the *push-forward* of $\mu$ via $T$ is given by $T_{\#} \mu := \mu \circ T^{-1}$. For $x = (x_1, \ldots, x_n) \in (\mathbb{R}^d)^n$, the projection to the $(i_1, \ldots, i_k)$th components is denoted by

$$\pi_{i_1, \ldots, i_k}(x) := (x_{i_1}, \ldots, x_{i_k}).$$

The *Wasserstein distance* $W_2 : \mathcal{P}_2(\mathbb{R}^d) \times \mathcal{P}_2(\mathbb{R}^d) \to [0, \infty)$ is given by

$$W_2^2(\mu, \nu) := \min_{\pi \in \Gamma(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_1 - x_2\|^2_2 \, d\pi(x_1, x_2), \quad \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d),$$

where

$$\Gamma(\mu, \nu) := \{ \pi \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d) : (\pi_1)_{\#} \pi = \mu, (\pi_2)_{\#} \pi = \nu \}.$$ 

The set of optimal transport plans $\pi$ realizing the minimum in (2) is denote by $\Gamma_{\text{opt}}(\mu, \nu)$. If $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$, then the optimal transport plan is unique and is moreover given by a so-called transport map, see [11] and [2, Thm 6.2.10]. Let $L_2(\mu, \mathbb{R}^d)$ denote the space of (equivalence classes of) functions $f : \mathbb{R}^d \to \mathbb{R}^d$ with $\int_{\mathbb{R}^d} \|f\|^2_2 \, d\mu(x) < \infty$. 

4
Theorem 1. Let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$. Then there is a unique plan $\pi \in \Gamma_{\text{opt}}(\mu, \nu)$ which is induced by a unique measurable optimal transport map $T: \mathbb{R}^d \to \mathbb{R}^d$, i.e.,

$$\pi = (\text{Id}, T)_{\#} \mu$$

and

$$W_2^2(\mu, \nu) = \min_{T: \mathbb{R}^d \to \mathbb{R}^d} \int_{\mathbb{R}^d} \|T(x) - x\|_2^2 \, d\mu(x) \quad \text{subject to} \quad T_{\#} \mu = \nu.$$ 

Further, $T = \nabla \psi$, where $\psi: \mathbb{R}^d \to (-\infty, +\infty]$ is convex, lower semi-continuous (lsc) and $\mu$-a.e. differentiable. Conversely, if $\psi$ is convex, lsc and $\mu$-a.e. differentiable with $\nabla \psi \in L_2(\mu, \mathbb{R}^d)$, then $T := \nabla \psi$ is an optimal map from $\mu$ to $\nu := T_{\#} \mu \in \mathcal{P}_2(\mathbb{R}^d)$.

**Wasserstein Geodesics** A curve $\gamma: I \to \mathcal{P}_2(\mathbb{R}^d)$ on an interval $I \subset \mathbb{R}$, is called a (length-minimizing) geodesic if there exists a constant $C \geq 0$ such that

$$W_2(\gamma(t_1), \gamma(t_2)) = C|t_2 - t_1|, \quad \text{for all} \quad t_1, t_2 \in I.$$

The constant $C$ is the speed of the geodesic. The Wasserstein space is geodesic, i.e. any two measures $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ can be connected by a geodesic. These geodesics may be characterized by optimal plans.

**Proposition 2** ([2, Thm 7.2.2]). Let $\epsilon > 0$. Any geodesic $\gamma: [0, \epsilon] \to \mathcal{P}_2(\mathbb{R}^d)$ connecting $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ is determined by an optimal plan $\pi \in \Gamma_{\text{opt}}(\mu, \nu)$ via

$$\gamma(t) := ((1 - \frac{t}{\epsilon}) \pi_1 + \frac{t}{\epsilon} \pi_2)_{\#} \pi, \quad t \in [0, \epsilon). \quad (3)$$

Conversely, any $\pi \in \Gamma_{\text{opt}}(\mu, \nu)$ gives rise to a geodesic $\gamma: [0, \epsilon] \to \mathcal{P}_2(\mathbb{R}^d)$ connecting $\mu$ and $\nu$.

The optimal $\pi$ in (3) may be replaced by non-optimal plans to obtain more general interpolating curves. For instance, based on the set of three-plans with base $\sigma \in \mathcal{P}_2(\mathbb{R}^d)$ given by

$$
\Gamma_{\sigma}(\mu, \nu) := \{ \alpha \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d) : (\pi_1)_{\#} \alpha = \sigma, (\pi_2)_{\#} \alpha = \mu, (\pi_3)_{\#} \alpha = \nu \},
$$

the so-called generalized geodesics $\gamma: [0, \epsilon] \to \mathcal{P}_2(\mathbb{R}^d)$ joining $\mu$ and $\nu$ (with base $\sigma$) is defined as

$$\gamma(t) := ((1 - \frac{t}{\epsilon})\pi_2 + \frac{t}{\epsilon} \pi_3)_{\#} \alpha, \quad t \in [0, \epsilon], \quad (4)$$

where $\alpha \in \Gamma_{\sigma}(\mu, \nu)$ with $(\pi_{1,2})_{\#} \alpha \in \Gamma_{\text{opt}}(\sigma, \mu)$ and $(\pi_{1,3})_{\#} \alpha \in \Gamma_{\text{opt}}(\sigma, \nu)$, see [2, Def 9.2.2]. The plan $\alpha$ may be interpreted as transport from $\mu$ to $\nu$ via $\sigma$. 

5
\(\lambda\)-Convexity along Wasserstein Geodesics  

Let \(\lambda \in \mathbb{R}\) be a fixed constant. A function \(F : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]\) is called \(\lambda\)-convex along geodesics [2, Def 9.1.1] if, for every \(\mu, \nu \in \text{dom} \ F := \{\mu \in \mathcal{P}_2(\mathbb{R}^d) : F(\mu) < \infty\}\), there exists at least one geodesic \(\gamma : [0, 1] \to \mathcal{P}_2(\mathbb{R}^d)\) between \(\mu\) and \(\nu\) such that

\[
F(\gamma(t)) \leq (1 - t) F(\mu) + t F(\nu) - \frac{\lambda}{2} t(1 - t) W_2^2(\mu, \nu), \quad t \in [0, 1].
\]

Analogously, a function \(F : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]\) is called \(\lambda\)-convex along generalized geodesics [2, Def 9.2.4], if for every \(\sigma, \mu, \nu \in \text{dom} \ F\), there exists at least one generalized geodesic \(\gamma : [0, 1] \to \mathcal{P}_2(\mathbb{R}^d)\) related to some \(\alpha\) as in (4) such that

\[
F(\gamma(t)) \leq (1 - t) F(\mu) + t F(\nu) - \frac{\lambda}{2} t(1 - t) W_2^2(\alpha, \mu, \nu), \quad t \in [0, 1],
\]

where

\[
W_2^2(\alpha, \mu, \nu) := \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_2 - x_3\|^2 \, d\alpha(x_1, x_2, x_3).
\]

Further, \(F\) is called convex (along generalized geodesics) if it is 0-convex (along generalized geodesics). Every function being \(\lambda\)-convex along generalized geodesics is also \(\lambda\)-convex along geodesics since generalized geodesics with base \(\sigma = \mu\) are actual geodesics. A \(\lambda\)-convex function \(F : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]\) is called coercive, cf. [2, (11.2.1b)], if there exists an \(r > 0\) such that

\[
\inf \left\{ F(\mu) : \mu \in \mathcal{P}_2(\mathbb{R}^d), \int_{\mathbb{R}^d} \|x\|^2 \, d\mu(x) \leq r \right\} > -\infty.
\]

### 3 Wasserstein Gradient Flows

A curve \(\gamma : I \to \mathcal{P}_2(\mathbb{R}^d)\) on the open interval \(I \subset \mathbb{R}\) is called absolutely continuous if there exists a function \(m \in L_1(I)\) such that

\[
W_2(\gamma(s), \gamma(t)) \leq \int_s^t m(s) \, ds, \quad s, t \in I.
\]

Absolutely continuous curves are characterized by the continuity equation [2, Thm 8.3.1]. More precisely, a continuous curve \(\gamma\) is absolutely continuous if and only if there exists a Borel velocity field \(v_t : \mathbb{R}^d \to \mathbb{R}^d, t \in I\) with \(\int_I \|v_t\|_{L^2(\gamma(t), \mathbb{R}^d)} \, dt < +\infty\) such that

\[
\partial_t \gamma(t) + \nabla \cdot (v_t (\gamma(t))) = 0
\]

holds on \(I \times \mathbb{R}^d\) in the distributive sense

\[
\int_I \int_{\mathbb{R}^d} \partial_t \varphi(t, x) + v_t(x) \cdot \nabla_x \varphi(t, x) \, d\gamma(t) \, dt = 0
\]
Moreover, there exists a unique velocity field, henceforth also denoted by $v_t$, such that $m(t) := \|v_t\|_{L_2(\gamma(t), \mathbb{R}^d)}$ becomes minimal in (5). Furthermore, the minimizing vector field is characterized by the condition $v_t \in T_{\gamma(t)}\mathcal{P}_2(\mathbb{R}^d)$ for almost every $t \in I$, where $T_{\mu}\mathcal{P}_2(\mathbb{R}^d)$ with $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ denotes the regular tangent space

$$T_{\mu}\mathcal{P}_2(\mathbb{R}^d) := \{ \nabla \phi : \phi \in C_c^\infty(\mathbb{R}^d) \}^{L_2(\mu, \mathbb{R}^d)}$$

$$= \{ \lambda(T-I) : (I, T)_{\#} \mu \in \Gamma^{opt}(\mu, T_{\#}\mu), \lambda > 0 \}^{L_2(\mu, \mathbb{R}^d)},$$

see [2, § 8]. Note that $T_{\mu}\mathcal{P}_2(\mathbb{R}^d)$ is an infinite dimensional subspace of $L_2(\mu, \mathbb{R}^d)$ if $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, and it is just $\mathbb{R}^d$ if $\mu = \delta_x$, $x \in \mathbb{R}^d$.

For a proper and lower semi-continuous (lsc) function $F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty]$ and $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, the reduced Fréchet subdifferential at $\mu$ is defined as the set $\partial F(\mu)$ consisting of all $\xi \in L_2(\mu, \mathbb{R}^d)$ satisfying

$$F(\nu) - F(\mu) \geq \inf_{\pi \in \Gamma^{opt}(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x_1), x_2 - x_1 \rangle \, d\pi(x_1, x_2) + o(W_2(\mu, \nu))$$

for all $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ or equivalently

$$\liminf_{\nu \to \mu} \frac{F(\nu) - F(\mu) - \inf_{\pi \in \Gamma^{opt}(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x_1), x_2 - x_1 \rangle \, d\pi(x_1, x_2)}{W_2(\mu, \nu)} \geq 0,$$

where $\nu$ converges to $\mu$ in $(\mathcal{P}_2(\mathbb{R}^d), W_2)$, see [2, (10.3.13)]. On the basis of this subdifferential, Wasserstein gradient flows may be defined as follows.

An absolutely continuous curve $\gamma: (0, +\infty) \to \mathcal{P}_2(\mathbb{R}^d)$ with velocity field $v_t \in T_{\gamma(t)}\mathcal{P}_2(\mathbb{R}^d)$ is called a Wasserstein gradient flow of $F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ if

$$v_t \in -\partial F(\gamma(t)), \text{ for a.e. } t > 0. \quad (6)$$

The existence of Wasserstein gradient flows is usually shown by using the generalized minimizing moment scheme [23,29], which can be considered as Euler backward scheme for computing the Wasserstein gradient flow (6). It is explained in the following. For a proper and lsc function $F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty]$ and fixed $\tau > 0$, the proximal mapping $\text{prox}_{\tau F}$ is defined as the set-valued function

$$\text{prox}_{\tau F}(\mu) = \arg\min_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \left\{ \frac{1}{2\tau} W_2^2(\mu, \nu) + F(\nu) \right\}, \quad \mu \in \mathcal{P}_2(\mathbb{R}^d). \quad (7)$$

Note that, for every $\mu \in \text{dom } F$, the existence and uniqueness of the minimizer in (7) is assured if $F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty]$ is $\lambda$-convex along generalized geodesics, where $\lambda > -1/\tau$, see [2, Lem 9.2.7].
Assuming that the proximal mapping is non-empty, and starting with some \( \mu_0 \in P_2(\mathbb{R}^d) \), we consider the piecewise constant curves given by the minimizing movement scheme (MMS), which is also known as Jordan–Kinderlehrer–Otto scheme:

\[
\gamma_\tau \big|_{((n-1)\tau,n\tau]} := \mu^n_\tau \quad \text{with} \quad \mu^n_\tau \in \text{prox}_{\tau F}(\mu^{n-1}_\tau).
\]

If \( F \) is \( \lambda \)-convex along generalized geodesics, then there exists a \( \tau^* > 0 \) such that \( \text{prox}_{\tau F}(\mu) \) becomes single-valued for all \( \tau < \tau^* \) and \( \mu \in P_2(\mathbb{R}^d) \). Then we can study the limit of the curves \( \gamma_\tau \).

**Theorem 3** ([2, Thm 11.2.1]). Let \( F : P_2(\mathbb{R}^d) \to (-\infty, +\infty] \) be proper, lsc, coercive, and \( \lambda \)-convex along generalized geodesics, and let \( \mu_0 \in \text{dom} F \). Then the curves \( \gamma_\tau \) defined via the minimizing movement scheme (8) converge for \( \tau \to 0 \) locally uniformly to a locally Lipschitz curve \( \gamma : (0, +\infty) \to P_2(\mathbb{R}^d) \) which is the unique Wasserstein gradient flow of \( F \) with \( \gamma(0+) = \mu_0 \).

Theorem 3 gives a pointwise definition of \( \gamma \) for all \( t \in [0, +\infty) \). However, we will see that the interaction functional with distance kernel is not \( \lambda \)-convex along geodesics.

**4 Geodesic Directions and Geodesic Tangents**

For general \( F \), the velocity field \( v_t \in T_{\gamma(t)}P_2(\mathbb{R}^d) \) in (6) is only determined for almost every \( t > 0 \), but we want to give a definition of so-called steepest descent flows pointwise. To this end, we recall the notion of the geometric tangent space, see [22, Chap 4] or [2, § 12.4], which generalizes tangent vector fields to so-called tangent velocity plans.

Note, any transport plan \( \pi \in \Gamma(\mu, \nu) \) is associated to a velocity plan \( v \in P_2(\mathbb{R}^d \times \mathbb{R}^d) \) by the relation

\[
v = (\pi_1, \pi_2 - \pi_1)\# \pi, \quad \text{or equivalently} \quad \pi = (\pi_1, \pi_1 + \pi_2)\# v.
\]

The set of all velocity plans at \( \mu \in P_2(\mathbb{R}^d) \) is defined by

\[
V(\mu) := \{ v \in P_2(\mathbb{R}^d \times \mathbb{R}^d) : (\pi_1)\# v = \mu \}.
\]

We equip \( V(\mu) \) with the metric \( W_\mu \) defined by

\[
W_\mu^2(v, w) := \inf_{\alpha \in \Gamma_\mu(v, w)} W_\alpha^2((\pi_2)\# v, (\pi_2)\# w),
\]

where

\[
\Gamma_\mu(v, w) := \{ \alpha \in P_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d) : (\pi_{1,2})\# \alpha = v, (\pi_{1,3})\# \alpha = w \}.
\]
Then, it was proven in [22, Thm 4.5] that \((V(\mu), W_\mu)\) is a complete metric space. For a velocity plan \(v \in V(\mu)\) and corresponding transport plan \(\pi = (\pi_1, \pi_1 + \pi_2)_\# v\), the curve \(\gamma_v: [0, \infty) \to P_2(\mathbb{R}^d)\) determined by

\[
\gamma_v(t) := (\pi_1 + t\pi_2)_\# v, \quad t \geq 0.
\]

is equal to the interpolation

\[
\gamma_v(t) = ((1 - t)\pi_1 + t\pi_2)_\# \pi, \quad \text{for } t \in [0, 1].
\]

In the case that the velocity plan \(v\) corresponds to an optimal transport plan \(\pi \in \Gamma^{opt}(\mu, \nu)\), we obtain by Proposition 2 that \(\gamma_v\) is a geodesic on \([0, 1]\).

In the following, we aim to characterize, for arbitrary \(\epsilon > 0\), a geodesic \(\gamma: [0, \epsilon] \to P_2(\mathbb{R}^d)\) by velocity plans. Therefore, we define the scaling of a velocity plan \(v \in V(\mu)\) by a factor \(c \in \mathbb{R}\) as

\[
c \cdot v := (\pi_1, c\pi_2)_\# v.
\]

Then, by definition the curve \(\gamma_{c \cdot v}\) fulfills

\[
\gamma_{c \cdot v}(t) = (\pi_1 + t\pi_2)_\# (c \cdot v) = (\pi_1 + t\pi_2)_\# (\pi_1, c\pi_2)_\# v = (\pi_1 + ct\pi_2)_\# v = \gamma_v(ct),
\]

i.e., \(\gamma_{c \cdot v}\) is the curve \(\gamma_v\) scaled by the factor \(c\). For \(c = 0\) we obtain that

\[
0_\mu := 0 \cdot v = \mu \otimes \delta_0.
\]

Using this scaling and (9), we obtain that a geodesic \(\gamma: [0, \epsilon] \to P_2(\mathbb{R}^d)\) related to \(\pi \in \Gamma^{opt}(\mu, \nu)\) by (3) belongs to the velocity plan

\[
v = \frac{1}{c} \cdot ((\pi_1, \pi_2 - \pi_1)_\# \pi) = (\pi_1, \frac{1}{c}(\pi_2 - \pi_1))_\# \pi.
\]

in the sense that \(\gamma_v \equiv \gamma\) on \([0, \epsilon]\). The main advantage of this characterization is that two geodesics \(\gamma_1: [0, \epsilon_1] \to P_2(\mathbb{R}^d)\) and \(\gamma_2: [0, \epsilon_2] \to P_2(\mathbb{R}^d)\) with \(\gamma_1|_{[0, \epsilon]} \equiv \gamma_2|_{[0, \epsilon]}\) for some \(\epsilon \leq \min\{\epsilon_1, \epsilon_2\}\) correspond to the same velocity plan \(v\). Hence, \(v\) may be interpreted as geodesic direction. We denote the subset \(V(\mu)\) consisting of all geodesic directions at \(\mu \in P_2(\mathbb{R}^d)\) by

\[
G(\mu) := \{ v \in V(\mu) : \exists \epsilon > 0 \text{ such that } \pi = (\pi_1, \pi_1 + \frac{1}{\epsilon}\pi_2)_\# v \in \Gamma^{opt}(\mu, (\pi_2)_\# \pi) \}
\]

\[
= \{ v \in V(\mu) : \exists \epsilon > 0 \text{ such that } \gamma_v \text{ is a geodesic on } [0, \epsilon] \}.
\]

Then the geometric tangent space at \(\mu \in P_2(\mathbb{R}^d)\) is given by

\[
T_\mu P_2(\mathbb{R}^d) := G(\mu)^{W_\mu}.
\]

Here are some special cases.
Proposition 4. (i) For $\mu \in \mathcal{P}_2^+(\mathbb{R}^d)$, it holds

$$T_\mu \mathcal{P}_2(\mathbb{R}^d) = \{ v = (\text{Id}, v)^\# \mu : v \in T_\mu \mathcal{P}_2(\mathbb{R}^d) \}$$

and $W_{\mu}^2(v, 0_\mu) = \| v \|^2_{L^2(\mu, \mathbb{R}^d)}$.

(ii) For $\mu = \delta_p$, $p \in \mathbb{R}^d$, it holds

$$T_{\delta_p} \mathcal{P}_2(\mathbb{R}^d) = \{ v = \delta_p \otimes \eta \in \mathcal{P}_2(\mathbb{R}^d) \}$$

and $W_{\delta_p}^2(v, 0_{\delta_p}) = \int_{\mathbb{R}^d} \| x \|^2 \, d\eta(x)$.

Proof. (i) The first part follows from [2, Thm 12.4.4], where it was shown that for $\mu \in \mathcal{P}_2^+(\mathbb{R}^d)$, the so-called barycentric projection is an isometric one-to-one correspondence between $T_\mu \mathcal{P}_2(\mathbb{R}^d)$ and $T_\mu \mathcal{P}_2(\mathbb{R}^d)$.

(ii) The second statement on the tangential space follows immediately from the fact that any probability measure with $\delta_p$ as one marginal is a product measure. Similarly, we obtain from $\Gamma_{\delta_p}(\delta_p \otimes \eta, \delta_p \otimes \delta_p) = \{ \alpha \}$, where $\alpha = \delta_p \otimes \eta \otimes \delta_p$, that

$$W_{\delta_p}(\delta_p \otimes \mu, \delta_p \otimes \delta_p) = W_\alpha(\eta, \delta_p) = \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \| x_2 - x_3 \|^2 \, d\alpha(x_1, x_2, x_3)$$

$$= \int_{\mathbb{R}^d} \| x \|^2_2 \, d\eta(x).$$

We define the exponential map $\exp_\mu : T_\mu \mathcal{P}_2(\mathbb{R}^d) \to \mathcal{P}_2(\mathbb{R}^d)$ by

$$\exp_\mu(v) := \gamma_v(1) = (\pi_1 + \pi_2)^\# v.$$ 

The inverse exponential map $\exp^{-1}_\mu : \mathcal{P}_2(\mathbb{R}^d) \to T_\mu \mathcal{P}_2(\mathbb{R}^d)$ is given by the (multivalued) function

$$\exp^{-1}_\mu(\nu) := \{ (\pi_1, \pi_2 - \pi_1)^\# \pi : \pi \in \Gamma_{\text{opt}}(\mu, \nu) \}$$

and consists of all velocity plans $v \in V(\mu)$ such that $\gamma_v|_{[0,1]}$ is a geodesic connecting $\mu$ and $\nu$. Note that

$$\exp^{-1}_\mu(\nu) = \{ v \in T_\mu \mathcal{P}_2(\mathbb{R}^d) : \exp_\mu(v) = \nu \} \cap \{ v \in G(\mu) : \gamma_v|_{[0,1]} \text{ is a geodesic} \}.$$ 

i.e., $\exp^{-1}_\mu$ is only the inverse of $\exp_\mu$ restricted to the set $\{ v \in G(\mu) : \gamma_v|_{[0,1]} \text{ is a geodesic} \}$.

For a curve $\gamma : I \to \mathcal{P}_2(\mathbb{R}^d)$, a velocity plan $v_t \in T_{\gamma(t)} \mathcal{P}_2(\mathbb{R}^d)$ is called a (geometric) tangent vector of $\gamma$ at $t \in I$ if, for every $h > 0$ and $v_{t,h} \in \exp^{-1}_{\gamma(t)}(\gamma(t + h))$, it holds

$$\lim_{h \to 0^+} W_{\gamma(t)}(v_t, \frac{1}{h} \cdot v_{t,h}) = 0.$$ (11)
If a tangent vector $v_t$ exists, then the above limit is uniquely determined since $W_{\gamma(t)}$ is a metric on $V(\gamma(t))$, and we write

$$\dot{\gamma}(t) := v_t.$$ 

In [22, Thm 4.19], it is shown that

$$\dot{\gamma}_v(0) = v$$  \text{ for all } v \in T_{\mu}P_2(\mathbb{R}^d). \quad (12)$$

Therefore, the definition of a tangent vector of a curve is consistent with the interpretation of $\gamma_v$ as a curve in direction of $v$. For $v \in G(\mu)$, we can also compute the tangent vector $\dot{\gamma}_v(t)$ for $t > 0$ by the following lemma.

**Lemma 5.** Let $v \in G(\mu)$ be a velocity plan and $\epsilon > 0$ such that $\gamma_v$ is a geodesic on $[0, \epsilon]$. Then the (geometric) tangent vector of $\gamma_v$ is given by

$$\dot{\gamma}_v(t) = (\pi_1 + t \pi_2, \pi_2)\#v, \quad t \in [0, \epsilon).$$

**Proof.** Let $t \in [0, \epsilon)$ and define $v_t := (\pi_1 + t \pi_2, \pi_2)\#v$. By definition, we have

$$\gamma_v(s) = (\pi_1 + s \pi_2)\#v_t = (\pi_1 + s \pi_2)\#(\pi_1 + t \pi_2, \pi_2)\#v$$

$$= (\pi_1 + (t + s) \pi_2)\#v = \gamma_v(s + t).$$

Since $\gamma_v$ is a geodesic on $[0, \epsilon]$ and $t < \epsilon$, this implies that $\gamma_v$ is a geodesic on $[0, t - \epsilon]$. In particular, it holds $v_t \in G(\gamma_v(0)) \subset T_{\gamma_v(0)}P_2(\mathbb{R}^d)$. Consequently, (12) implies $\dot{\gamma}_v(0) = v_t$. On the other hand, it follows from $\gamma_v(t + s) = \gamma_v(s)$ and the definition (11) of the tangent vector that $\dot{\gamma}_v(t) = \dot{\gamma}_v(0)$ which yields the assertion $\dot{\gamma}_v(t) = v_t$. \qed

For reparameterization, we need the following chain rule of differentiation which proof is given in Appendix A.

**Lemma 6.** Let $\nu : [0, T) \rightarrow P_2(\mathbb{R}^d)$, $T > 0$ and $f : J \rightarrow [0, T)$ be differentiable and monotone increasing. If the tangent vector of $\gamma$ at $f(t)$, $t \in J$, exists, then it holds

$$\dot{\nu}(t) = \dot{f}(t) \cdot \dot{\gamma}(f(t)), \quad \nu(t) := \gamma(f(t)).$$

5 **Wasserstein Steepest Descent Flows**

In this section, we provide an alternative view on Wasserstein gradient flows (6) based on the geometric interpretation that at any point $t \geq 0$ the tangent vector $\dot{\gamma}(t)$ points into an appropriately defined direction of steepest descent. Our approach allows the use of Euler forward schemes which are often easier to implement in comparison to MMSs, which are based on the Euler backward scheme. In particular, the computation of particle gradient flows by simple gradient descent methods, can be seen as space and time discretization of the Euler forward scheme, see Section 8. We like to mention that measure differential
equations with a different definition of the “solution” inclusive Euler forward schemes were considered, e.g. in [40].

For $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$, we define the direction of steepest descent using the following two notations of directional derivatives, where the naming is adopted from [17, proposition. The proof is outlined in Appendix B.2. First, we consider the derivative along the curves $\gamma_{w}$, where $w$ belongs to the (geometric) tangent space. More precisely, the Dini derivative of $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ at $\mu \in \text{dom } \mathcal{F}$ in direction $w \in \mathbf{T}_\mu(\mathcal{P}_2(\mathbb{R}^d))$ is defined (if it exists) by

$$D_w \mathcal{F}(\mu) := \lim_{t \to 0+} \frac{\mathcal{F}(\gamma_{w}(t)) - \mathcal{F}(\mu)}{t} = \frac{d}{dt} \mathcal{F} \circ \gamma_{w}(t) \bigg|_{t=0+}.$$ 

Unfortunately, already in Euclidean spaces the derivative of a function along a curve $\gamma$ at $t$ does not necessarily coincide with the Dini derivative in direction of the tangent of $\gamma$ at $t$. Therefore, we will need a more technical definition. The lower/upper Hadamard derivative of $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ at $\mu \in \text{dom } \mathcal{F}$ in direction $w \in \mathbf{T}_\mu \mathcal{P}_2(\mathbb{R}^d)$ is defined by

$$H^-_w \mathcal{F}(\mu) := \liminf_{w \to v, t \to 0+, \gamma_{w} \to \gamma_{v}, \gamma_{w} \text{ is geodesic}} \frac{\mathcal{F}(\gamma_{w}(t)) - \mathcal{F}(\mu)}{t}, \quad H^+_w \mathcal{F}(\mu) := \limsup_{w \to v, t \to 0+, \gamma_{w} \to \gamma_{v}, \gamma_{w} \text{ is geodesic}} \frac{\mathcal{F}(\gamma_{w}(t)) - \mathcal{F}(\mu)}{t}$$

and the Hadamard derivative (if the upper and lower limit coincide) by

$$H_w \mathcal{F}(\mu) := \lim_{w \to v, t \to 0+, \gamma_{w} \to \gamma_{v}, \gamma_{w} \text{ is geodesic}} \frac{\mathcal{F}(\gamma_{w}(t)) - \mathcal{F}(\mu)}{t},$$

where the convergence $w \to v$ is with respect to $W_\mu$. The functional $\mathcal{F}$ is called Dini or Hadamard differentiable at $\mu$ if its Dini or Hadamard derivative exists for all directions $v \in \mathbf{T}_\mu \mathcal{P}_2(\mathbb{R}^d)$. Note that all these directional derivatives are positively homogeneous (of degree 1) in $v$. If $\mathcal{F}$ is Hadamard differentiable, then it is also Dini differentiable and Hadamard and Dini derivative coincide. For locally Lipschitz continuous functions we have also the opposite direction. Recall that a function $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ is called locally Lipschitz continuous at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, if there exist $L, r > 0$ such that

$$|\mathcal{F}(\nu_1) - \mathcal{F}(\nu_2)| \leq LW_2(\nu_1, \nu_2), \quad \nu_1, \nu_2 \in B_r(\mu)$$

for all $\nu_1, \nu_2 \in B_r(\mu) := \{\nu \in \mathcal{P}_2(\mathbb{R}^d) : W_2(\nu, \mu) < r\} \subset \text{dom } \mathcal{F}$ and locally Lipschitz continuous, if this holds true for all $\mu \in \text{dom } \mathcal{F}$. Note that if $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ is locally Lipschitz, then it is also coercive since

$$\mathcal{F}(\delta_0) - \mathcal{F}(\mu) \leq LW_2(\mu, \delta_0),$$

i.e.

$$F(\mu) \geq \mathcal{F}(\delta_0) - LW_2(\mu, \delta_0) \geq \mathcal{F}(\delta_0) - L\sqrt{r}$$

for all $\mu$ with $W_2^2(\mu, \delta_0) = \int_{\mathbb{R}^d} \|x\|^2 ||d\mu(x) \leq r$. Then it is not hard to show the following proposition. The proof is outlined in Appendix B.2.
Proposition 7. Let $F: \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be locally Lipschitz continuous around $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. If $D_v F(\mu)$ exists for $v \in T_\mu \mathcal{P}_2(\mathbb{R}^d)$, then $D_v F(\mu) = H_v F(\mu)$.

For $F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$, the set of directions of steepest descent at $\mu \in \text{dom } F$ is defined by

$$H_{-} F(\mu) := \left\{ (H^+_v F(\mu))^- \cdot v : v \in \underset{w \in T_\mu \mathcal{P}_2(\mathbb{R}^d),}{\arg \min} H^-_w F(\mu) \right\},$$

if $H^-_v F(\mu)$ exists in $(-\infty, \infty]$ for all $v \in T_\mu \mathcal{P}_2(\mathbb{R}^d)$, where $(t)^- := \max\{-t, 0\}$ for $t \in \mathbb{R}$. There may be no minimal direction, i.e. $H_{-} F(\mu)$ may be empty. On the basis of the introduced directional directions, we are now interested in curves whose tangent $\dot{\gamma}(t)$ points into the direction of steepest descent.

Definition 8. A locally absolutely continuous curve $\gamma: [0, +\infty) \to \mathcal{P}_2(\mathbb{R}^d)$ is called a Wasserstein steepest descent flow with respect to $F$ if $\dot{\gamma}(t)$ exists and satisfies

$$\dot{\gamma}(t) \in H_{-} F(\gamma(t)), \quad t \in [0, +\infty).$$

(13)

It is an open question if every Wasserstein steepest descent flow (13) also satisfies the (weaker) Wasserstein gradient flow equation (6). Note that steepest descent directions can exist also in cases where the so-called extended Fréchet subdifferential related to the Wasserstein gradient flow is empty. However, under certain assumptions on $F$, there exists a unique Wasserstein steepest descent flow and it coincides with the Wasserstein gradient flow of $F$ in (6) for all $t \in [0, +\infty)$.

Proposition 9. Let $F: \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be locally Lipschitz continuous and $\lambda$-convex along generalized geodesics and $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$. Then, there exists a unique Wasserstein steepest descent flow of $F$ starting at $\mu_0$. Moreover, it coincides with the unique Wasserstein gradient flow of $F$ starting at $\mu_0$ determined by Theorem 3.

The assumption of the local Lipschitz continuity can be weakened. However, as the exact formulation of the weaker assumptions requires some more technical notations, we include the more general version of the proposition as well as the proof in B.3.

Remark 10. Definition 8 allows the existence of Wasserstein gradient flows $\gamma$ with initial point $\mu_0 = \lim_{t \to 0^+} \gamma(t) \not\in \text{dom } F$ (if it exists) and slope $\lim_{t \to 0^+} \|\dot{\gamma}(t)\|_{\gamma(t)} = \infty$. That means the steepest descent direction at $\mu_0$ may not exist. In Definition 8 we excluded such curves, since we assume the existence of tangent velocity plans $\dot{\gamma}(t)$ for any $t \geq 0$.

6 Discrepancies

In this paper, we are interested in Wasserstein flows of so-called discrepancies defined with respect to kernels. We restrict our attention to symmetric and conditionally positive definite...
kernels $K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ of order one, i.e., for any $n \in \mathbb{N}$, any pairwise different points $x^1, \ldots, x^n \in \mathbb{R}^d$ and any $a_1, \ldots, a_n \in \mathbb{R}$ with $\sum_{i=1}^n a_i = 0$ the following relation is satisfied:

$$\sum_{i,j=1}^n a_ia_j K(x^i, x^j) \geq 0. \quad (14)$$

If (14) is fulfilled for all $a_1, \ldots, a_n \in \mathbb{R}$, the kernel is just called positive definite. We speak about (conditionally) strictly positive definiteness if we have strict inequality in (14) except for all $a_j$, $j = 1, \ldots, n$ being zero. Examples of strictly positive definite kernels are the Gaussian $K(x_1, x_2) := \exp(\|x_1 - x_2\|/c)$, $c > 0$ and the inverse multiquadric $K(x_1, x_2) := (c^2 + \|x_1 - x_2\|^2)^{-r}$, $c, r > 0$. Strictly conditionally positive definite kernels are the multiquadric $K(x_1, x_2) := -\|x_1 - x_2\|^r$, $r \in (0, 2)$ and the Riesz kernels

$$K(x_1, x_2) := -\|x_1 - x_2\|^r, \quad r \in (0, 2), \quad (15)$$

see [52, p 115] and for more information on Riesz kernels [42].

The $L^2$-discrepancy $D^2_K: \mathcal{P}(\mathbb{R}^d) \times \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$ between two measures $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ is defined by

$$D^2_K(\mu, \nu) := E_K(\mu - \nu)$$

with the so-called $K$-energy on signed measures

$$E_K(\sigma) := \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x_1, x_2) d\sigma(x_1) d\sigma(x_2), \quad \sigma \in \mathcal{M}(\mathbb{R}^d).$$

The relation between discrepancies and Wasserstein distances is discussed in [35]. For fixed $\nu \in \mathcal{P}(\mathbb{R}^d)$, the $L^2$-discrepancy is a functional in $\mu$ and can be decomposed as

$$F_\nu(\mu) = D^2_K(\mu, \nu) = E_K(\mu) + V_{K,\nu}(\mu) + \underbrace{E_K(\nu)}_{\text{const.}} \quad (16)$$

with the interaction energy on probability measures

$$E_K(\mu) = \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x_1, x_2) d\mu(x_1) d\mu(x_2), \quad \mu \in \mathcal{P}_2(\mathbb{R}^d) \quad (17)$$

and the potential energy of $\mu$ with respect to the potential of $\nu$,

$$V_{K,\nu}(\mu) := \int_{\mathbb{R}^d} V_{K,\nu}(x_1) d\mu(x_1), \quad V_{K,\nu}(x_1) := -\int_{\mathbb{R}^d} K(x_1, x_2) d\nu(x_2). \quad (18)$$

By the following proposition, the discrepancy of the Riesz kernel (15) with $r \in [1, 2)$ is locally Lipschitz continuous in each argument for $r \in [1, 2)$. The proof is given in Appendix C.
Proposition 11. For the Riesz kernel (15) with \( r \in [1, 2) \), the interaction energy \( \mathcal{E}_K \) in (17) and the potential energy \( \mathcal{V}_{K, \nu} \), \( \nu \in \mathcal{P}_2(\mathbb{R}^d) \), in (18) are locally Lipschitz continuous.

Since the negative Riesz kernel (15) is convex for \( r \in [1, 2) \), the negative interaction energy \( -\mathcal{E}_K \) is convex along generalized geodesics by [2, Prop 9.3.5]. Similarly, the potential energy \( \mathcal{V}_{K, \nu} \) is convex along (generalized) geodesics by [2, Prop 9.3.2]. However, by the following proposition, \( \mathcal{E}_K \) itself and then discrepancies \( D^2_K \) are not \( \lambda \)-convex along geodesics.

Proposition 12. Let \( K \) be the Riesz kernel (15) on \( \mathbb{R}^d \), \( d \geq 2 \). Then we have for any \( \lambda \in \mathbb{R} \) the following:

(i) The interaction energy \( \mathcal{E}_K \) is not \( \lambda \)-convex along geodesics.

(ii) The discrepancy \( D^2_K(\cdot, \delta_x) \), \( x \in \mathbb{R}^d \) is not \( \lambda \)-convex along geodesics.

**Proof.** Part (i). To this end, we consider the line segments

\[
x_s(t) := (s, (1 - 2t) \frac{s}{2}, 0, \ldots, 0) \in \mathbb{R}^d, \quad t \in [0, 1],
\]

and the geodesics between \( \mu := \frac{1}{2} \delta_0 + \frac{1}{2} \delta_{x_s(0)} \) and \( \nu := \frac{1}{2} \delta_0 + \frac{1}{2} \delta_{x_s(1)} \) for \( s > 0 \). Since the unique optimal transport between \( \mu \) and \( \nu \) is induced by the map \( 0 \mapsto 0 \) and \( x_s(0) \mapsto x_s(1) \), these geodesics may be written as \( \gamma_s(t) := \frac{1}{2} \delta_0 + \frac{1}{2} \delta_{x_s(t)} \), see Proposition 2. Furthermore, the Wasserstein distance is given by \( W^2_2(\mu, \nu) = \frac{1}{2} s^2 \). Evaluating the interaction energy gives

\[
\mathcal{E}_K(\mu) = \mathcal{E}_K(\nu) = -\frac{\|x_s(0)\|}{4} = -\left(\frac{5}{16}\right) \frac{1}{4} s^2 \quad \text{and} \quad \mathcal{E}_K(\gamma_s(\frac{1}{2})) = -\frac{s^2}{4}.
\]

If \( \mathcal{E}_K \) is \( \lambda \)-convex along \( \gamma_s \), then, for \( \lambda = \frac{1}{2} \), it has to fulfill

\[
-\frac{s^2}{4} \leq -\left(\frac{5}{16}\right) \frac{1}{4} s^2 - \lambda \frac{s^2}{16} \quad \text{and thus} \quad \lambda \leq \left(1 - \left(\frac{5}{16}\right)\right) \frac{4}{s^2 - s^2}.
\]

Considering the limit \( s \to 0^+ \), we notice that \( \lambda \) cannot be bounded from above.

Part (ii). Without loss of generality, we consider the case \( x := -e_1 \), where \( e_1 \in \mathbb{R}^d \) is the first unit vector. Then we obtain

\[
D^2_K(\gamma_s(t), \delta_{-e_1}) = \frac{\|e_1\|^r}{2} + \frac{\|e_1 + x_s(t)\|^r}{2} - \frac{\|x_s(t)\|^r}{4}
\]

and thus

\[
D^2_K(\mu, \delta_{-e_1}) = D^2_K(\nu, \delta_{-e_1}) = \frac{1}{2} + \left(1 + \frac{1}{s}\right)^2 + \frac{1}{4} \frac{s^r}{2} - \left(\frac{5}{16}\right) \frac{1}{4} s^r,
\]

\[
D^2_K(\gamma_s(\frac{1}{2}), \delta_{-e_1}) = \frac{1}{2} + \left(1 + \frac{1}{s}\right)^2 \frac{s^r}{2} - \frac{s^r}{4}.
\]
If $D_K^2$ is $\lambda$-convex along $\gamma_s$, then, for $\lambda = \frac{1}{2}$, it has to fulfill
\[
\frac{1}{2} + \left(\left(1 + \frac{1}{s}\right)^2 + \frac{s^r}{2} - \frac{s^r}{4}\right) \leq \frac{1}{2} + \left(\left(1 + \frac{1}{s}\right)^2 + \frac{1}{4}\right)^{\frac{r}{s}} - \left(\frac{5}{4}\right)^{\frac{r}{s}} (s^r - \lambda s^2) \frac{16}{16}
\]
and thus
\[
\lambda \leq \left[2 \left(\left(1 + \frac{1}{s}\right)^2 + \frac{1}{4}\right)^{\frac{r}{s}} - 2 \left(\left(1 + \frac{1}{s}\right)^2 + 1 - \left(\frac{5}{4}\right)^{\frac{r}{s}}\right)\right]\frac{4}{s^{2r}}. \tag{19}
\]

The first difference in the bracket may be estimated using the mean value theorem and the monotonicity of the derivative of the exponential $e^{x^2}$, which yields
\[
\left|\left(\left(1 + \frac{1}{s}\right)^2 + \frac{1}{4}\right)^{\frac{r}{s}} - \left(\left(1 + \frac{1}{s}\right)^2\right)^{\frac{r}{s}}\right| \leq \frac{1}{4} \cdot \frac{r}{2} \left(1 + \frac{1}{s}\right)^{2r}.
\]
Thus the first difference converges to zero for $s \to 0+$. Since the second difference is a negative constant, the right-hand side of (19) tend to $-\infty$; so $\lambda$ cannot be a global constant. \qed

### 7 Interaction Energy Flows

In this section, we focus on the explicit calculation of Wasserstein steepest descent flows of the interaction energy $E_K$ for the Riesz kernels (15) in particular, when starting at $\mu = \delta_p$, $p \in \mathbb{R}^d$. Since the functional $E_K$ is no longer $\lambda$-convex along geodesics in $d \geq 2$ dimensions, the analysis of [2] is not applicable for this case. However, we show that the MMS (8) still converges, and that the limit curve is a Wasserstein steepest descent flow for $r \in [1, 2)$. We like to mention that this strengthens the convergence result in [8, Prop 4.2.2], where it is only shown that the MMS has a cluster point for $r = 1$.

Recall that the set $H^- E_K(\mu)$ of steepest descent directions is given by all $(H_v^- E_K(\mu))^* \cdot v^*$, where $v^*$ solves the constrained optimization problem
\[
\arg \min_{v \in T_{\mu}\mathcal{P}_2(\mathbb{R}^d)} H^- v E_K(\mu) \quad \text{s.t.} \quad \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_2\|^2 dv(x_1, x_2) = 1. \tag{20}
\]
Therefore, we start by computing the directional derivatives of $E_K$.

**Theorem 13.** Let $K$ be a Riesz kernel (15). Then the Hadamard derivative at $\delta_p$ in direction $v = \delta_p \otimes \eta \in T_{\delta_p}\mathcal{P}_2(\mathbb{R}^d)$ is given by
\[
H_v E_K(\delta_p) = \begin{cases} E_K(\eta), & r = 1, \\ 0, & r \in (1, 2). \end{cases}
\]
For $r \in (0, 1)$, we have for the Dini derivative at $\delta_p$ in direction $v = \delta_p \otimes \eta \in T_{\delta_p}\mathcal{P}_2(\mathbb{R}^d)$ that
\[
H^- v E_K(\delta_p) \leq D_v E_K(\delta_p) = \begin{cases} -\infty, & \eta \not\in \{\delta_q : q \in \mathbb{R}^d\}, \\ 0, & \eta \in \{\delta_q : q \in \mathbb{R}^d\}. \end{cases}
\]
Proof. For $v = \delta_p \otimes \eta$, we have $\gamma(v)(t) = \gamma_{t, v}(1) = ((1 - t)p + t \text{Id})_{\#} \eta$ and then

$$E_K(\gamma(v)(t)) = -\frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \|x_1 - x_2\|^2 d[\gamma(v)](x_1) d[\gamma(v)](x_2)$$

$$= -|t|^r \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \|x_1 - x_2\|^2 d\eta(x_1) d\eta(x_2).$$

Then the assertion follows for the Dini derivative by taking the right-hand side derivative of $E_K \circ \gamma(v)$ at $t = 0$. By Proposition 11, we know that $E_K$ is locally Lipschitz for Riesz kernels (15) with $r \in [1, 2]$. Then, by Proposition 7, the Dini- and Hadamard derivative coincide which completes the proof. \hfill \Box

Part (i) of the theorem implies in particular, that there exists no Wasserstein steepest descent flow of $E_K$ starting at $\delta_p$, if $K$ is a Riesz kernel (15) with $r \in (0, 1)$. Moreover, for $r \in (1, 2)$, a possible Wasserstein steepest descent flow starting at $\delta_p$ is given by the constant curve $\gamma(t) = \delta_p$. This curves are moreover Wasserstein gradient flows in the sense of (6).

**Proposition 14.** Let $K$ be the Riesz kernel (15) for $r \in (1, 2]$ and $p \in \mathbb{R}^d$. Then $\gamma: [0, +\infty) \to \mathcal{P}_2(\mathbb{R}^d): t \mapsto \delta_p$ is a Wasserstein gradient flow.

**Proof.** Wlog, let $p = 0$. The velocity field $v_t \in \mathbb{T}_{\gamma(t)}\mathcal{P}_2(\mathbb{R}^d)$ corresponding to $\gamma$ is given by $v_t = 0$. Thus, we have to show that $0 \in \partial E_K(\delta_0)$, i.e., that $\liminf_{\nu \to \delta_0} E_K(\nu)/W_2(\nu, \delta_0) \geq 0$. To this end, we bound $E(\nu)$ from below. Since $E_K$ is locally Lipschitz continuous, there exist $L > 0$ and $\epsilon > 0$ such that for all $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ with $W_2(\nu, \delta_0) \leq \epsilon$ it holds $E_K(\nu) = E_K(\nu) - E_K(\delta_0) \geq -L W_2(\nu, \delta_0) \geq -L \epsilon$. Moreover, we have by the definition of $E_K$ for $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ and $c \geq 0$ that

$$E_K((c \text{Id})_{\#} \nu) = c c' E_K(\nu), \quad W_2((c \text{Id})_{\#} \nu, \delta_0) = c W_2(\nu, \delta_0).$$

Now let $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ with $W_2(\nu, \delta_0) \leq \epsilon$. Then, we get for $c = \epsilon/W_2(\nu, \delta_0)$ that $W_2((c \text{Id})_{\#} \nu, \delta_0) = \epsilon$, which implies

$$E_K(\nu) = E_K((c^{-1} \text{Id})_{\#}(c \text{Id})_{\#} \nu) = c^{-r} E_K((c \text{Id})_{\#} \nu) 
\geq -c^{-r} L \epsilon = -L \epsilon^{1-r} W_2(\nu, \delta_0)^r.$$ 

Finally, we conclude

$$\liminf_{\nu \to \delta_0} \frac{E_K(\nu)}{W_2(\nu, \delta_0)} \geq \liminf_{\nu \to \delta_0} -L \epsilon^{1-r} W_2(\nu, \delta_0)^{r-1} = 0. \hfill \Box$$
For simplicity, we restrict our attention to the case $p = 0$, but similar conclusions can be drawn for arbitrary $p \in \mathbb{R}^d$. For $r = 1$ and $\mu = \delta_0$, we obtain by Theorem 13 that the solution of constrained problem (20) is given by $v^* = \delta_0 \otimes \eta^*$, where
\[
\eta^* \in \arg \min_{\eta \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{E}_K(\eta) \quad \text{s.t.} \quad \int_{\mathbb{R}^d} \|x\|^2_2 \, d\eta(x) = 1. \quad (21)
\]
On the other hand, the first step of the MMS (8) for $\mathcal{F} = \mathcal{E}_K$ starting at $\mu_0 = \delta_0$ reads as
\[
\eta^*_\tau := \text{prox}_{\tau \mathcal{E}_K}(\delta_0) \in \arg \min_{\eta \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{E}_K(\eta) + \frac{1}{2\tau} \int_{\mathbb{R}^d} \|x\|^2_2 \, d\eta(x), \quad (22)
\]
which appears to be the penalized form of (21). The minimization problem (22) is a special case of the classical potential theory problem
\[
\inf_{\eta \in \mathcal{P}(A)} \mathcal{E}_K(\eta) + \int_A V(x) \, d\eta(x), \quad (23)
\]
where $\mathcal{P}(A)$ denotes the set of Borel probability measures on $A \subset \mathbb{R}^d$, see [10, 43]. This problem is still a field of active research, see, e.g., [14, 15, 34]. If the minimizer of (23) exists, then it is called an equilibrium measure for the external field $V$. In this context, the existence and uniqueness of solutions of the penalized problem (22) are immediate consequences of well-established results in potential theory as we will see in the next proposition.

**Proposition 15.** Let $K$ be the Riesz kernel with $r \in (0, 2)$ and $\tau > 0$ be given. Then problem (22) has a unique solution $\eta^*_\tau \in \mathcal{P}_2(\mathbb{R}^d)$ which fulfills
\begin{enumerate}[(i)]  
  \item $|\mathcal{E}_K(\eta^*_\tau)| < \infty$,  
  \item $\text{supp}(\eta^*_\tau)$ is compact,  
  \item orthogonal invariance $O \# \eta^*_\tau = \eta^*_\tau$, where $O \in O(d) := \{O \in \mathbb{R}^{d \times d} : O^T O = I\}$.  
\end{enumerate}
Furthermore, $\eta^*_\tau$ is the minimizer of (22) if and only if there exist $C_{K, \tau} \in \mathbb{R}$ such that
\[
\begin{align*}
\int_{\mathbb{R}^d} K(x_1, x_2) \, d\eta^*_\tau(x_2) + \frac{1}{2\tau} \|x_1\|^2_2 & \geq C_{K, \tau}, \quad x_1 \in \mathbb{R}^d,  \\
\int_{\mathbb{R}^d} K(x_1, x_2) \, d\eta^*_\tau(x_2) + \frac{1}{2\tau} \|x_1\|^2_2 & = C_{K, \tau}, \quad x_1 \in \text{supp}(\eta^*_\tau).  
\end{align*} \quad (24)
\]
**Proof.** Considering (23) with $V(x) = \frac{1}{2\tau} \|x\|^2_2$ and $A = \mathbb{R}^d$, we obtain (22) up to the subtle difference that the minimization takes place over $\mathcal{P}(\mathbb{R}^d)$ instead of $\mathcal{P}_2(\mathbb{R}^d)$. The unique minimizer $\eta^*_\tau \in \mathcal{P}(\mathbb{R}^d)$ of this problem satisfies (i) and (ii), see [10, Cor 4.4.16(c)], such that $\eta^*_\tau \in \mathcal{P}_2(\mathbb{R}^d)$ is also the (unique) minimizer of (22). In particular, for any compact
Let obtain the second claim. \(A \subset \mathbb{R}^d\) with \(\text{supp}(\eta^*_r) \subset A\), the minimizer of (23) is \(\eta^*_r|_A\). Moreover, \(\eta^*_r|_A\) is characterized by the optimality conditions (24) (restricted to \(x \in A\)), cf. \([10, \text{Thm 4.2.14–Thm 4.2.16}]\). Since \(A\) can be arbitrarily large, the optimality conditions characterize also \(\eta^*_r\) on \(\mathbb{R}^d\), which concludes the proof.

The following proposition shows how the penalized problem is related to the constrained.

**Proposition 16.** Let \(K\) be a Riesz kernel \((15)\) with \(r \in (0, 2)\).

(i) Then \(\eta^* \in \mathcal{P}_2(\mathbb{R}^d)\) minimizes (21) if and only if \(\eta^* = (c_\tau \text{ Id})\# \eta^*\) minimizes (22), where \(c_\tau := (-\tau r \mathcal{E}_K(\eta^*))^{1/(2-r)}\).

(ii) Vice versa, \(\eta^*_r \in \mathcal{P}_2(\mathbb{R}^d)\) minimizes (22) if and only if \(\eta^* = (c_\tau^{-1} \text{ Id})\# \eta^*_r\) minimizes (21), where \(c_\tau := (\int_{\mathbb{R}^d} \|x\|^2 \, d\eta^*_r(x))^{1/2}\).

**Proof.** Let \(\tau > 0\) be the fixed step in (22). For any \(c_\tau > 0\) and \(\eta^*_r \in \mathcal{P}_2(\mathbb{R}^d)\), we have \(\mathcal{E}_K((c_\tau \text{ Id})\#\eta^*_r) = c_\tau^2 \mathcal{E}_K(\eta^*_r)\). Then the objective in (22) can be rewritten as

\[
\inf_{c_\tau > 0} \inf_{\eta^*_r \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{E}_K(\eta^*_r) + \frac{1}{2\tau} c_\tau^2 \quad \text{s.t.} \quad \int_{\mathbb{R}^d} \|x\|^2 \, d\eta^*_r(x) = c_\tau^2
\]

\[
= \inf_{c_\tau > 0} \inf_{\eta^*_r \in \mathcal{P}_2(\mathbb{R}^d)} c_\tau^2 \mathcal{E}_K((c_\tau^{-1} \text{ Id})\#\eta^*_r) + \frac{1}{2\tau} c_\tau^2 \quad \text{s.t.} \quad \int_{\mathbb{R}^d} \|x\|^2 \, d(c_\tau^{-1} \text{ Id})\#\eta^*_r(x) = 1
\]

\[
= \inf_{c_\tau > 0} c_\tau \left( \inf_{\eta \in \mathcal{P}_2(\mathbb{R}^d)} \mathcal{E}_K(\eta) \right) + \frac{1}{2\tau} c_\tau^2 \quad \text{s.t.} \quad \int_{\mathbb{R}^d} \|x\|^2 \, d\eta(x) = 1,
\]

where \(\eta = (c_\tau^{-1} \text{ Id})\#\eta^*_r\). Now, the set of minimizer with respect to \(\eta\) is given by the set of all solutions \(\eta^*\) of (21). Thus, the set of solutions of (22) is empty if and only if the set of solutions of (21) is empty. Further, setting the derivative with respect to \(c_\tau\) to 0 yields that the minimizer \(c_\tau^*\) has to fulfills

\[0 = r (c_\tau^*)^{r-1} \mathcal{E}_K(\eta^*) + \frac{1}{\tau} c_\tau^* \quad \iff \quad c_\tau^* = (-\tau r \mathcal{E}_K(\eta^*))^{1/(2-r)}\).

It is easy to verify that \(\eta^* \neq \delta_0\) such that \(\mathcal{E}_K(\eta^*) < 0\) and \(2 - r > 0\) ensuring that this expression is well-defined. In summary, we obtain that \(\eta^*_r\) is a solution of (22) if and only if \(\eta^*_r = (c_\tau \text{ Id})\#\eta^*\) for some solution \(\eta^*\) of (21) and \(c_\tau = (-\tau r \mathcal{E}_K(\eta^*))^{1/(2-r)}\). Following the arguments in the reverse direction and noting that (25) implies \(c_\tau^2 = \int_{\mathbb{R}^d} \|x\|^2 \, d\eta^*_r\), we obtain the second claim.

In the following, we denote by \(U_A\) the uniform distribution on \(A\).

**Theorem 17.** Let \(K\) be a Riesz kernel \((15)\) with \(r \in (0, 2)\). Then the solution \(\eta^*_r\) of (22) is
(i) for $d + r < 4$ given by
\[
\eta^*_r = \rho_s \mathcal{U}_{s, \mathbb{S}^d}, \quad \rho_s(x) := A_s (s^2 - \|x\|^2)^{1 - \frac{r}{2}}, \quad x \in s \mathbb{S}^d,
\]
where $\mathbb{S}^d := \{x \in \mathbb{R}^d : \|x\|_2 \leq 1\}$ and
\[
A_s := \frac{\Gamma(\frac{d}{2})}{\pi^{\frac{d}{2}} B\left(\frac{d}{2}, 2 - \frac{r}{2}\right)} s^{-(2-r)}, \quad s_r := \left(\frac{\Gamma(2 - \frac{r}{2}) \Gamma(\frac{d + r}{2}) r \tau}{2 \Gamma(\frac{d}{2})}\right)^{\frac{1}{2-r}}
\]
with the Beta function $B$ and the Gamma function $\Gamma$.

(ii) for $d + r \geq 4$ given by
\[
\eta^*_r = \mathcal{U}_{c_r, \mathbb{S}^{d-1}}, \quad c_r := (-\tau r \mathcal{E}_K(\eta^*))^{1/(2-r)},
\]
where $\eta^* = \mathcal{U}_{\mathbb{S}^{d-1}}, \mathcal{E}_K(\eta^*) = -\frac{1}{2} F_1(-\frac{r}{2}, \frac{2-r-d}{2}; \frac{d}{2}; 1)$ with the hypergeometric function $\mathcal{E}_K(\eta^*)$.

The proof is given in D.1. The special case $d = 3$ and $r = 1$ was recently also handled in [16]. Note that for $d \geq 3$ and $r \in [1, 2)$ the densities $\rho_s$ are not integrable anymore.

Interestingly, for $d = 3$, we observe a so-called condensation phenomenon starting at $r = 1$, where the absolutely continuous measure switches to a singular one. A similar phenomenon was recognized for the logarithmic kernel $K(x_1, x_2) = -\log \|x_1 - x_2\|$, corresponding to $r = 0$ and $d \geq 4$ in [16, Thm 1.2: (i)(b)].

For the case $r = 1$, in which we are mainly interested, we obtain the following analytic expressions for the solution $\eta^*$ of the constrained problem and the steepest descent direction $H_{-\mathcal{E}_K(\delta_p)}$. The corollary straightforwardly follows from the relation $\eta^* = (c_r^{-1} \text{Id})_{\mathbb{S}^d} \eta^*_r$ in Proposition 16 and since $-H_{\delta_p \otimes \eta^*} \mathcal{E}_K(\delta_p) = -\mathcal{E}_K(\eta^*)$ and $H_{-\mathcal{E}_K(\delta_p)} = (-H_{\delta_p \otimes \eta^*} \mathcal{E}_K(\delta_p)) \cdot (\delta_p \otimes \eta^*)$ by Theorem 13.

**Corollary 18.** Let $K$ be a Riesz kernel (15) with $r = 1$. Then the solution $\eta^*$ of (21) and the steepest descent directions of $\mathcal{E}_K$ at $\delta_p$ are given as follows:

- (i) For $d = 1$: $\eta^* = \mathcal{U}_{[-\sqrt{3}, \sqrt{3}]^2}$ and $H_{-\mathcal{E}_K(\delta_p)} = \{\delta_p \otimes \mathcal{U}_{[-1, 1]}\}$.

- (ii) For $d = 2$: $\eta^* = \rho \sqrt{3/2} \mathcal{U}_{\sqrt{3/2} \mathbb{S}^2}$ and $H_{-\mathcal{E}_K(\delta_p)} = \{\delta_p \otimes \rho \mathcal{U}_{\mathbb{S}^2}\}$, where $\rho_s$ is the density function $\rho_s(x) := \frac{1}{2\pi s} (s^2 - \|x\|^2)^{-\frac{1}{2}}, \quad x \in s \mathbb{S}^2$.

- (iii) For $d \geq 3$: $\eta^* = \mathcal{U}_{\mathbb{S}^{d-1}}$ and $H_{-\mathcal{E}_K(\delta_p)} = \{\delta_p \otimes \mathcal{U}_{R_d \mathbb{S}^{d-1}}\}$, where $R_d := \frac{1}{2} F_1(-\frac{1}{2}, -\frac{d-1}{2}; \frac{d}{2}; 1)$ with the hypergeometric function $\mathcal{E}_K(2F_1)$.

There is the following interesting link between the measures $\eta^*$ in dimensions $d = 1, 2, 3$ which states that they follow by projecting the measure from the higher dimensional space to the lower dimensional one.
Corollary 19. Consider the rescaled measure \( \mu_d := (C_d \text{Id})_\# \eta^* \) of Corollary 17 with \( r = 1 \), where \( C_d > 0 \) is chosen such that

\[
\text{supp}(\mu_d) = \begin{cases} 
\mathbb{B}^d, & d = 1, 2, \\
\mathbb{S}^2, & d = 3.
\end{cases}
\]

Then \( \mu_d \) can be considered as a projection of \( \mu_{d'} \) onto a \( d \)-dimensional subspace \( X_d \subset \mathbb{R}^{d'} \), more precisely \( \mu_d = (\pi_1, \ldots, \pi_d)_\# \mu_{d'}, \ 1 \leq d \leq d' \leq 3 \).

Proof. For the case \( d = 2 \), we obtain for the sets

\[
A_{\theta_1, \theta_2}^{\varphi_1, \varphi_2} := \{ x \in \mathbb{R}^2 : x = (\sin(\theta) \cos(\varphi), \sin(\theta) \sin(\varphi)) \}, \ \theta_1 \leq \theta \leq \theta_2, \ \varphi_1 \leq \varphi \leq \varphi_2 \},
\]

where \( 0 \leq \theta_1 \leq \theta \leq \theta_2 \leq \frac{\pi}{2} \), \( \varphi_1 \leq \varphi \leq \varphi_2 \) that

\[
(\pi_{1,2})_\# \mathcal{U}_{\mathbb{S}^2}(A_{\theta_1, \theta_2}^{\varphi_1, \varphi_2}) = \frac{2}{4\pi} \int_{\theta_1}^{\theta_2} \int_{\varphi_1}^{\varphi_2} d\varphi \sin(\theta) d\theta = \frac{1}{2\pi} (\varphi_2 - \varphi_1)(\cos(\theta_1) - \cos(\theta_2)).
\]

Since

\[
\rho_1 \mathcal{U}_{\mathbb{B}^2}(A_{\theta_1, \theta_2}^{\varphi_1, \varphi_2}) = \frac{1}{2\pi} \int_{\sin(\theta_1)}^{\sin(\theta_2)} \int_{\varphi_1}^{\varphi_2} \sin(\theta_1) d\varphi (1 - r^2)^{-\frac{3}{2}} dr \]

\[
= \frac{1}{2\pi} (\varphi_2 - \varphi_1)(\sqrt{1 - \sin(\theta_1)^2} - \sqrt{1 - \sin(\theta_2)^2}),
\]

we have \((\pi_{1,2})_\# \mathcal{U}_{\mathbb{S}^2}(A_{\theta_1, \theta_2}^{\varphi_1, \varphi_2}) = \rho_1 \mathcal{U}_{\mathbb{B}^2}(A_{\theta_1, \theta_2}^{\varphi_1, \varphi_2})\) and arrive at the assertion since the sets \( A_{\theta_1, \theta_2}^{\varphi_1, \varphi_2} \) generate the Borel \( \sigma \)-algebra on \( \mathbb{B}^2 \).

For the case \( d = 1 \), using \((\pi_{1})_\# \mathcal{U}_{\mathbb{S}^2} = (\pi_{1})_\# (\pi_{1,2})_\# \mathcal{U}_{\mathbb{S}^2} = (\pi_{1})_\# \rho_1 \mathcal{U}_{\mathbb{B}^2} \), it is sufficient to show that \((\pi_{1})_\# \rho_1 \mathcal{U}_{\mathbb{B}^2} = \frac{1}{2\pi} \mathcal{U}_{[-1,1]} \). This follows from integration of the density \( \rho_1(x) \) along the lines \( l_s = \{ x = (x_1, x_2) \in \mathbb{R}^2 : x_1 = s \} \) giving

\[
\frac{2}{2\pi} \int_{0}^{\sqrt{1-s^2}} (1 - (s^2 + t^2))^{-\frac{1}{2}} dt = \int_{0}^{s'} (s'^2 - t^2)^{-\frac{1}{2}} dt = \frac{1}{2}, \quad -1 < s < 1,
\]

which is the density of \( \mathcal{U}_{\mathbb{B}^1} \).

\[ \square \]

To determine the whole steepest descent flow, we need also the steepest descent directions at more general measures than just point measures. The proof is in D.2.

Theorem 20. Let \( K \) be a Riesz kernel (15) with \( r \in [1, 2] \) and \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \), where we assume that \( \mu(\{x\}) = 0, \ x \in \mathbb{R}^d \) in case \( r = 1 \). Then the unique steepest descent direction is given by

\[
H_\mathcal{E}_K(\mu) = \{ (\text{Id}, -\nabla G)_\# \mu \}, \quad G(x_1) := \int_{\mathbb{R}^d} K(x_1, x_2) d\mu(x_2).
\]
For the one-dimensional setting, a complete formula for the steepest descent direction was given in [9, Prop 5.4]. Now we are in the position to show the existence of non-trivial Wasserstein steepest descent flows for $r \in [1, 2)$.

**Theorem 21.** Let $K$ be a Riesz kernel with $r \in [1, 2)$ and $\eta^*$ be the unique solution of the constrained problem (21). Then the curve $\gamma : [0, \infty) \to \mathcal{P}_2(\mathbb{R}^d)$ given by

$$
\gamma(t) := (\alpha_t \text{Id}) \# \eta^*, \quad \alpha_t := (-t r (2 - r) E_K(\eta^*))^{1/2},
$$

(26)
is a steepest descent flow starting at $\gamma(0) = \delta_0$.

The proof is given in D.3.

In the case $r = 1$, we obtain for example the curves

$$
\gamma(t) = (-t \mathcal{E}_K(\eta^*) \text{Id}) \# \eta^* = \begin{cases} 
\mathcal{U}_{(-t,t)}, & d = 1, \\
\frac{\pi^2}{8} (\frac{2 \pi^2 t^2}{16} - ||x||^2_2)^{-\frac{3}{2}} U_{t \frac{\pi^2}{8} \mathbb{B}^2}, & d = 2, \\
\mathcal{U}_{t R_d \mathbb{S}^{d-1}}, & d \geq 3,
\end{cases}
$$

where the constant $R_d$ is given in Corollary 17(iii).

**Remark 22.** (i) With the same proof, we can see that the curve (26) also fulfills the steepest descent condition $\dot{\gamma}(t) \in H_{-\mathcal{E}_K}(\gamma(t))$ for $r \in (0, 1)$ if $t > 0$. However, by Theorem 13, the set $H_{-\mathcal{E}_K}(\gamma(0)) = H_{-\mathcal{E}_K}(\delta_0)$ is empty for $r \in (0, 1)$, so that this curve is not a Wasserstein steepest descent flow in the sense of Definition 8.

(ii) For $r \in (1, 2)$, we obtain together with the trivial solution an infinite family of Wasserstein steepest descent flows starting at $\delta_0$. These are parameterized by the 'length of stay' $t_0 \in \mathbb{R}_{\geq 0}$ at $\delta_0$ due to

$$
\gamma(t) = \begin{cases} 
\delta_0, & \text{for } t < t_0, \\
(\alpha_{t-t_0} \text{Id}) \# \eta^*, & \text{for } t \geq t_0.
\end{cases}
$$

(27)

**Remark 23** (Relation to MMS and Wasserstein Gradient Flows). In [1], the MMS steps for $\mathcal{E}_K$ are computed analytically, and it turns out that the scheme converges to the curves in (26). Note that Theorem 3 here cannot be applied since $\mathcal{E}_K$ is not $\lambda$-convex along geodesics. Indeed, Proposition 14 shows the existence of Wasserstein gradient flows that cannot be represented as MMS limits. Vice versa, it is an open question if limits of MMS are Wasserstein gradient flows. For this direction, the $\lambda$-convexity requirement can be weakened towards a regularity assumption by [2, Thm 11.3.2]. Nevertheless, it is still unclear if $\mathcal{E}_K$ fulfills this regularity assumption.
8 Discrepancy Flows

In the following, we determine steepest descent flows of the discrepancy functional \( F_\nu := D^2_K(\cdot, \nu) \) for the Riesz kernel \( K \) with \( r \in [1, 2) \). For \( r \in (1, 2) \), where the Riesz kernel is differentiable, we characterize the Wasserstein steepest descent flow of \( F_\delta_q \) starting at \( \delta_p \). We provide a numerical simulation via particle flows for \( r \in [1, 2) \). In contrast to the case \( r \geq 2 \), the particle explodes here.

The next theorem, which proof is given in E, describes the steepest descent direction of the discrepancy functional.

**Theorem 24.** Let \( F_\nu := D^2_K(\cdot, \nu) \), where \( \nu \in P_2(\mathbb{R}^d) \) and \( K \) is the Riesz kernel (15) with \( r \in [1, 2) \). Then the following holds true.

(i) For \( \mu \in P_2(\mathbb{R}^d) \), where \( \mu(x) = 0 \) for all \( x \in \mathbb{R}^d \) in case \( r = 1 \), the unique steepest descent direction is given by

\[
H_{-F_\nu}(\mu) = \{ (\text{Id}, -\nabla G)_{\#}\mu \}, \quad G(x_1) := \int_{\mathbb{R}^d} K(x_1, x_2) \, d\mu(x_2) + V_{K, \nu}(x_1).
\]

(ii) For \( p \in \mathbb{R}^d \) with \( \nu(\{p\}) = 0 \), the steepest descent direction at \( \delta_p \) is given by

\[
H_{-F_\nu}(\delta_p) = \begin{cases} 
\delta_p \otimes (-\mathcal{E}_K(\eta^*) \text{Id} - \nabla V_{K, \nu}(p))_{\#}\eta^*, & r = 1, \\
\delta_p \otimes \delta_{-\nabla V_{K, \nu}(p)}, & r \in (1, 2),
\end{cases}
\]

where \( \eta^* \) is defined in Corollary 17 and \( V_{K, \nu} \) in (18).

Based on these steepest descent directions, we see in the next proposition that, for differentiable Riesz kernels, there exists a steepest descent flow for \( D^2_K(\cdot, \delta_q) \), \( q \in \mathbb{R}^d \), which has the form of a particle flow.

**Proposition 25.** Let \( F_\nu := D^2_K(\cdot, \delta_q) \), where \( q \in \mathbb{R}^d \), and let \( K \) be the Riesz kernel with \( r \in (1, 2) \). A Wasserstein steepest descent flow starting at \( \delta_p, p \in \mathbb{R}^d \), is given by

\[
\gamma(t) := \begin{cases} 
\delta_{x(t)}, & t \in [0, t_*), \\
\delta_q, & t \in [t_*, \infty),
\end{cases} \quad \text{with} \quad t_* := \frac{q - p}{r(2 - r)} \left( \frac{2^{-r}}{2} - r(2 - r)t \right)^{\frac{1}{2-r}},
\]

where

\[
x(t) := q - \frac{q - p}{\|q - p\|_2^2} \left( \frac{2^{-r}}{2} - r(2 - r)t \right)^{\frac{1}{2-r}}.
\]

**Proof.** The tangent vector of the curve \( t \mapsto x(t) \) in (29) is given by

\[
\dot{x}(t) = r \frac{q - p}{\|q - p\|_2^2} \left( \frac{2^{-r}}{2} - r(2 - r)t \right)^{\frac{1}{2-r}-1}
= r (q - x(t)) \left( \frac{2^{-r}}{2} - r(2 - r)t \right)^{-1}.
\]
Therefore, the particle \( x(t) \) solves the gradient flow equation
\[
\dot{x}(t) = -\nabla V_{K,\delta_q}(x(t)), \quad t \in [0, t_*), \quad x(0) = p,
\]
where
\[
V_{K,\delta_q}(x) := \|q - x\|_2^r, \quad \nabla V_{K,\delta_q}(x) = -r(q - x)\|q - x\|_2^{r-2}, \quad x \in \mathbb{R}^d \setminus \{q\}.
\]
Thus, by Theorem 24, the curve (28) is a Wasserstein steepest descent flow for \( t \in [0, t_*) \).

For \( t \geq t_* \), we have \( \dot{\gamma}(t) = \delta_q \otimes \delta_0 \), which is here the direction of steepest descent since \( \delta_q \) is the global minimizer of \( D^2_K(\cdot, \delta_q) \).

Moreover, we expect that there exists an infinite family of Wasserstein steepest descent flows similar to the family given in (27) for the interaction energy. That means at any time point \( 0 \leq t_0 < t_* \), the point mass \( \gamma(t) \) in (28) may explode to an absolutely continuous measure leading to another Wasserstein steepest descent flow. Unfortunately, the analytic computation of the whole flow describing this effect is much more difficult than for the interaction energy. Therefore, we provide some numerical simulations using an Euler forward scheme.

**Numerical simulation.** Let \( K \) be again the Riesz kernel (15) with \( r \in [1, 2) \), and let \( e_1 \) be the first unit vector. In the following, we want to approximate the discrepancy flow with respect to \( F_{\delta_{e_1}} = D^2_K(\cdot, \delta_{e_1}) \) in \( \mathbb{R}^d \). To this end, we restrict the set of feasible measures to the set of point measures located at exactly \( M \) points, i.e., to the set
\[
S_M := \left\{ \frac{1}{M} \sum_{i=1}^M \delta_{x_i} : x_i \in \mathbb{R}^d, x_i \neq x_j \text{ for all } i \neq j \right\}.
\]
Then, we compute the Wasserstein gradient flow of the functional
\[
F_M(\mu) := \begin{cases} 
D^2_K(\mu, \delta_{e_1}), & \text{if } \mu \in S_M \\
+\infty, & \text{otherwise}.
\end{cases}
\]
By taking the mean field limit \( M \to \infty \), we expect that gradient flows with respect to \( F_M \) approximate the gradient flows with respect to \( F_{\delta_{e_1}} \). In order to compute the gradient flows with respect to \( F_M \) for some fixed \( M \in \mathbb{N} \), we consider the (rescaled) particle gradient flow for the function \( F_M : \mathbb{R}^{dM} \to [0, \infty) \) given by
\[
F_M(x) := F_{\delta_{e_1}} \left( \frac{1}{M} \sum_{i=1}^M \delta_{x_i} \right) = -\frac{1}{2M^2} \sum_{i,j=1}^M \|x_i - x_j\|^2 + \frac{1}{M} \sum_{i=1}^M \|x_i - e_1\|^2.
\]
More precisely, we are interested in solutions of the ODE
\[
\dot{u} = -M \nabla F_M(u).
\]
Figure 2: 2D particle gradient flow of $D^2_R (\cdot, \delta e_1)$ for the Riesz kernel with $r = 1$ starting around $\delta - e_1$. The black circles depict the border of $\text{supp} \gamma_u(t)$ related to the steepest descent direction $v$ at $t = 0$ given in (32).

Then, we see that the solutions $u = (u_1, \ldots, u_M): (0, \infty) \rightarrow \mathbb{R}^{dM}$ of (30) and the Wasserstein gradient flows $\gamma: (0, \infty) \rightarrow \mathcal{P}_2(\mathbb{R}^d)$ with respect to $\mathcal{F}_M$ are related by

$$\gamma(t) := \frac{1}{M} \sum_{i=1}^M \delta_{u_i(t)}.$$ 

For further details see [1]. Finally, we approximate the solutions of (30) by the explicit Euler-forward scheme

$$x^{(n+1)} := -\tau^{(n)} M \nabla F_M (x^{(n)}), \quad n \in \mathbb{N}_0.$$ 

(31)

**Example 26.** We take $\tau^{(0)} := \frac{1}{10M}$ and set $\tau^{(n)} := \min\{n\tau^{(0)}, \tau_{\text{max}}\}$, where $\tau_{\text{max}} \sim \frac{1}{M}$ is some maximal step size. We aim to compute gradient flows starting at $\delta - e_1$. In order to start in a set $S_M$, we first perform a forward step from $\delta - e_1$ in the known steepest descent direction, see Theorem 24. So the initial points $x_i^{(0)}$ for $d = 2$ and $d = 3$ are nearly distributed on a small ball and sphere, respectively. We apply the explicit Euler scheme (31) for $M = 2000$ points for initial points in a cube of radius $R = 10^{-9}$ and maximal step size $\tau_{\text{max}} = \frac{10}{M}$. The results are depicted in

- Figure 2 for $d = 2$, $r = 1$,
Figure 3: 3D particle gradient flow of $D^2_K(\cdot, \delta e_1)$ for the Riesz kernel with $r = 1$ starting around $\delta - e_1$. The left columns show the projection to the $x_1 x_2$-plane, the right columns to the $x_3 x_2$-plane. The black circles depict the border of $\text{supp} \gamma_v(t)$ related to the steepest descent direction $v$ at $t = 0$ given in (32).

- Figure 3 for $d = 3$, $r = 1$, and
- Figure 4 for $d = 2$, $r = \frac{3}{2}$.

To compare the computed flows with the initial steepest descent direction in Theorem 24, we illustrate the support of

$$\gamma_v(t) = ((t - 1) e_1 - E_K(\eta^*) t \text{Id}) \# \eta^*$$

with $\eta^*$ from Corollary 17, where $v := H_{-\mathcal{F}\delta_e} (\delta - e_1)$. We observe a good accordance with the numerical Euler forward scheme indicating that the particle explosion in discrepancy flows behaves similarly as for interaction energy flows. □

For smoother kernels than the considered Riesz kernels, the repulsion effect leading to particle explosions does not occur. For instance, Arbel et al. [3] consider Lipschitz-continuously differentiable kernels and show the existence of a unique Wasserstein gradient flow for the corresponding discrepancy. Moreover, the forward Euler scheme given in [3,
Figure 4: 2D particle gradient flow of $\mathcal{D}_K^2(\cdot, \delta_{e_1})$ for the Riesz kernel with $r = \frac{3}{2}$ starting around $\delta_{-e_1}$.

§ 2.2] converges locally uniformly to this flow. In particular, this shows that the Wasserstein gradient flow $\gamma$ remains atomic if the initial measure $\gamma(0) = \mu_0$ is atomic. The behavior changes completely for the Riesz kernel with $r = 1$. Here the repulsion effect is directly encoded in the steepest descent direction given in Theorem 24(ii). For $r \in (1, 2)$, the repulsion is weaker such that the steepest descent flow can have the form of a particle flow, see Proposition 25; but our numerical experiments indicate the existence of an infinite family of Wasserstein descent flows similar to the family (27) observed for the interaction energy, where at any time the particle may decide to explode.

A Proof of Lemma 6

Let $v_{t+h} \in \exp_{\nu(t)}^{-1}(\nu(t+h))$. Then it holds

$$\nu(t+h) = \gamma(f(t+h)) = \gamma\left(f(t) + h\dot{f}(t) + r(h)\right),$$

where $r(h)/h \to 0$ as $h \to 0$. Consequently, the optimal transport plans from $\nu(t)$ to $\nu(t+h)$ and from $\gamma(f(t))$ to $\gamma\left(f(t) + h\dot{f}(t) + r(h)\right)$ coincide such that

$$v_{t,h} = \tilde{v}_{f(t), h\dot{f}(t) + r(h)} \in \exp_{\gamma(f(t))}^{-1}\left(\gamma\left(f(t) + h\dot{f}(t) + r(h)\right)\right).$$
We consider the case \( \dot{f}(t) > 0 \). Since \( r(h)/h \to 0 \) as \( h \to 0+ \), we have that \( h\dot{f}(t) + r(h) > 0 \) for \( h > 0 \) small enough. Thus, it holds by homogeneity of \( W_{\nu(t)} \), see Lemma 27, that

\[
0 \leq W_{\nu(t)}(\dot{f}(t) \cdot \dot{\gamma}(f(t)), \frac{1}{h} \cdot \nu_{t,h})
\]

\[
= \frac{h\dot{f}(t) + r(h)}{h} W_{\gamma(f(t))}\left(\frac{h\dot{f}(t)}{h\dot{f}(t) + r(h)} \cdot \dot{\gamma}(f(t)), \frac{1}{h\dot{f}(t) + r(h)} \cdot \nu_{t,h}\right)
\]

\[
\leq \frac{h\dot{f}(t) + r(h)}{h} \rightarrow 0 + f(t)
\]

\[
\left[ W_{\gamma(f(t))}\left(\frac{h\dot{f}(t)}{h\dot{f}(t) + r(h)} \cdot \dot{\gamma}(f(t)), \frac{1}{h\dot{f}(t) + r(h)} \cdot \nu_{t,h}\right) + W_{\gamma(f(t))}\left(\frac{\dot{\gamma}(f(t))}{h\dot{f}(t) + r(h)} \cdot \tilde{\nu}_{f(t),h\dot{f}(t) + r(h)}\right)\right].
\]

The term (II) converges to zero, as \( \dot{\gamma}(f(t)) \) is a tangent vector of \( \gamma \) at \( f(t) \) and since \( h \to 0+ \) implies \( h\dot{f}(t) + r(h) \to 0+ \). Further, the term (I) can be computed as

\[
(I) = \left\| \frac{\dot{f}(t)}{h\dot{f}(t) + r(h)} \cdot \dot{\gamma}(f(t)) \right\|^2_{\gamma(f(t))} + \left\| \dot{\gamma}(f(t)) \right\|^2_{\gamma(f(t))} - 2 \left( \frac{\dot{f}(t)}{h\dot{f}(t) + r(h)} \cdot \dot{\gamma}(f(t)) \right) \cdot \dot{\gamma}(f(t)) = \gamma(f(t))
\]

\[
= \left(1 - \frac{\dot{f}(t)}{h\dot{f}(t) + r(h)}\right)^2 \left\| \gamma(f(t)) \right\|^2_{\gamma(f(t))} \to 0 \quad \text{as} \quad h \to 0+. \]

Consequently, \( W_{\gamma(f(t))}(\dot{f}(t) \cdot \dot{\gamma}(f(t)), \frac{1}{h} \cdot \nu_{t,h}) \) converges to zero.

Finally, we consider the case that \( \dot{f}(t) = 0 \). Then we have \( \dot{f}(t) \cdot \dot{\gamma}(f(t)) = \gamma(f(t)) \otimes \delta_0 \).

Thus it holds

\[
W_{\nu(t)}(\dot{f}(t) \cdot \dot{\gamma}(f(t)), \frac{1}{h} \cdot \nu_{t,h}) = W_{\nu(t)}(\gamma(f(t)) \otimes \delta_0, \frac{1}{h} \cdot \nu_{t,h})
\]

\[
= \left\| \frac{1}{h} \cdot \tilde{\nu}_{f(t),r(h)}\right\|_{\gamma(f(t))}
\]

which is zero if \( r(h) = 0 \) for \( h > 0 \) small enough. Otherwise, we have that \( r(h) > 0 \) for \( h > 0 \). Then we obtain, that the above expression is equal to

\[
\frac{r(h)}{h} \left\| \frac{1}{r(h)} \cdot \gamma_{f(t),r(h)}\right\|_{\gamma(f(t))}.
\]

Now, the first factor converges to zero and the second factor converges to some number \( C > 0 \) since it holds \( \frac{1}{r(h)} \cdot \gamma_{f(t),r(h)} \to \dot{\gamma}(f(t)) \) with respect to \( W_{\gamma(f(t))} \). Hence the whole expression converges to zero and we are done.

\[ \square \]

B Proofs from Section 5

In order to prove the results from Section 5, we require the notion of a scalar product, metric velocity as well as some further properties of the metric \( W_\mu \) in \( \mathbf{V}(\mu) \). We give these definitions and properties in B.1. Afterwards, we prove Proposition 9 in B.3.
B.1 Scalar product, Metric velocity and Properties of \(W_\mu\)

Besides the metric, we may define the scalar product of two velocity plans \(v, w \in V(\mu)\) by
\[
\langle v, w \rangle_\mu := \max_{\alpha \in \Gamma_{\mu}(v,w)} \langle v, w \rangle_\alpha \quad \text{with} \quad \langle v, w \rangle_\alpha := \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} x_2^2 x_3 d\alpha(x_1, x_2, x_3) \tag{33}
\]
and the metric velocity as
\[
\|v\|^2_\mu := \langle v, v \rangle_\mu = \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_2\|^2_2 dv(x_1, x_2).
\]
In particular, we have for \(v \in \exp^{-1}(\nu)\) that
\[
W^2_2(\mu, \nu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2_2 d(\pi_1, \pi_1 + \pi_2) v(x, y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \|y\|^2_2 dv(x, y) = \|v\|^2_\mu. \tag{34}
\]

The next lemma summarizes further properties. Some of them are proven in [22], for the others we provide a proof.

**Lemma 27.** Let \(\mu \in \mathcal{P}_2(\mathbb{R}^d)\). For all \(v, w \in V(\mu)\), the following relations hold true:

(i) **Homogeneity:**
\[
\langle c \cdot v, w \rangle_\mu = c \langle v, w \rangle_\mu = \langle v, c \cdot w \rangle_\mu, \quad c \geq 0,
\]
\[
\|c \cdot v\|_\mu = |c| \|v\|_\mu, \quad c \in \mathbb{R},
\]
\[
W_\mu(c \cdot v, c \cdot w) = |c| W_\mu(v, w), \quad c \in \mathbb{R}.
\]

(ii) **Properties of \(W_\mu\):**
\[
W^2_\mu(v, w) = \|v\|_\mu^2 + \|w\|_\mu^2 - 2\langle v, w \rangle_\mu,
\]
\[
W_\mu(v, w) \geq W_2(\gamma_v(1), \gamma_w(1)),
\]
\[
W^2_\mu(v, 0_\mu) = \|v\|_\mu^2 = \int_{\mathbb{R}^d} \|x_2\|^2_2 dv(x).
\]

(iii) **Cauchy–Schwarz inequality:**
\[
|\langle v, w \rangle_\mu| \leq \|v\|_\mu \|w\|_\mu,
\]
where it holds \(\langle v, w \rangle_\mu = \|v\|_\mu \|w\|_\mu\) if and only if there exists some \(c \geq 0\) such that \(v = c \cdot w\).
Proof. i) The homogeneity proof was given in [22, Prop 4.17, 4.27].

ii) The first result was shown in [22, Prop 4.2] and the second one in [22, (4.23)]. The third item follows by the definition of \( \|v\|^2_\mu \) and the first item as it holds by i) that \( \|0\|_\mu = 0 \). iii) It holds

\[
\langle v, w \rangle_\mu = \sup_{\alpha \in \Gamma_\mu(v,w)} \langle v, w \rangle_\alpha = \sup_{\alpha \in \Gamma_\mu(v,w)} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} y^T z d\alpha(x, y, z)
\]

\[
\leq \sup_{\alpha \in \Gamma_\mu(v,w)} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|y\|_2 \|z\|_2 d\alpha(x, y, z)
\]

\[
\leq \sup_{\alpha \in \Gamma_\mu(v,w)} \left( \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|y\|_2^2 d\alpha(x, y, z) \right)^{1/2} \left( \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|z\|_2^2 d\alpha(x, y, z) \right)^{1/2}
\]

\[
= \sup_{\alpha \in \Gamma_\mu(v,w)} \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|y\|_2^2 dv(x, y) \right)^{1/2} \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|z\|_2^2 dw(x, z) \right)^{1/2} = \|v\|_\mu \|w\|_\mu,
\]

where the first inequality is Cauchy–Schwarz’ inequality in \( \mathbb{R}^d \) and the second inequality is Cauchy–Schwarz’s inequality on the functions \((x, y, z) \mapsto \|y\|_2 \) and \((x, y, z) \mapsto \|z\|_2 \) in \( L^2(\alpha) \). Consequently, it holds equality if and only if for \( \alpha \)-almost every \((x, y, z)\) there exists some \( c \geq 0 \) such that \( y = cz \) and if there exists some \( c \geq 0 \) such that \( \|y\|_2 = c \|z\|_2 \) \( \alpha \)-almost everywhere. That is, we have equality if and only if there exist some \( c \geq 0 \) such that \( y = cz \) \( \alpha \)-almost everywhere, which is equivalent to \( v = c \cdot w \). Finally, it follows

\[
-\|v\|_\mu \|w\|_\mu = -\|v\|_\mu \|w\|_\mu \leq -\langle -v, w \rangle_\mu \leq \langle v, w \rangle_\mu \leq \|v\|_\mu \|w\|_\mu.
\]

\[\square\]

B.2 Proof of Proposition 7

Let \((v_n)_{n \in \mathbb{N}}\) be a sequence in \( V(\mu) \) with \( W_\mu(v_n, v) \to 0 \) and let \((t_n)_{n \in \mathbb{N}}\) with \( t_n > 0 \) such that \( t_n \to 0 \). Then, we find \( n_0 \in \mathbb{N} \) such that

\[
\gamma v(t_n), \gamma v_n(t_n) \in B_t(\mu), \quad n \geq n_0.
\]

Using the local Lipschitz continuity of \( F \), formula (10), the second item of Lemma 27 ii) and the third item of Lemma 27 i), we infer that

\[
\lim_{n \to \infty} \frac{|F(\gamma v(t_n)) - F(\gamma v_n(t_n))|}{t_n} \leq \lim_{n \to \infty} \frac{L W_2(\gamma v(t_n), \gamma v_n(t_n))}{t_n}
\]

\[
= \lim_{n \to \infty} \frac{L W_2(\gamma t_n v(1), \gamma t_n v_n(1))}{t_n} \leq \lim_{n \to \infty} \frac{L W_\mu(t_n v, t_n v_n)}{t_n}
\]

\[
= \lim_{n \to \infty} \frac{L t_n W_\mu(v, v_n)}{t_n} = \lim_{n \to \infty} L W_\mu(v, v_n) = 0. \quad (35)
\]
On the other hand, by the definition of \( \lim \inf \) and \( \lim \sup \) there exist sequences \( t_n^\pm \to 0^+ \) in \( \mathbb{R}_{\geq 0} \) and \( \gamma_v^\pm \) in \( V(\mu) \) such that \( \gamma_v^\pm |_{[0,t_n^\pm]} \) are geodesics, \( W_\mu(v_n^\pm, v) \to 0 \) and

\[
H^-_v F(\mu) := \lim_{n \to \infty} \frac{F(\gamma_{v_n^-}(t_n^-)) - F(\mu)}{t_n^-},
\]

\[
H^+_v F(\mu) := \lim_{n \to \infty} \frac{F(\gamma_{v_n^+(t_n^+)} - F(\mu))}{t_n^+}.
\]

Then, it holds by (35) that

\[
|D_v F(\mu) - H^+_v F(\mu)| = \lim_{n \to \infty} \frac{|F(\gamma_{v_n^+(t_n^+)) - F(\gamma_{v_n^-(t_n^-))})|}{t_n^\pm} = 0.
\]

Since both the lower and the upper Hadamard derivative coincide with the Dini derivative we arrive at the assertion. \( \square \)

### B.3 Proof of Proposition 9

Proposition 9 is a special case of Theorem 33 at the end of this subsection. In order to relate Wasserstein steepest descent flows to Wasserstein gradient flows, we need more technicalities, in particular the notation of subdifferentials for velocity plans. The extended Fréchet subdifferential of a function \( F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty] \) at \( \mu \) is defined by

\[
\partial F(\mu) := \{ v \in V(\mu) : F(\nu) \geq F(\mu) - \sup_{v \in \exp^{-1}_\mu(\nu)} \langle (-1) \cdot h, v \rangle_{\mu} + o(W_2(\mu, \nu)) \},
\]

cf. [2, Def 10.3.1]. In particular, it is shown in [2, Thm 10.3.11] that for functions \( F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty] \), which are \( \lambda \)-convex functions along generalized geodesics, and a measure \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) with \( \partial F(\mu) \neq \emptyset \) there exists an unique element of the subdifferential with minimal norm, i.e., \( \arg \min_{v \in \partial F} \| v \|_{\mu} \) contains exactly one element. Moreover, the local slope \( |\partial F|: \mathcal{P}_2(\mathbb{R}^d) \to [0, \infty] \) of \( F \) is defined by

\[
|\partial F|(\mu) := \lim_{v \to \mu} \frac{F(\mu) - F(\nu)^+}{W_2(\mu, \nu)},
\]

where \( (t)^+ := \max\{t, 0\} \).

Using these notations, the following theorem from [2, Thm 11.2.1] characterizes the tangent vectors of Wasserstein gradient flows for all \( t \in [0, +\infty) \). Note that the original theorem is formulated for \( W_2 \) instead of \( W_\gamma(t) \) in (36), but the proofs in those book provide indeed the relation below.
Theorem 28. Let $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ be proper, lsc, coercive and $\lambda$-convex along generalized geodesics. Further, denote by $\gamma: (0, \infty) \to \mathcal{P}_2(\mathbb{R}^d)$ the unique Wasserstein gradient flow from Theorem 3. Then, for every $t, h > 0$ and $v_{t,h} \in \exp_{\gamma(t)}^{-1}(\gamma(t + h))$, the right limit

$$\dot{\gamma}(t) = v_t := \lim_{h \to 0^+} -\frac{1}{h} \cdot v_{t,h}, \text{ i.e., } \lim_{h \to 0^+} W_{\gamma(t)}(v_t, -\frac{1}{h} \cdot v_{t,h}) = 0 \quad (36)$$

exists and satisfies for all $t > 0$ the relations

$$v_t = \text{arg min}_{v \in \partial \mathcal{F}(\gamma(t))} \|v\|_{\gamma(t)} \quad (37)$$

and

$$\lim_{h \to 0^+} \frac{\mathcal{F}(\gamma(t + h)) - \mathcal{F}(\gamma(t))}{h} = -\|v_t\|_{\gamma(t)}^2 = -|\partial \mathcal{F}|^2(\gamma(t)) \quad (38)$$

Further, (36), (37) and (38) hold true at $t = 0$ if and only if $\partial \mathcal{F}(\mu_0) \neq \emptyset$.

Using this theorem, we can show that in some cases Wasserstein gradient flows are Wasserstein steepest descent flows.

Lemma 29. Let $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ be proper, lsc, coercive and $\lambda$-convex along generalized geodesics. Then, for $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ with $\partial \mathcal{F}(\mu) \neq \emptyset$ and

$$v := \text{arg min}_{w \in \partial \mathcal{F}(\mu)} \|w\|_{\mu}, \quad (39)$$

it holds

$$h := (-1) \cdot v \in H^-_{\mathcal{F}(\mu)} \text{ and } H^-_{\frac{\|h\|_{\mu}}{\|v\|_{\mu}}} \mathcal{F}(\mu) = -|\partial \mathcal{F}|(\mu).$$

In particular, for all $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$ with $\partial \mathcal{F}(\mu_0) \neq \emptyset$, the Wasserstein gradient flow of $\mathcal{F}$ starting at $\mu_0$ is a Wasserstein steepest descent flow of $\mathcal{F}$.

Proof. Theorem 28 implies the existence of a unique Wasserstein gradient flow $\gamma: (0, \infty) \to \mathcal{P}_2(\mathbb{R}^d)$ with $\gamma(0) := \gamma(0^+) = \mu$. Since $\partial \mathcal{F}(\mu) \neq \emptyset$, we know that $v \in \mathcal{V}(\mu)$ in (39) is the velocity field $v_t$ with (36), (37) and (38) at $t = 0$.

We consider two cases. If $v = 0_{\gamma(0)}$, then the assertion is straightforward. If $v \neq 0_{\gamma(0)}$, we conclude by (38) and the definition of $H^-_v \mathcal{F}$ that

$$-|\partial \mathcal{F}|^2(\mu) = \lim_{h \to 0^+} \frac{\mathcal{F}(\gamma(h)) - \mathcal{F}(\gamma(0))}{h} = \lim_{h \to 0^+} \frac{\mathcal{F}(\gamma(-1) \cdot v_{0,h}(h)) - \mathcal{F}(\gamma(0))}{h} \geq H^-_{\gamma(0)} \mathcal{F}(\gamma(0)) = H^-_{\gamma(0)} \mathcal{F}(\gamma(0)),$$

and further by dividing by $|\partial \mathcal{F}|(\gamma(0)) = \|v\|_{\gamma(0)} = \|h\|_{\gamma(0)}$ that

$$\frac{1}{\|h\|_{\gamma(0)}} H^-_{\gamma(0)} \mathcal{F}(\gamma(0)) \leq -|\partial \mathcal{F}|(\gamma(0)).$$

32
On the other hand, we have by (34) that \( W_2(\mu, \gamma_{\tilde{w}}(t)) = \| t \cdot \tilde{w} \|_{\mu} = t \| \tilde{w} \|_{\mu}, \tilde{w} \in T_\mu(\mathcal{P}_2(\mathbb{R}^d)) \), such that for every \( w \in T_\mu(\mathcal{P}_2(\mathbb{R}^d)), w \neq 0_\mu, \)

\[
\frac{(H_{\tilde{w}}^w F(\mu))^-}{\| \tilde{w} \|_{\mu}} \leq \left( \liminf_{\tilde{w} \to w, t \to 0^+, \gamma_{\tilde{w}} \in [0, t]} \frac{F(\gamma_{\tilde{w}}(t)) - F(\mu)}{t \| \tilde{w} \|_{\mu}} \right)^-
\]

\[
= \limsup_{\tilde{w} \to w, t \to 0^+, \gamma_{\tilde{w}} \in [0, t]} \frac{(F(\mu) - F(\gamma_{\tilde{w}}(t)))^+}{W_2(\mu, \gamma_{\tilde{w}}(t))} \leq |\partial F|(\mu).
\]

Combining both inequalities, we get

\[
\frac{1}{\| h \|_{\gamma(0)}} H_{h}^- F(\gamma(0)) = H_{h}^- F(\gamma(0)) = -|\partial F|(\gamma(0)).
\]

Let \( w \in \arg \min_{\tilde{w} \in T_{\gamma(0)} \mathcal{P}_2(\mathbb{R}^d)} \| \tilde{w} \|_{\gamma(0)} = 1 \) \( H_{\tilde{w}}^w F(\mu) \). Then we obtain by (40) that

\[
H_{\tilde{w}}^w F(\gamma(0)) \geq -|\partial F|(\gamma(0)),
\]

so that \( \frac{1}{\| h \|_{\gamma(0)}} \cdot h \in \arg \min_{\tilde{w} \in T_{\gamma(0)} \mathcal{P}_2(\mathbb{R}^d)} \| \tilde{w} \|_{\gamma(0)} = 1 \) \( H_{\tilde{w}}^w F(\mu) \) and \( h \in H_{\mu} F(\gamma(0)) = H_{\mu} F(\mu). \)

To show the reverse direction, namely that every Wasserstein steepest descent flow is a Wasserstein gradient flow, we need some additional assumptions.

We say that \( F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, \infty] \) is continuous along geodesics if \( F \circ \gamma: [0, \epsilon] \to (-\infty, \infty] \) is continuous for all geodesics \( \gamma: [0, \epsilon] \to \mathcal{P}_2(\mathbb{R}^d) \) with \( F \circ \gamma(0), F \circ \gamma(\epsilon) < \infty \). The following lemma states that \( h \) from the previous lemma is the only element in \( H_{-\mu} F(\mu) \) if \( F \) is additionally continuous along geodesics. This will be the basis of the proof that under mild assumptions Wasserstein steepest descent flows are Wasserstein gradient flows.

**Lemma 30.** Let \( F: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty] \) be proper, lsc, coercive, \( \lambda \)-convex along generalized geodesics and continuous along geodesics. Then, it holds for any \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) with \( \partial F(\mu) \neq \emptyset \) that \( H_{-\mu} F(\mu) = \{ h \} \), where \( h \) is defined as in Lemma 29.

**Proof.** Consider some \( g \in H_{-\mu} F(\mu) \). Since \( h \in H_{-\mu} F(\mu) \), we have

\[
H_{-g}^- F(\mu) = H_{-h}^- F(\mu) = -\| h \|_{\mu} |\partial F|(\mu) = -\| g \|_{\mu} |\partial F|(\mu).
\]

Further, by definition of \( H_{-g}^- \), there exist \( \tilde{t}_n \to 0 \) and \( g_n \in G(\mu) \) with \( g_n \to g \) in \( W_\mu \) such that \( \tilde{t}_n \cdot g_n \in \exp_{-1}(\gamma_{g_n}(\tilde{t}_n)) \) and

\[
\lim_{n \to \infty} \frac{F(\gamma_{g_n}(\tilde{t}_n)) - F(\mu)}{\tilde{t}_n} = H_{-g}^- F(\mu) = -\| g \|_{\mu} |\partial F|(\mu).
\]

33
Since the limit is finite, we assume wlog that $F(\gamma_{g_0}(t_n)) < \infty$. Thus, by continuity of $F$ along geodesics, the functions

$$\phi_n: [0, 1] \rightarrow \mathbb{R}, \quad \phi_n(s) := F(\gamma_{g_0}(s\bar{t}_n)), \quad s \in [0, 1],$$

are continuous. Hence we can find a sequence $(s_n)_{n \in \mathbb{N}}$ with $s_n \rightarrow 1$ as $n \rightarrow \infty$ such that

$$|\phi_n(s_n) - \phi_n(1)| = |F(\gamma_{g_0}(s_n\bar{t}_n)) - F(\gamma_{g_0}(\bar{t}_n))| \leq \bar{t}_n^2$$

with $\exp^{-1}(\gamma_{g_0}(s_n\bar{t}_n)) = \{s_n\bar{t}_n \cdot v_n\}$, cf. [2, Lem 7.2.1]. Now, replacing the sequence $\bar{t}_n$ by $t_n := s_n\bar{t}_n$ does not alter the limit, i.e.,

$$\lim_{n \rightarrow \infty} \frac{F(\gamma_{g_0}(t_n)) - F(\mu)}{t_n} = \lim_{n \rightarrow \infty} \frac{F(\gamma_{g_0}(s_n\bar{t}_n)) - F(\mu)}{s_n\bar{t}_n} - \lim_{n \rightarrow \infty} \frac{F(\gamma_{g_0}(s_n\bar{t}_n)) - F(\gamma_{g_0}(\bar{t}_n))}{s_n\bar{t}_n} = \lim_{n \rightarrow \infty} \frac{F(\gamma_{g_0}(\bar{t}_n)) - F(\mu)}{\bar{t}_n} = H_F(\mu).$$

Since $(-1) \cdot h \in \partial F(\mu)$ and $\exp^{-1}(\gamma_{g_0}(t_n)) = \{t_n \cdot g_n\}$ it holds with (34) that

$$F(\gamma_{g_0}(t_n)) - F(\mu) \geq -\langle h, t_n \cdot g_n \rangle_{\mu} + o(t_n\|g_n\|_{\mu}) = -t_n\langle h, g_n \rangle_{\mu} + o(t_n\|g_n\|_{\mu}).$$

As $g_n \rightarrow g$ in $W_{\mu}$ implies $\|g_n\|_{\mu} \rightarrow \|g\|_{\mu}$, we obtain by dividing both sides by $t_n$ and letting $n \rightarrow \infty$ that

$$-\|g\|_{\mu} \partial F(\mu) = \lim_{n \rightarrow \infty} \frac{F(\gamma_{g_0}(t_n)) - F(\mu)}{t_n} \geq -\langle h, g \rangle_{\mu} \geq -\|h\|_{\mu}\|g\|_{\mu},$$

where the second implication is the Cauchy–Schwarz inequality from Lemma 27 (iii). Since $\|g\|_{\mu} = \|h\|_{\mu} = \|\partial F(\mu)\|_{\mu}$ we have equality. By the equality condition of the Cauchy–Schwarz relation, this yields $h = g$ such that $H_{\mu}F(\mu) = \{h\}$. \hfill \square

Now, we can show that under certain assumptions Wasserstein steepest descent flows are Wasserstein gradient flows.

**Lemma 31.** Let $F: P_2(\mathbb{R}^d) \rightarrow (-\infty, +\infty]$ be proper, lsc, coercive, $\lambda$-convex along generalized geodesics and continuous along geodesics and let $\mu_0 \in P_2(\mathbb{R}^d)$ such that $\partial F(\mu_0) \neq \emptyset$. Further assume that $\partial F(\mu) \neq \emptyset$ for any $\mu \in P_2(\mu)$ with $H_{\mu}F(\mu) \neq \emptyset$. Then, there exists a unique Wasserstein steepest descent flow of $F$ starting at $\mu_0$, which coincides with the Wasserstein gradient flow of $F$ starting at $\mu_0$.

**Proof.** By Theorem 3, there exists a unique Wasserstein gradient flow starting at $\mu_0$, which is by Lemma 29 a steepest descent flow. Thus, it suffices to show that any Wasserstein steepest descent flow $\gamma: [0, \infty) \rightarrow P_2(\mathbb{R}^d)$ is a Wasserstein gradient flow. Since $\gamma(t) \in H_{\gamma(t)}F$, we have $\langle h, g \rangle_{\gamma(t)} \geq -\|h\|_{\gamma(t)}\|g\|_{\gamma(t)}$ for all $h, g$. Hence, $\gamma(t)$ is a Wasserstein gradient flow starting at $\mu_0$. \hfill \square
we have that $H_-(\gamma(t))$ is non-empty, which implies by assumption that the subdifferential $\partial F(\gamma(t))$ is non-empty. By Lemma 29 and 30, we obtain $\dot{\gamma}(t) \in H_- F(\gamma(t)) = \{(1) \cdot v\}$, where $v := \arg\min_{w \in \partial F(\gamma(t))} \|w\|_{\gamma(t)}$ which implies that $(-1) \cdot \dot{\gamma}(t) \in \partial F(\gamma(t))$. Since $\gamma$ is by definition absolutely continuous, there exists a Borel velocity field $v_t : \mathbb{R}^d \to \mathbb{R}^d$, $t \in I$ with

$$
\partial_t \gamma(t) + \nabla_x \cdot (\gamma(t)v_t) = 0 \quad \text{in } I \times \mathbb{R}^d.
$$

Moreover, [2, Prop 8.4.6] implies that $(\text{Id}, v_t)_\# \gamma(t) = \dot{\gamma}(t)$ for almost-every $t \in I$ such that

$$(\text{Id}, -v_t)_\# \gamma(t) = (-1) \cdot (\text{Id}, v_t)_\# \gamma(t) = (-1) \cdot \dot{\gamma}(t) \in \partial F(\gamma(t)).$$

Finally, we know by [2, Rem 10.3.3] that $(\text{Id}, v)_\# \mu \in \partial F(\mu)$ if and only if $v \in \partial F(\mu)$, so that $-v_t \in \partial F(\gamma(t))$, i.e., $v_t \in -\partial F(\gamma(t))$. Together with (41), we can conclude that $\gamma$ is the unique Wasserstein gradient flow with respect to $F$. \hfill $\square$

**Remark 32.** The assumption that $\partial F(\mu) \neq \emptyset$ for any $\mu \in \mathcal{P}_2(\mu)$ with $H_- F(\mu) \neq \emptyset$ is automatically fulfilled if the slope $|\partial F(\mu)|$ is finite for every $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ as [2, Thm 10.3.10] states that the subdifferential at $\mu$ is non-empty for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ with $|\partial F(\mu)| < \infty$. This includes in particular locally Lipschitz continuous functions $F$ since local Lipschitz continuity implies by definition that $|\partial F(\mu)|$ is finite for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$.

Summarizing Lemma 29, 30 and 31 we obtain the following theorem.

**Theorem 33.** Let $F : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ be proper, lsc, coercive and $\lambda$-convex along generalized geodesics and let $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$ such that $\partial F(\mu_0) \neq \emptyset$. Then, the unique Wasserstein gradient flow starting at $\mu_0$ is a Wasserstein steepest descent flow. Moreover, if $F$ is additionally continuous along geodesics and fulfills $\partial F(\mu) \neq \emptyset$ for any $\mu \in \mathcal{P}_2(\mu)$ with $H_- F(\mu) \neq \emptyset$, then there exists a unique Wasserstein steepest descent flow starting at $\mu_0$ which coincides with the Wasserstein gradient flow.

### C Proof of Proposition 11

In the following, we denote the Lipschitz constant of $F : \mathbb{R}^d \to \mathbb{R}$ on $A \subset \mathbb{R}^d$ by

$$\text{Lip}(F, A) := \sup \left\{ \frac{|F(x) - F(y)|}{\|x - y\|_2} : x, y \in A, x \neq y \right\}.$$ 

To prove the Proposition 11, we need three auxiliary lemmata.

**Lemma 34.** Let $V : \mathbb{R}^d \to \mathbb{R}$ be locally Lipschitz continuous and $L > 0$ such that

$$\text{Lip}(V, B_r(x)) \leq L(1 + \|x\|_2 + r), \quad x \in \mathbb{R}^d, \quad r > 0. \quad (42)$$

35
Then the functional $\mathcal{V} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ given by

$$
\mathcal{V}(\mu) := \int_{\mathbb{R}^d} V(x) d\mu(x), \quad \mu \in \mathcal{P}_2(\mathbb{R}^d),
$$

is locally Lipschitz continuous.

Proof. For $r > 0$ and $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, let $\nu_1, \nu_2 \in B_r(\mu)$. Choosing $\pi \in \Gamma^{\text{opt}}(\nu_1, \nu_2)$ and $v = (\pi_1, \pi_2 - \pi_1)_\# \pi \in \exp_{\nu_1}^{-1}(\nu_2)$, we estimate first applying the triangular inequality

$$
|\mathcal{V}(\nu_1) - \mathcal{V}(\nu_2)| \leq \int_{\mathbb{R}^d \times \mathbb{R}^d} |V(x_1) - V(x_2)| d\pi(x_1, x_2)
$$

$$
= \int_{\mathbb{R}^d \times \mathbb{R}^d} |V(x_1) - V(x_1 + x_2)| dv(x_1, x_2)
$$

$$
\leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \text{Lip}(V, B_{\|x_2\|_2}(x_1)) \|x_2\|_2 dv(x_1, x_2)
$$

$$
\leq L \int_{\mathbb{R}^d \times \mathbb{R}^d} (1 + \|x_1\|_2 + \|x_2\|_2) \|x_2\|_2 dv(x_1, x_2).
$$

Using the Cauchy-Schwarz inequality, we get

$$
|\mathcal{V}(\nu_1) - \mathcal{V}(\nu_2)| \leq L \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_2\|_2^2 dv(x_1, x_2) \right)^{\frac{1}{2}} + L \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_2\|_2^2 dv(x_1, x_2)
$$

$$
+ L \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_1\|_2^2 dv(x_1, x_2) \right)^{\frac{1}{2}} \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_2\|_2^2 dv(x_1, x_2) \right)^{\frac{1}{2}}
$$

$$
= L \left( 1 + \left( \int_{\mathbb{R}^d} \|x_1\|_2^2 dv_1(x_1) \right)^{\frac{1}{2}} + W_2(\nu_1, \nu_2) \right) W_2(\nu_1, \nu_2)
$$

$$
= L \left( 1 + 2r + \left( \int_{\mathbb{R}^d} \|x_1\|_2^2 dv_1(x_1) \right)^{\frac{1}{2}} \right) W_2(\nu_1, \nu_2).
$$

To estimate the remaining integral, let $\tilde{\pi} \in \Gamma^{\text{opt}}(\nu_1, \mu)$. Using the triangle inequality, we obtain

$$
\int_{\mathbb{R}^d} \|x_1\|_2^2 dv_1(x_1) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_1\|_2^2 d\tilde{\pi}(x_1, x_2)
$$

$$
\leq 2 \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_1 - x_2\|_2^2 d\tilde{\pi}(x_1, x_2) + 2 \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_2\|_2^2 d\tilde{\pi}(x_1, x_2)
$$

$$
= 2W_2(\mu, \nu_1) + 2 \int_{\mathbb{R}^d} \|x_2\|_2^2 d\mu(x_2),
$$

and consequently

$$
|\mathcal{V}(\nu_1) - \mathcal{V}(\nu_2)| \leq L \left( 1 + \frac{2r + 2 \left( \int_{\mathbb{R}^d} \|x_2\|_2^2 d\mu(x_2) \right)^{\frac{1}{2}}}{1 + 2r + \left( \int_{\mathbb{R}^d} \|x_1\|_2^2 dv_1(x_1) \right)^{\frac{1}{2}}} \right) W_2(\nu_1, \nu_2).
$$
Note, if $V: \mathbb{R}^d \to \mathbb{R}$ is differentiable such that there exists $L > 0$ with
\[
\|\nabla V(x)\|_2 \leq L(1 + \|x\|_2), \quad x \in \mathbb{R}^d,
\]
then for $x_1, x_2 \in B_r(x)$ with $r > 0$, $x \in \mathbb{R}^d$, it holds
\[
|V(x_2) - V(x_1)| = \left| \int_0^1 \nabla V(x_1 + t(x_2 - x_1))^T(x_2 - x_1)dt \right|
\]
\[
\leq \int_0^1 \|\nabla V(x_1 + t(x_2 - x_1))\|_2 \|x_2 - x_1\|_2 dt
\]
\[
\leq \int_0^1 L(1 + \|x_1 + t(x_2 - x_1)\|_2) \|x_2 - x_1\|_2 dt
\]
\[
\leq \int_0^1 L(1 + \|x_1\|_2 + t\|x_2 - x_1\|_2) \|x_2 - x_1\|_2 dt
\]
\[
= L(1 + \|x_1\|_2 + \frac{1}{2} \|x_2 - x_1\|_2) \|x_2 - x_1\|_2 \leq L(1 + \|x_1\|_2 + r) \|x_2 - x_1\|
\]
and the condition (42) is satisfied.

**Lemma 35.** Let $K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be locally Lipschitz continuous and $L > 0$ such that
\[
\text{Lip}(K, B_r(x) \times B_s(y)) \leq L(1 + \|x\|_2 + \|y\|_2 + r + s), \quad x, y \in \mathbb{R}^d, \quad r, s \geq 0. \quad (44)
\]
Then the interaction energy $E_K: \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ in (17) is locally Lipschitz continuous.

**Proof.** For $r > 0$, let $\nu_1, \nu_2 \in B_r(\mu)$. Choosing $\pi \in \Gamma_{\text{opt}}(\nu_1, \nu_2)$ and $v = (\pi_1, \pi_2 - \pi_1)\# \pi \in \exp_{\nu_1}(\nu_2)$, we estimate
\[
|E_K(\nu_1) - E_K(\nu_2)|
\]
\[
\leq \int_{\mathbb{R}^d} |K(x_1, x_2) - K(y_1, y_2)| d\pi(x_1, y_1) d\pi(x_2, y_2)
\]
\[
\leq \int_{\mathbb{R}^d} |K(x_1, x_2) - K(x_1 + y_1, x_2 + y_2)| d\nu(x_1, y_1) d\nu(x_2, y_2)
\]
\[
\leq \int_{\mathbb{R}^d} \text{Lip}(K, B_{\|y_1\|_2}(x_1) \times B_{\|y_2\|_2}(x_2))(\|y_1\|_2 \|y_2\|_2) d\nu(x_1, y_1) d\nu(x_2, y_2)
\]
\[
\leq \int_{\mathbb{R}^d} \text{Lip}(K, B_{\|y_1\|_2}(x_1) \times B_{\|y_2\|_2}(x_2))(\|y_1\|_2 + \|y_2\|_2) d\nu(x_1, y_1) d\nu(x_2, y_2)
\]
\[
\leq L \int_{\mathbb{R}^d} (1 + \|x_1\|_2 + \|x_2\|_2 + \|y_1\|_2 + \|y_2\|_2) d\nu(x_1, y_1) d\nu(x_2, y_2)
\]
\[
\leq L \left( 2 + 2 \int_{\mathbb{R}^d} \|x\|_2 d\nu_1(x) + 2 \left( \int_{\mathbb{R}^d} \|x\|_2^2 d\nu_1(x) \right)^{\frac{1}{2}} + 4W_2(\nu_1, \nu_2) \right) W_2(\nu_1, \nu_2)
\]
\[
\leq L \left( 2 + 8r + 2 \int_{\mathbb{R}^d} \|x\|_2 d\nu_1(x) + 2 \left( \int_{\mathbb{R}^d} \|x\|_2^2 d\nu_1(x) \right)^{\frac{1}{2}} \right) W_2(\nu_1, \nu_2)
\]
37
Using the Cauchy–Schwarz inequality, we have
\[
\int_{\mathbb{R}^d} \|x\|_2^2 d\nu_1(x) \leq \left( \int_{\mathbb{R}^d} \|x\|_2^2 d\nu_1(x) \right)^{\frac{1}{2}}
\]
Exploiting (43), we have
\[
|\mathcal{E}_K(\nu_1) - \mathcal{E}_K(\nu_2)| \leq L \left( 2 + 8r + 4 \left( 2r + 2 \int_{\mathbb{R}^d} \|y\|_2^2 d\mu(x) \right)^{\frac{1}{2}} \right) W_2(\nu_1, \nu_2)
\]
and arrive at the assertion.

Lemma 36. Let \( K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) be differentiable such that there exists \( L > 0 \) with
\[
\|\nabla K(x, y)\|_2 \leq L(1 + \|x\|_2 + \|y\|_2).
\]
Then condition (44) is satisfied.

Proof. Fix \( x, y, \in \mathbb{R}^d, r, s > 0 \) and let \( (x_1, y_1), (x_2, y_2) \in B_r(x) \times B_s(y) \) then we estimate
\[
|K(x_2, y_2) - K(x_1, y_1)|
\]
\[
= \left| \int_0^1 \nabla K(x_1 + t(x_2 - x_1), y_1 + t(y_2 - y_1))^T(x_2 - x_1, y_2 - y_1) dt \right|
\]
\[
\leq \int_0^1 \|\nabla K(x_1 + t(x_2 - x_1), y_1 + t(y_2 - y_1))\|_2 \|(x_2 - x_1, y_2 - y_1)\|_2 dt
\]
\[
\leq \int_0^1 L(1 + \|x_1 + t(x_2 - x_1)\|_2 + \|y_1 + t(y_2 - y_1)\|_2) \|(x_2 - x_1, y_2 - y_1)\|_2 dt
\]
\[
\leq \int_0^1 L(1 + \|x_1\|_2 + t\|x_2 - x_1\|_2 + \|y_1\|_2 + t\|y_2 - y_1\|_2) \|(x_2 - x_1, y_2 - y_1)\|_2 dt
\]
\[
\leq L(1 + \|x_1\|_2 + r + \|y_1\|_2 + s) \|(x_2 - x_1, y_2 - y_1)\|_2
\]
which yields the assertion.

Proof of Proposition 11: Part (\( \mathcal{E}_K \)): By Lemma 35 it is sufficient to show that the kernel \( K(x, y) = -\|x - y\|_2 \), satisfies for \( r \in [1, 2) \) the condition (44). For \( r = 1 \) the condition follows from the fact that \( K \) is Lipschitz continuous with Lipschitz constant \( L = 1 \). For \( r \in (1, 2) \) the kernels \( K \) are differentiable with gradient
\[
\nabla K(x, y) = (\nabla_1 K(x, y), -\nabla_1 K(x, y))^T, \quad \nabla_1 K(x, y) = \begin{cases} 0, & x = y, \\ \frac{r(x-y)}{\|x-y\|_2^2 - r}, & x \neq y. \end{cases}
\]
Lemma 36 leads with the estimate
\[ \| \nabla K(x, y) \|_2 = \sqrt{2} r \| x - y \|_2^{-1} \leq \sqrt{2} r (1 + \| x - y \|_2) \leq L (1 + \| x \|_2 + \| y \|_2), \quad L := \sqrt{2} r, \]
for \( r \in (1, 2) \) and the previous observation for \( r = 1 \) for \( s_1, s_2 > 0 \) to the assertion
\[ \text{Lip}(K, B_{s_1}(x) \times B_{s_2}(y)) \leq L (1 + \| x \|_2 + \| y \|_2 + s_1 + s_2), \quad x, y \in \mathbb{R}^d. \] (45)

Part \((V_{K, \nu})\): By Proposition 34 it is sufficient to show that the potential \( V_{K, \nu}(x) = \int_{\mathbb{R}^d} K(x, y) \, d\nu(y), \ \nu \in \mathcal{P}_2(\mathbb{R}^d) \) satisfies the condition (42). Fix \( x \in \mathbb{R}^d, \ s > 0 \) and let \( x_1, x_2 \in B_s(x) \) with \( x_1 \neq x_2 \). Then by the previous findings (45) we estimate
\[
\frac{|V_{K, \nu}(x_1) - V_{K, \nu}(x_2)|}{\|x_1 - x_2\|_2} \leq \int_{\mathbb{R}^d} \frac{|K(x_1, y) - K(x_2, y)|}{\|x_1 - x_2\|_2} \, d\nu(y) \leq \int_{\mathbb{R}^d} \text{Lip}(K, B_s(x) \times \{ y \}) \, d\nu(y)
\]
\[
\leq \int_{\mathbb{R}^d} L (1 + \| x \|_2 + s + \| y \|_2) \, d\nu(y)
\]
\[
\leq L (1 + \int_{\mathbb{R}^d} \| y \|_2 \, d\nu(y) + \| x \|_2 + s).
\]
\[ \square \]

D Proofs from Section 7

D.1 Proof of Theorem 17

To establish the claim, we require the following integrals over the sphere.

**Proposition 37.** Let \( d \in \mathbb{N} \) with \( d \geq 2, \ r \in (0, 2) \) and \( R > 0 \). Then it holds
\[
\int_{S^{d-1}} \| x - y \|_2 \, dU_{S^{d-1}}(y) = \begin{cases} R^r \, _2F_1 \left( -\frac{r}{2}, \frac{2-r-d}{2}; \frac{d}{2}; \frac{\| x \|_2^2}{R^2} \right), & \| x \|_2 \leq R, \\ \| x \|_2^2 \, _2F_1 \left( -\frac{r}{2}, \frac{2-r-d}{2}; \frac{d}{2}; \frac{R^2}{\| x \|_2^2} \right), & R \leq \| x \|_2. \end{cases}
\]

**Proof.** In order to prove the claim, we consider the orthogonal polynomials \( P_n^{(d-2)} \) with respect to the weight function \((1-t^2)^{\frac{d-2}{2}}\). For \( d > 2 \), these are the Gegenbauer polynomials with normalization
\[
\int_{-1}^{1} P_n^{(d-2)}(t) P_m^{(d-2)}(t)(1-t^2)^{\frac{d-3}{2}} \, dt = \begin{cases} \frac{\pi 2^{3-d} \Gamma(n+d-2)}{n!(d-2)!} \Gamma(\frac{d-3}{2})^2, & n = m, \\ 0, & n \neq m. \end{cases}
\]

In particular, we have for \( n = 0 \) that
\[
\int_{-1}^{1} P_0^{(d-2)}(t) P_0^{(d-2)}(t)(1-t^2)^{\frac{d-3}{2}} \, dt = \frac{\pi 2^{3-d} \Gamma(d-2)}{d-2} = \frac{\pi 2^{3-d} \Gamma(d-\frac{3}{2}) \Gamma(\frac{d-1}{2})}{d-2} \Gamma(\frac{d}{2})^2 \\
= \frac{\pi^{1/2} \Gamma(\frac{d-1}{2})}{\Gamma(\frac{d}{2})} = B(\frac{1}{2}, \frac{d-1}{2}), \quad (46)
\]

39
where we used \( z\Gamma(z) = \Gamma(z + 1) \) and \( \Gamma(z)\Gamma(z + 1/2) = 2^{1-2z}\pi^{1/2}\Gamma(2z) \) and where \( B(a,b) \) is the beta function. For \( d = 2 \), we obtain the Chebyshev polynomials of first kind with normalization

\[
\int_{-1}^{1} P_n^{(0)}(t)P_m^{(0)}(t)(1 - t^2)^{-1/2}dt = \begin{cases} 
\pi, & n = m = 0, \\
\pi/2, & n = m \neq 0 \\
0, & n \neq m.
\end{cases}
\]

By definition, we obtain also for \( d = 2 \) that

\[
\int_{-1}^{1} P_0^{(d-2)}(t)P_0^{(d-2)}(t)(1 - t^2)^{d-3} dt = \pi = B\left(\frac{1}{2}, \frac{1}{2}\right) = B\left(\frac{d-1}{2}, \frac{d-3}{2}\right).
\]

Now, it holds by [7, Section 2] that for any \( c > 0 \) the function \( t \mapsto (2 - 2t + c^2)^{r/2} \) can be expanded for \( t \in [-1,1] \) as

\[
(2 - 2t + c^2)^{r/2} = \sum_{n=0}^{\infty} a_n\left(\frac{r}{2}, \frac{d-2}{2}\right) P_n^{(d-2)}(t),
\]

for some coefficients \( a_n\left(\frac{r}{2}, \frac{d-2}{2}\right) \). By definition of Chebyshev and Gegenbauer polynomials it holds that \( P_0^{(d-2)}(t) = 1 \) for all \( t \). Therefore, we can compute this coefficient for \( n = 0 \) as

\[
a_0\left(\frac{r}{2}, \frac{d-2}{2}\right) = \frac{1}{B\left(\frac{1}{2}, \frac{d-1}{2}\right)} \int_{-1}^{1} (2 - 2t + c^2)^{r/2} P_0^{(d-2)}(t)(1 - t^2)^{d-3} dt
\]

\[
= \frac{2}{B\left(\frac{1}{2}, \frac{d-1}{2}\right)} \int_{0}^{1} (4 + c^2 - 2t)^{r/2}(2t - t^2)^{d-3} dt
\]

\[
= \frac{2^{d-2}(4 + c^2)^{r/2}}{B\left(\frac{1}{2}, \frac{d-1}{2}\right)} \int_{0}^{1} \left(1 - \frac{4}{4 + c^2} t\right)^{r/2} t^{d-3} (1 - t)^{d-3} dt,
\]

where we substitute \( t \) by \( t - 1 \) in the first and \( t \) by \( 2t \) in the second equality. Using Euler’s integral formula [6, § 2.1.3, (10)], this is equal to

\[
a_0\left(\frac{r}{2}, \frac{d-2}{2}\right) = (4 + c^2)^{r/2} 2 F_1\left(-\frac{r}{2}, \frac{d-1}{2}, d-1, -\frac{4}{4 + c^2}\right).
\]

Note that for \( d > 2 \), this is consistent with the computations from [7, Section 2.1]. Now, let \( x \in \mathbb{R}^d \setminus \{0\} \), \( y \in S^{d-1} \) and choose \( t = x^Ty/\|x\|_2 \) and \( c^2 = (\|x\|_2 - 1)^2/\|x\|_2 \). Then, it holds

\[
(2 - 2t + c^2) = \frac{2\|x\|_2 - 2x^Ty + \|x\|_2^2 + 1 - 2\|x\|_2}{\|x\|_2} = \frac{\|x - y\|_2^2}{\|x\|_2}
\]

and

\[
(4 + c^2) = \frac{4\|x\|_2 + \|x\|_2^2 - 2\|x\|_2 + 1}{\|x\|_2} = \frac{(\|x\|_2 + 1)^2}{\|x\|_2}.
\]

40
In particular, we have

\[
\|x - y\|_r^r = \sum_{n=0}^{\infty} a_n \left( \frac{r}{2}, \frac{d-2}{2} \right) \|x\|_r^r \mathcal{P}_n^{(d-2)} \left( \frac{x^T y}{\|x\|_r^2} \right)
\]  

(48)

with

\[
a_0 \left( \frac{r}{2}, \frac{d-2}{2} \right) = \frac{\|x\|_r^r + 1}{\|x\|_r^r} 2 F_1 \left( -\frac{r}{2}, -\frac{d-1}{2}, d - 1; \frac{4\|x\|_r^r}{\|x\|_r^r + 1} \right).
\]

(49)

Due to symmetry, we can choose wlog \( y = y_1 e + y_{(d-1)} \) with \( y_1 \in [0, 1] \) and \( y_{(d-1)} \in \{0\} \times S^{d-2} \). Then, we compute the integral over the unit sphere by [4, (1.16)] as

\[
\int_{S^{d-1}} \|x - y\|_r^r dS^{d-1}(y) = \int_{-1}^{1} \int_{S^{d-2}} \|x - y\|_r^r dS^{d-2}(y_{(d-1)})(1 - y_1^2)^{\frac{d-3}{2}} dy_1.
\]

By inserting (48) and using \( \frac{x^T y}{\|x\|_r^2} = y_1 \), the above formula becomes

\[
\|x\|_r^r \int_{-1}^{1} \sum_{n=0}^{\infty} a_n \left( \frac{r}{2}, \frac{d-2}{2} \right) \mathcal{P}_n^{(d-2)}(y_1) dS^{d-2}(y_{(d-1)})(1 - y_1^2)^{\frac{d-3}{2}} dy_1.
\]

This does not depend on \( y_{(d-1)} \). Therefore, by using the volume formula over the sphere

\[
\int_{S^{d-2}} 1 dS^{d-2} = \frac{2\pi^{(d-1)/2}}{\Gamma \left( \frac{d-1}{2} \right)},
\]

it is equal to

\[
\|x\|_r^r \frac{2\pi^{(d-1)/2}}{\Gamma \left( \frac{d-1}{2} \right)} \int_{-1}^{1} \sum_{n=0}^{\infty} a_n \left( \frac{r}{2}, \frac{d-2}{2} \right) \mathcal{P}_n^{(d-2)}(y_1)(1 - y_1^2)^{\frac{d-3}{2}} dy_1.
\]

By interchanging the sum and the integral and adding the factor \( \mathcal{P}_0^{(d-2)}(y_1) = 1 \), this is equal to

\[
\|x\|_r^r \sum_{n=0}^{\infty} a_n \left( \frac{r}{2}, \frac{d-2}{2} \right) \frac{2\pi^{(d-1)/2}}{\Gamma \left( \frac{d-1}{2} \right)} \int_{-1}^{1} \mathcal{P}_0^{(d-2)}(y_1) \mathcal{P}_n^{(d-2)}(y_1)(1 - y_1^2)^{\frac{d-3}{2}} dy_1.
\]

Due to the orthogonality property of the polynomials \( \mathcal{P}_n^{(d-2)} \), all summands despite \( n = 0 \) are zero. Moreover, we can insert for \( n = 0 \) the formulas (46) and (47). Then, the above term is equal to

\[
\|x\|_r^r \frac{2\pi^{(d-1)/2}}{\Gamma \left( \frac{d-1}{2} \right)} B(1^2, \frac{d-1}{2}) a_0 \left( \frac{r}{2}, \frac{d-2}{2} \right) = \|x\|_r^r \frac{2\pi^{(d-1)/2}}{\Gamma \left( \frac{d-1}{2} \right)} \frac{\pi^{1/2} \Gamma \left( \frac{d-1}{2} \right)}{\Gamma \left( \frac{d}{2} \right)} a_0 \left( \frac{r}{2}, \frac{d-2}{2} \right)
\]

\[
= \|x\|_r^r \frac{2\pi^{d/2}}{\Gamma \left( \frac{d}{2} \right)} a_0 \left( \frac{r}{2}, \frac{d-2}{2} \right).
\]

Summarizing, we obtain by inserting (49)

\[
\int_{S^{d-1}} \|x - y\|_r^r dS^{d-1}(y) = \frac{2\pi^{d/2}}{\Gamma \left( \frac{d}{2} \right)} (||x|| + 1)^r 2 F_1 \left( -\frac{r}{2}, -\frac{d-1}{2}, d - 1; \frac{4||x||}{||x|| + 1} \right).
\]
By normalizing the volume of $S^{d-1}$ and rescaling with a factor $R$ this is equivalent to
\[
\int_{S^{d-1}} \|x-y\|_2^d \, dU_{S^{d-1}}(y) = (\|x\| + R)^2 \, F_2F_1\left(-\frac{d}{2}, \frac{d-1}{2}; d-1; \frac{4\|x\|R}{(\|x\|+R)^2}\right).
\]
Finally, the claim follows by the quadratic transformation rule due to Gauss [19, (2.11(5))] given by
\[
(1 + t)^{-2a} \, F_2F_1\left(a, b; 2b; 4t/(1 + t)^2\right) = \, F_2F_1\left(a, a + \frac{1}{2} - b; b + \frac{1}{2}; t^2\right), \quad t \in [0, 1],
\]
with $t = \|x\|/R$ for $\|x\| \leq R$ and $t = R/\|x\|_2$ for $R \leq \|x\|_2$.

Further, we will need some auxiliary results on hypergeometric functions.

**Lemma 38.** Let $d + r < 4$. Then, it holds for any $x \in [0, 1]$ that
\[
2F_1\left(1 - \frac{r}{2}, 2 - \frac{d+r}{2}; 3 - \frac{r}{2}; x\right) \geq \sup_{N_{\max} \in \mathbb{N}} \left\{ \sum_{n=0}^{N_{\max}} \frac{(1 - \frac{r}{2})_n (2 - \frac{d+r}{2})_n}{(3 - \frac{r}{2})_n n!} x^n \right\},
\]
where the last equality is due to the fact that all coefficients are non-negative. Further, the non-negativity of the coefficients implies that
\[
\sum_{n=1}^{N_{\max}} \frac{(1 - \frac{r}{2})_n (2 - \frac{d+r}{2})_n}{(3 - \frac{r}{2})_n n!} x^n
\]
is convex on $[0, 1]$ for any $N_{\max}$. Therefore $x \mapsto 2F_1\left(1 - \frac{r}{2}, 2 - \frac{d+r}{2}; 3 - \frac{r}{2}; x\right)$ is convex as a supremum of convex functions. Now the claim follows by the identity $f(x) \geq f(1) + (x - 1)f'(1)$ for convex functions and the derivative rule for hypergeometric functions.

We need the following lemma to prove Proposition 40 below.

**Lemma 39.** Let $d \in \mathbb{N}$ and $r \in (0, 2)$ with $d + r \geq 4$. Then it holds
\[
(i) \quad \frac{1}{2} \, F_2F_1\left(-\frac{r}{2}, \frac{-d-r-2}{2}; \frac{d}{2}; 1\right) = \frac{d+r-2}{d} \, F_2F_1\left(\frac{2-r}{2}, \frac{-d-r-4}{2}; \frac{d+2}{2}; 1\right), \quad \text{and}
\]
\[
(ii) \quad F_2F_1\left(\frac{4-x}{2}, \frac{6-d-x}{2}; \frac{d}{2} + 2; x\right) \geq 0 \quad \text{and} \quad F_2F_1\left(\frac{2-r}{2}, \frac{4-d-r}{2}; \frac{d}{2} + 1; x\right) \geq 0 \quad \text{for any} \quad x \in (0, 1).
\]
The hypergeometric function $f(x) = 2F_1\left(\frac{2-r}{2}, \frac{-d-r-4}{2}; \frac{d+2}{2}; x\right)$ is here decreasing on $[0, 1]$.
Proof. (i) By Gauss’s summation formula for hypergeometric functions [30, (3.1)], we have

$$\binom{a}{b} \binom{c}{d} = \binom{a+b}{c} \binom{a}{b} \binom{c}{d} \binom{c-a}{d-b}$$

Thus, we obtain together with $\Gamma(x + 1)/x = \Gamma(x)$ the first assertion

$$1 - \frac{\Gamma(d/2)\Gamma(d + r - 1)}{2\Gamma((d + r)/2)\Gamma(d + r/2 - 1)} = \frac{d}{\Gamma((d + r)/2)\Gamma(d + r/2 - 1)}$$

(ii) First, we show that $\binom{4-r}{2}, \binom{6-d-r}{2} + 2; x > 0$. Since $\binom{1}{0}$ is by definition symmetric in the first two arguments, we obtain

$$\binom{4-r}{2}, \binom{6-d-r}{2} + 2; x = \binom{1}{0}(4-r, 6-d-r; 2 + 2; x).$$

By Euler’s integral formula [6, § 2.1.3, (10)], this is equal to

$$\frac{\Gamma(d/2 + 2)}{\Gamma((d - r)/2)\Gamma(d + r/2)} \int_0^1 t^{(d-r)/2}(1-t)^{d/2-(d-r)/2}dt.$$

Since the $\Gamma$-function is positive on $\mathbb{R}_{>0}$ and since for $t, x \in (0, 1)$ it holds $t, (1-t), (1-tx > 0$, this is greater than zero and the first claim is proven. The proof of the second inequality works analogously. Finally, by the derivative rule for hypergeometric functions and $d + r \geq 4$, it follows

$$f'(x) = -\frac{(x+r)(d-r-4)}{2d+4} \binom{4-r}{2}, \binom{6-d-r}{2} + 2; x \leq 0,$$

so that $f$ is decreasing. □

Proposition 40. Let $d \in \mathbb{N}$ and $r \in (0, 2)$ with $d + r \geq 4$ and

$$h(x) := -\binom{4-r}{2}, \binom{6-d-r}{2} + 2; x^2$$

Then it holds $1 \in \arg \min_{x \in [0, 1]} h(x)$ and $1 \in \arg \min_{x \in [1, \infty]} \tilde{h}(x)$.

Proof. (i) Using the derivative rule for hypergeometric functions, we obtain

$$h'(x) = \frac{(d-r-2)}{2} x \left(2F_1 \left(\frac{2}{2}, \frac{6-d-r}{2}; 1 \right) - 2 \binom{4-r}{2}, \binom{6-d-r}{2} + 2; x^2 \right)$$

and in particular $h'(1) = 0$. By Lemma 39(ii) and since $x \mapsto x^2$ is strictly increasing on $[0, 1]$, the function $2F_1 \left(\frac{2}{2}, \frac{6-d-r}{2}; 1 \right)$ is decreasing on $[0, 1]$. In particular, we conclude

$$\binom{4-r}{2}, \binom{6-d-r}{2} + 2; x \leq 0, \text{ for } x = 1,$$

This implies $h'(x) \leq 0$ on $(0, 1)$ such that $h$ is decreasing on $[0, 1]$ which yields the first claim.
(ii) We show that \( \tilde{h}'(x) \geq 0 \) for \( x \in [1, \infty) \). We obtain
\[
\tilde{h}'(x) = -rx^{-2}F_1(-\frac{r}{2}, -\frac{d+r-2}{2}; \frac{d}{2}; \frac{1}{x^2}) + \frac{r^2(\frac{d+r-2}{2})}{d} \frac{d+r-4}{2} \frac{2}{2} F_1(\frac{2-r}{2}, -\frac{d+r-4}{2}; \frac{d+2}{2}; 1).
\]
Now \( h'(x) \geq 0 \) on \( [1, \infty) \) is equivalent to \( \frac{h'(x)}{x^2} \geq 0 \) on \( [1, \infty) \). By Lemma 39(ii) and since \( x \mapsto 1/x^2 \) is decreasing, the function \( x \mapsto 2F_1(\frac{2-r}{2}, -\frac{d+r-4}{2}; \frac{d+2}{2}; 1) \) is increasing on \( [1, \infty) \) such that we have for \( x \in [1, \infty) \) that
\[
\frac{\tilde{h}'(x)}{x^2} \geq g(x) := -2F_1(-\frac{r}{2}, -\frac{d+r-2}{2}; \frac{d}{2}; \frac{1}{x^2}) + \frac{2(\frac{d+r-2}{2})}{d} \frac{d+r-4}{2} \frac{2}{2} F_1(\frac{2-r}{2}, -\frac{d+r-4}{2}; \frac{d+2}{2}; 1)
\]
For \( x = 1 \), we obtain by Lemma 39(i) that
\[
g(1) = -2F_1(-\frac{r}{2}, -\frac{d+r-2}{2}; \frac{d}{2}; 1) + \frac{2(\frac{d+r-2}{2})}{d} \frac{d+r-4}{2} \frac{2}{2} F_1(\frac{2-r}{2}, -\frac{d+r-4}{2}; \frac{d+2}{2}; 1) = 0.
\]
Thus, it suffices to show that \( g \) is increasing on \( [1, \infty) \). Taking the derivative of \( g \) on \( [1, \infty) \) gives
\[
g'(x) = \frac{2}{x} (\frac{d+r-2}{2}) \frac{d+r-4}{2} \frac{2}{2} F_1(\frac{2-r}{2}, -\frac{d+r-4}{2}; \frac{d+2}{2}; 1)
\]
and we are done. \( \square \)

**Proof of Theorem 17(i):** In [13] it was shown that for \( d + r < 4 \) the measure \( \eta^*_\tau \) in (i) fulfills the equality condition in (24), see also [25, Lem 2.4]. We have to show the inequality condition.

**Case:** \( d = 1 \): Since \( \text{supp}(\eta^*_\tau) = [-s_\tau, s_\tau] \), it remains to show that
\[
f(x_1) := \int_{\mathbb{R}} K(x_1, x_2) d\eta^*_\tau(x_2) + \frac{1}{2\tau} ||x_1||^2
\]
is increasing on \( [s_\tau, \infty) \) and decreasing on \( (-\infty, s_\tau] \). Due to the symmetry, it suffices to show that \( f \) is increasing on \( [s_\tau, \infty) \). For \( x_1 \in [s_\tau, \infty) \), we have \( x_1 > x_2 \) for all \( x_2 \in \text{supp}(\eta^*_\tau) \) such that we can reformulate \( f \) as
\[
f(x_1) = -A_{s_\tau} \int_{-s_\tau}^{s_\tau} (x_1 - x_2)^2 (s_\tau^2 - x_2^2)^{(1-r)/2} dx_2 + \frac{1}{2\tau} x_1^2
\]
for all \( x_1 \geq s_\tau \). For \( x_1 \leq s_\tau \) we can use a similar argument.\( \square \)
Thus, its derivative on \((s_r, \infty)\) is given by

\[
f'(x_1) = g(x_1) := -rA_{s_r} \int_{-s_r}^{s_r} (x_1 - x_2)^{-1}(s_r^2 - x_2^2)^{(1-r)/2}dx_2 + \frac{1}{r}x_1 \quad (51)
\]

Now, we show first that \(g(s_r) = 0\) and second that \(g\) is increasing on \((s_r, \infty)\). Together this shows that \(f' > 0\) such that \(f\) is increasing on \([s_r, \infty)\) and we are done.

By [25, Cor. 2.5], with \(m = 1\), \(\beta = r - 1\) and \(\alpha = r\) it holds

\[
g(s_r) = -rA_{s_r} \frac{\pi^2}{\Gamma^2(\frac{1}{2})} \text{B}(\frac{3-r}{2}, \frac{r}{2})_2 F_1(1-r, -\frac{1}{2}; 1, \frac{1}{2}) + \frac{1}{r}
\]

Using Gauss’s summation formula for hypergeometric functions (50), the above equation can be reformulated as

\[
g(s_r) = -rA_{s_r} \frac{-2(r-1)\Gamma(\frac{1}{2})\Gamma(2-r)}{\pi^2 \Gamma(\frac{1}{2}) \Gamma(\frac{3-r}{2})} \frac{\Gamma(\frac{1}{2}) \Gamma(\frac{3-r}{2}) \Gamma(\frac{1-r}{2}) \Gamma(\frac{r}{2})}{\Gamma(\frac{1}{2}) \Gamma(1)} + \frac{1}{r}
\]

\[
= -rA_{s_r} \frac{2(r-1)\Gamma(\frac{1}{2})\Gamma(\frac{3-r}{2})}{\pi^2 \Gamma(\frac{1}{2}) \Gamma(\frac{3-r}{2})} \Gamma(\frac{1}{2}) \Gamma(\frac{3-r}{2}) \Gamma(\frac{1-r}{2}) \Gamma(\frac{r}{2}) + \frac{1}{r}
\]

This implies that \(g(s_r) = 0\).

Further, it holds for \(r \in (0, 1]\) that \((x_1 - x_2)^{-1}\) is decreasing on \([s_r, \infty)\) for any \(x_2 \in [-s_r, s_r]\). Therefore both terms in (51) are increasing and we are done for this case. For \(r \in (1, 2)\), we take again the derivative of \(g\) and arrive at

\[
g'(x_1) := -r(r-1)A_{s_r} \int_{-s_r}^{s_r} (x_1 - x_2)^{r-2}(s_r^2 - x_2^2)^{(1-r)/2}dx_2 + \frac{1}{r}
\]

By the same arguments as above we have that \(g'\) is increasing on \((s_r, \infty)\) and using [25, Cor. 2.5], with \(m = 1\), \(\beta = r - 2\) and \(\alpha = r\) and Gauss’s summation formula, we obtain

\[
g'(s_r) = -r(r-1)A_{s_r} \frac{\pi^2}{\Gamma^2(\frac{1}{2})} \text{B}(\frac{3-r}{2}, \frac{r}{2})_2 F_1(2-r, 0, \frac{1}{2}; 1) + \frac{1}{r}
\]

\[
= -r(r-1)A_{s_r} \frac{2(r-1)\Gamma(\frac{1}{2})\Gamma(2-r)}{\pi^2 \Gamma(\frac{1}{2}) \Gamma(\frac{3-r}{2})} \frac{\Gamma(\frac{1}{2}) \Gamma(\frac{3-r}{2}) \Gamma(\frac{1-r}{2}) \Gamma(\frac{r}{2})}{\Gamma(\frac{1}{2}) \Gamma(2-r)} + \frac{1}{r}
\]

This implies that \(g\) is increasing on \([s_r, \infty)\) and we are done.

**Case \(d \geq 2\):** Let \(e_1\) be the first unit vector in \(\mathbb{R}^d\). Choose \(\tau\) such that \(s_r = 1\) and let \(t \geq 1\), i.e.,

\[
\tau = \frac{4\Gamma(\frac{1}{2})}{\Gamma(2-\frac{1}{2}) \Gamma(\frac{1}{2})} = \frac{\Gamma(1+\frac{1}{2})}{\Gamma(2-\frac{1}{2}) \Gamma(\frac{1}{2})}.
\]
We consider
\[ h(t) := -\int_{\mathbb{R}^d} ||te_1 - x||^\tau \, d\mathcal{H}_d(x) + \frac{1}{2\tau} t^2 = -A_1 \int_{B_1} ||te_1 - x||^{\tau} (1 - ||x||^{2})^{1 - \frac{2\tau}{d}} \, dx + \frac{1}{2\tau} t^2. \]

We aim to show that \( h(t) \geq h(1) \) for all \( t \geq 1 \). Changing the order of integration, the integral over \( B_1 \) is equal to
\[ I(t) = \int_0^1 \int_{\mathbb{R}^{d-1}} ||te_1 - x||^\tau \, d\mathcal{H}_{d-1}(x) \frac{2\pi^{\frac{d}{2}} R^{d-1}}{\Gamma(\frac{d}{2})} (1 - R^2)^{1 - \frac{r+d}{2}} dR. \]

Now, the inner integral can be computed by Proposition 37. Then the above formula becomes
\[ I(t) = \frac{\pi^{\frac{d}{2}} R^r}{\Gamma(\frac{d}{2})} \int_0^1 2F_1 \left( -\frac{r}{2}, 1 - \frac{r+d}{2}; \frac{d}{2}; \frac{R^2}{t^2} \right) R^{d-2} (1 - R^2)^{1 - \frac{r+d}{2}} 2R dR. \]

Using the substitution \( S = R^2 \) \( (\, dS = 2RdR) \), this is equal to
\[ I(t) = \frac{\pi^{\frac{d}{2}} t^r}{\Gamma(\frac{d}{2})} \int_0^1 2F_1 \left( -\frac{r}{2}, 1 - \frac{r+d}{2}; \frac{d}{2}; \frac{S}{t^2} \right) S^{\frac{d}{2}-1} (1 - S)^{1 - \frac{d+r}{2}} dS. \]

Now using Euler’s integral transform [47, eqn (4.1.2)] for generalized hypergeometric functions
\[ _3F_2(a_1, a_2, a_3; b_1, b_2; z) = \frac{\Gamma(b_2)}{\Gamma(a_3) \Gamma(b_2 - a_3)} \int_0^1 S^{a_3 - 1} (1 - S)^{b_2 - a_3 - 1} 2F_1(a_1, a_2; b_1; Sz) \, d S \]
with \( a_1 = -\frac{r}{2}, \, a_2 = 1 - \frac{r+d}{2}, \, a_3 = \frac{d}{2}, \, b_1 = \frac{d}{2}, \, b_2 = 2 - \frac{r}{2} \) and \( z = \frac{1}{t^2} \), we obtain
\[ I(t) = \frac{\pi^{\frac{d}{2}} t^r}{\Gamma(\frac{d}{2})} \frac{\Gamma(\frac{4}{2}) \Gamma(\frac{2-r-d}{2})}{\Gamma(\frac{2-2r}{2})} _3F_2 \left( -\frac{r}{2}, 1 - \frac{r+d}{2}; \frac{d}{2}, \frac{2}{2}, 2 - \frac{r}{2}; \frac{1}{t^2} \right). \]

Using the definition of generalized hypergeometric functions
\[ _3F_2(a_1, a_2, c; b; z) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n (c)_n}{(b)_n n!} z^n = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n}{(b)_n n!} z^n = _2F_1(a_1, a_2; b; z) \]
with Pochhammer symbol \((z)_0 = 1\) and \((z)_n = (z + n - 1) (z)_{n-1}\), we conclude
\[ I(t) = \frac{\pi^{\frac{d}{2}} t^r \Gamma(\frac{2-r-d}{2})}{\Gamma(\frac{2-2r}{2})} _2F_1 \left( -\frac{r}{2}, 1 - \frac{r+d}{2}; 2 - \frac{r}{2}; \frac{1}{t^2} \right). \]

Thus, the function \( h \) can be rewritten as
\[ h(t) = -A_1 \frac{\pi^{\frac{d}{2}} t^r \Gamma(\frac{2-r-d}{2})}{\Gamma(\frac{2-2r}{2})} _2F_1 \left( -\frac{r}{2}, 1 - \frac{r+d}{2}; 2 - \frac{r}{2}; \frac{1}{t^2} \right) + \frac{t^2}{2\tau} \]
\[ = -\frac{\Gamma(2-r)}{\pi^{\frac{d}{2}} \Gamma(\frac{2-2r}{2})} \frac{\pi^{\frac{d}{2}} t^r \Gamma(\frac{2-r-d}{2})}{\Gamma(\frac{2-2r}{2})} _2F_1 \left( -\frac{r}{2}, 1 - \frac{r+d}{2}; 2 - \frac{r}{2}; \frac{1}{t^2} \right) + \frac{r \Gamma(2-r) \Gamma(\frac{4-r}{2}) t^2}{2t (1+r)} \]
\[ = -r^2 _2F_1 \left( -\frac{r}{2}, 1 - \frac{r+d}{2}; 2 - \frac{r}{2}; \frac{1}{t^2} \right) + \frac{r \Gamma(2-r) \Gamma(\frac{4-r}{2}) t^2}{2t (1+r)}. \]
In order to show that $h$ is increasing on $[1, \infty)$, we consider its derivative. It is given by

\[ h'(t) = -rt^{-1} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) \]

\[ + \frac{r^{3} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) + r^{3} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r})}{\Gamma(1 + \frac{1}{2})}. \]

Since $r + d - 2 \geq 0$, we have by Lemma 38 that

\[ \frac{h'(t)}{rt^2} \geq g(t) := -2 F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) \]

\[ - (t^{-2} - t^{-4}) \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) + \frac{r^{3} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r})}{\Gamma(1 + \frac{1}{2})}. \]

Next, we show that $g$ is non-negative on $[1, \infty)$, which implies that $h'$ is non-negative such that $h$ is increasing on $[1, \infty)$. Using Gauss's summation formula for hypergeometric functions (50), we can evaluate $g(1)$ using the identity $\Gamma(z) = \Gamma(z + 1)$ as

\[ g(1) = -\frac{\Gamma(2 - z) \Gamma(1 + z)}{\Gamma(1 + \frac{3}{2})} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) \]

\[ - (t^{-2} - t^{-4}) \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) + \frac{r^{3} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r})}{\Gamma(1 + \frac{1}{2})} \]

\[ = \frac{\Gamma(2 - z) \Gamma(1 + z)}{\Gamma(1 + \frac{3}{2})} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) \]

\[ = 0. \]

Thus it suffices to show that $g$ is increasing. The derivative of $g$ is given by

\[ g'(t) = t^{-2} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) \]

\[ + \frac{(2t^{-2} - 4t^{-5}) \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r})}{\Gamma(1 + \frac{1}{2})}. \]

The inequality is again the application of Lemma 38. Reformulation yields

\[ g'(t) \geq (2 - r) t^{-3} \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) \]

\[ + (2t^{-2} - 4t^{-5}) \binom{2}{2} F_{1}(1 - \frac{r}{2}, 2 - \frac{r+d}{2}; 3 - \frac{r}{2}; \frac{1}{r}) + \frac{(2-r) \Gamma(2 - z) \Gamma(1 + z)}{\Gamma(1 + \frac{3}{2})}. \]

Applying Gauss's summation formula for hypergeometric functions and $\Gamma(z) = \Gamma(z + 1)$, 47
the above formula becomes
\[ g'(t) \geq -(2 - r) t^{-3} + \frac{d - r - 2}{4} \frac{\Gamma\left(\frac{d - r - 2}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} + \frac{(2 - r) \Gamma\left(\frac{d - r - 2}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} t^{-r} \]
\[ + \frac{(2t - r - 3 - 4t - 5 + 5t t - 5) + d - 2}{4} \frac{\Gamma\left(\frac{d + r - 1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} t^{-r} \]
\[ = -(2 - r) t^{-3} \frac{(r + d - 2) \Gamma\left(\frac{d + r - 1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} + \frac{(2 - r) \Gamma\left(\frac{d + r - 1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} t^{-r} \]
\[ = -(2 - r) t^{-3} \frac{(r + d - 2) \Gamma\left(\frac{d + r - 1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} t^{-r} \]
\[ = (2 - r) \frac{\Gamma\left(\frac{d + r - 1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} \left(t^{1-r} \frac{4}{4} \right) \]
\[ \geq (2 - r) \frac{\Gamma\left(\frac{d + r - 1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} \left(t^{1-r} + \frac{(2 - r)(4 - r - d)}{4} t^{-3} - \frac{(4 - r)(4 - r - d)}{4} t^{-3} \right) \]
\[ = (2 - r) \frac{\Gamma\left(\frac{d + r - 1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} (t^{1-r} - t^{-3}) \geq 0. \]

In summary, we have that \( g(1) = 0 \) and that \( g \) is increasing on \([1, \infty)\). Therefore, \( g \) is non-negative on \([1, \infty)\) which yields that \( f' \) is non-negative on \([1, \infty)\). In particular \( f \) is increasing on \([1, \infty)\) and we are done.

**Proof of Theorem 17(ii):** We have to check that \( \eta^*_r \) fulfills the conditions in (24). Since the constraint for \( \eta^* \) in (21) is fulfilled for \( R = 1 \), it remains to show (24) just for \( R = 1 \) and the appropriate \( \tau \), and then use Proposition 16(i) to get \( \eta^*_r \). To this end, we consider the functions

\[ h(x) = -2 F_1\left(-\frac{r}{2}, \frac{2 - r + d}{2}; \frac{d}{2}; x^2\right) + \frac{1}{2} x^2, \]
\[ \tilde{h}(x) = -2 F_1\left(-\frac{r}{2}, \frac{2 - r + d}{2}; \frac{d}{2}; \frac{1}{x^2}\right) x^r + \frac{1}{2} x^2. \]

Clearly, the equality condition in (24) is fulfilled with the constant \( C_r = h(1) = \tilde{h}(1) \). We have to show that \( h(x) \geq h(1) \) for \( x \in [0, 1] \) and \( \tilde{h}(x) \geq \tilde{h}(1) \) for \( x \in [1, \infty) \). With

\[ \frac{1}{r} = \frac{r(d + r - 2)}{d} 2 F_1\left(\frac{2 - r}{2}, -\frac{d + r - 4}{2}; \frac{d + 2}{2}; 1\right) \]

this is shown in Proposition 40. This implies \( \eta^* = U_{\eta^*} \) and it follows directly from Proposition 37 that \( \mathcal{E}_K(\eta^*) = -\frac{1}{2} F_1\left(-\frac{r}{2}, \frac{2 - r + d}{2}; \frac{d}{2}; 1\right) \).

**D.2 Proof of Theorem 20**

We prove the more general statement that for any symmetric and locally Lipschitz continuous kernel \( K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) with Lipschitz constant

\[ \text{Lip}(F, A) := \sup \left\{ \frac{|F(x) - F(y)|}{\|x - y\|_2} : x, y \in A, x \neq y \right\}. \]

fulfilling

\[ \text{Lip}(K, B_r(x) \times B_s(y)) \leq L(1 + \|x\|_2 + \|y\|_2 + r + s), \quad x, y \in \mathbb{R}^d, \quad r, s \geq 0, \]

48
and any $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ with $\mu(X) = 0$, where $X \subseteq \mathbb{R}^d \times \mathbb{R}^d$ is the set, where $K$ is not differentiable, it holds

$$H_v\mathcal{E}_K(\mu) = D_v\mathcal{E}_K(\mu) = \langle (\text{Id}, \nabla G)\#_\mu, v \rangle_\mu, \quad v \in T_\mu\mathcal{P}_2(\mathbb{R}^d).$$

(52)

Since the Riesz kernel with $r \in [1, 2]$ fulfills these properties, this implies by the equality condition of the Cauchy–Schwarz inequality from Lemma 27 (iii) that

$$\arg\min_{v \in T_\mu\mathcal{P}_2(\mathbb{R}^d), \|v\|_\mu = 1} H_v\mathcal{E}_K(\mu) = \left\{ -\|\text{Id}, \nabla G\#_\mu\|_{\mu}^{-1} \cdot (\text{Id}, \nabla G)\#_\mu \right\}$$

such that

$$H_{-}\mathcal{E}_K(\mu) = \{(-1) \cdot (\text{Id}, \nabla G)\#_\mu \} = \{(\text{Id}, -\nabla G)\#_\mu \}.$$

Observe that the Riesz kernel is everywhere differentiable for $r \in (1, 2)$ and that it is not differentiable exactly at $\{(x, x) : x \in \mathbb{R}^d\}$ for $r = 1$. Moreover, by Fubini’s Theorem the assertion $\mu(\{x\}) = 0$ for all $x \in \mathbb{R}^d$ leads to

$$\mu \otimes \mu(\{(x, x) : x \in \mathbb{R}^d\}) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} 1_{\{(x, x) : x \in \mathbb{R}^d\}}(y, z) d\mu(y) d\mu(z)$$

$$= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} 1_{\{z\}}(y) d\mu(y) d\mu(z) = \int_{\mathbb{R}^d} \mu(\{z\}) d\mu(z) = 0,$$

which proves Theorem 20. Thus, it remains to show (52).

Since $K$ is locally Lipschitz, it holds for a.e. $(x, y) \in \mathbb{R}^{2d}$ that $K$ is differentiable, hence

$$\lim_{t \to 0^+} \frac{K(x + tv, y + tw) - K(x, y)}{t} = \nabla K(x, y)^T(v, w), \quad (v, w) \in \mathbb{R}^{2d}.$$

We can apply the dominated convergence theorem, since the right hand side in

$$\left| \frac{K(x + tv, y + tw) - K(x, y)}{t} \right| \leq \text{Lip}(K, B_{\|v\|_2}(x) \times B_{\|w\|_2}(y)) \|v, w\|_2$$

is absolutely integrable. Hence, for any measure $\mu$ with $\mu \otimes \mu(X) = 0$ and direction $v \in T_\mu\mathcal{P}_2(\mathbb{R}^d)$, we obtain by symmetry of $K$ and Fubini’s theorem that

$$\lim_{t \to 0^+} \frac{\mathcal{E}_K(\gamma_{v}(t)) - \mathcal{E}_K(\mu)}{t} = \lim_{t \to 0^+} \frac{\mathcal{E}_K(\gamma_{v}(1)) - \mathcal{E}_K(\mu)}{t}$$

$$= \lim_{t \to 0^+} \frac{1}{2} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} K(x + tv, y + tw) - K(x, y) \frac{d\mu(x, v)d\mu(y, w)}{t}$$

$$= \frac{1}{2} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \nabla K(x, y)^T(v, w) d\mu(x, v) d\mu(y, w)$$

$$= \frac{1}{2} \int_{\mathbb{R}^{2d}} \int_{\mathbb{R}^{2d}} \nabla_1 K(x, y)^Tv + \nabla_2 K(x, y)^Tw d\mu(x, v) d\mu(y, w)$$

$$= \int_{\mathbb{R}^{2d}} v^T \left( \int_{\mathbb{R}^d} \nabla_1 K(x, y) d\mu(y) \right) d\mu(x, v).$$

49
Using again the dominating convergence theorem with (53) we note that
\[
\int_{\mathbb{R}^d} \nabla_1 K(x, y) d\mu(y) = \nabla \int_{\mathbb{R}^d} K(x, y) d\mu(y), \quad \mu - \text{a.e.} \quad x \in \mathbb{R}^d,
\]
so that
\[
\lim_{t \to 0^+} \frac{\mathcal{E}_K(\gamma_t(t)) - \mathcal{E}_K(\mu)}{t} = \int_{\mathbb{R}^{2d}} v^T \nabla G(x) dv(x, v) = \int_{\mathbb{R}^d} x_2^T x_3 d\alpha(x_1, x_2, x_3)
\]
with \(\alpha = (\pi_1, \pi_2, \nabla G \circ \pi_1)\#v\). Since \(\alpha\) is the unique plan with \((\pi_1, 2)\#\alpha = v\) and \((\pi_1, 3)\#\alpha = (\text{Id}, \nabla G)\#\mu\) and we arrive at (52) by definition (33).

\[\square\]

### D.3 Proof of Theorem 21

The curve of interest (26) is of the form \(\gamma_{c_2-r}\), where \(c_\tau := (-\tau r \mathcal{E}_K(\eta^*))^{\frac{1}{1-r}}\) and
\[
\gamma_c(t) := \gamma_{\delta_0 \otimes \eta^*}(ct^{\frac{1}{1-r}}) = (ct^{\frac{1}{1-r}} \text{Id})\#\eta^*, \quad c > 0.
\]
In order to apply Theorem 20, we compute the gradient of the function
\[
G_{\gamma_{c_\tau}}(t)(x) := \int_{\mathbb{R}^d} K(x, y) d\gamma_{c_\tau}(t)(y).
\]
Here, we distinguish two cases. First, in case \(d + r < 4\), Theorem 18 yields that \(\eta^*\) is absolute continuous. Moreover, we know from Proposition 15 and Proposition 16 that \(\eta_\tau^* = (c_\tau \text{Id})\#\eta^*\) satisfies the optimality conditions (24), in particular,
\[
\int_{\mathbb{R}^d} K(x, y) d(c_\tau \text{Id})\#\eta_\tau^*(y) = \int_{\mathbb{R}^d} K(x, y) d\eta_\tau^*(y) = C_{K, \tau} - \frac{1}{2t} \|x\|_2^2
\]
for all \(x \in \text{supp} \eta_\tau^*\). Then we can compute
\[
G_{\gamma_{c_\tau}}(t)(x) = -\int_{\mathbb{R}^d} \|x - y\|_2 \ d(c_\tau t^{\frac{1}{1-r}} \text{Id})\#\eta^*(y)
= t^{\frac{2}{1-r}} \int_{\mathbb{R}^d} K(x t^{\frac{1}{1-r}}, y) d(c_\tau \text{Id})\#\eta^*(y)
= t^{\frac{2}{1-r}} \left( C_{K, \tau} - \frac{t^{\frac{2}{1-r}}}{2t} \|x\|_2^2 \right)
= t^{\frac{2}{1-r}} C_{K, \tau} - \frac{1}{2t} \|x\|_2^2, \quad x \in \text{supp}(\gamma_{c_\tau}(t)).
\]
In the interior of \(\text{supp}(\gamma_{c_\tau}(t))\), we thus have
\[
\nabla G_{\gamma_{c_\tau}}(t)(x) = -\frac{x}{t}, \quad t > 0,
\]
which holds also true \( \gamma_{c_r}(t) \text{-a.e.} \) since \( \eta^* \) is absolutely continuous.

Second, if \( d+r \geq 4 \), we have \( \eta^* = U_{d-1} \) by Theorem 18. Proposition 37 for \( R = c_r t^{2-r} \) and \( x \in \mathbb{R}^d \) with \( \|x\|_2 \leq R \) implies

\[
G_{\gamma_{c_r}(t)}(x) = -\int_{R^{d-1}} \|x - y\|_2^2 \, dU_{R^{d-1}}(y) = -R^r 2 F_1\left( -\frac{r}{2}, \frac{2-r-d}{2}; d; \frac{\|x\|_2^2}{R^2} \right).
\]

Using the derivative rule for hypergeometric functions and the chain rule, we have

\[
\nabla G_{\gamma_{c_r}(t)}(x) = -R^{r-2} \frac{r(d+r-2)}{d} 2 F_1\left( \frac{2-r}{2}, \frac{4-r-d}{2}; \frac{d+2}{2}; \frac{\|x\|_2^2}{R^2} \right) x,
\]

for \( x \in \text{supp}(\gamma_{c_r}(t)) = R S^{d-1} \). On the basis of Proposition 37, we have \( \mathcal{E}_K(\eta^*) = -\frac{1}{2} 2 F_1\left( -\frac{r}{2}, \frac{2-r-d}{2}; \frac{d}{2}; 1 \right) \) so that

\[
\frac{(d+r-2)}{d} 2 F_1\left( \frac{2-r}{2}, \frac{4-r-d}{2}; \frac{d+2}{2}; \frac{\|x\|_2^2}{R^2} \right) \mathcal{E}_K(\eta^*) = -1
\]

by Lemma 39(i). Inserting this in the previous equation, we obtain also in this case that

\[
\nabla G_{\gamma_{c_r}(t)}(x) = -\frac{r}{t}.
\]

Setting \( s := (2-r)^{-1} \), and using Lemma 6 and 5, we deduce

\[
\dot{\gamma}_{c_r}(t) = c s t^s - \dot{\gamma}_{c_0} \otimes \eta^*(c t^s)
\]

(54)

Inserting the computed gradient for \( t > 0 \), we get

\[
\dot{\gamma}_{c_2-r}(t) = (\text{Id}, (2-r)^{-1} t^{-1} \text{Id}) \# \gamma_{c_2-r}(t) = (\text{Id}, -\nabla G_{\gamma_{c_2-r}(t)} \# \gamma_{c_2-r}(t),
\]

which is the unique element of \( H \mathcal{E}(\gamma_{c_2-r}(t)) \) by Theorem 20.
Finally, we consider the case \( t = 0 \). For \( t \to 0 \) in (54), we obtain
\[
\dot{\gamma}_{c_2,r}(0) = \begin{cases} (-E_K(\eta^*)) \cdot \delta_0 \otimes \eta^*, & r = 1, \\ 0 \cdot \delta_0 \otimes \eta^*, & r \in (1, 2), \end{cases}
\]
which is by Theorem 13 exactly the direction of steepest descent at \( \delta_0 \). This concludes the proof. \( \square \)

\section*{E Proof of Theorem 24}

\textbf{Part (i)} We note that the discrepancy may be written as \( D^2_K(\mu, \nu) = E_K(\mu) \) with
\[
\tilde{K}(x_1, x_2) = K(x_1, x_2) + V_{K,\nu}(x_1) + V_{K,\nu}(x_2) + E_K(\nu), \quad x_1, x_2 \in \mathbb{R}^d.
\]
For \( r \in (1, 2) \) we have that the kernel \( \tilde{K} \) is by definition differentiable. In the case \( r = 1 \), the first term is not differentiable for \( (x_1, x_2) \notin X_1 := \{(x, x) : x \in \mathbb{R}^d\} \), the second term is not differentiable for \( (x_1, x_2) \notin X_2 := \{(q, x) \in \mathbb{R}^d \times \mathbb{R}^d : \nu(\{q\}) \neq 0\} \) and the third term is not differentiable when \( (x_1, x_2) \notin X_3 := \{(x, q) \in \mathbb{R}^d \times \mathbb{R}^d : \nu(\{q\}) \neq 0\} \). In the following, we prove that \( X_1, X_2 \) and \( X_3 \) are zero-sets under \( \mu \otimes \mu \). Then, the statement follows analogously to the proof of Theorem 20 in D.2.

As in the proof of Theorem 20, we have \( \mu \otimes \mu(X_1) = 0 \) since \( \mu(\{x\}) = 0 \) for all \( x \in \mathbb{R}^d \). Moreover, we have \( X_2 = \{q \in \mathbb{R}^d : \nu(\{q\}) \neq 0\} \times \mathbb{R}^d \) such that
\[
\mu \otimes \mu(X_2) = \mu(\{q \in \mathbb{R}^d : \nu(\{q\}) \neq 0\}) = \sum_{q \in \mathbb{R}^d \text{ with } \nu(\{q\}) \neq 0} \mu(\{q\}) = 0,
\]
where we used that \( \{q \in \mathbb{R}^d : \nu(\{q\}) \neq 0\} \) is countable as any probability measure has only countable many points with positive mass. Finally, \( \mu \otimes \mu(X_3) = 0 \) follows analogously.

\textbf{Part (ii)} The discrepancy functional is locally Lipschitz. Therefore, to compute the Hadamard derivative, we can exploit Proposition 7 and the decomposition (16). As in the proof of Theorem 20, the function \( V_{K,\nu} \) is differentiable in \( p \) if \( \nu(\{p\}) = 0 \). In view of Lebesgue’s dominated convergence theorem, the Dini derivative of the interaction energy in direction \( v := \delta_p \otimes \eta, \eta \in \mathcal{P}_2(\mathbb{R}^d) \), is thus given by
\[
D_v V_{K,\nu}(\delta_p) = \lim_{t \to 0^+} \frac{V_{K,\nu}(\gamma_v(t)) - V_{K,\nu}(\delta_p)}{t}
= \lim_{t \to 0^+} \frac{1}{t} \int_{\mathbb{R}^d \times \mathbb{R}^d} V_{K,\nu}(x_1 + tx_2) - V_{K,\nu}(x_1) \, d\nu(x_1, x_2)
= \int_{\mathbb{R}^d} \langle \nabla V_{K,\nu}(p), x_2 \rangle \, d\eta(x_2) = \langle \nabla V_{K,\nu}(p), v_0 \rangle,
\]

52
where \( v_\eta := \int_{\mathbb{R}^d} x \, d\eta(x) \). The steepest descent directions \( H_{-\delta_p} \mathcal{F}_\nu(\mu) \) are now given by the tangents \( (H_{-\delta_p} \mathcal{F}_\nu(\delta_p))^\perp \cdot (\delta_p \otimes \hat{\eta}) \), where \( \hat{\eta} \) solves
\[
\min_{\eta \in \mathcal{P}_2(\mathbb{R}^d)} H_{-\delta_p} \mathcal{F}_\nu(\delta_p) + \nabla V_{K,\nu}(p)^T v_\eta \quad \text{s.t.} \quad \int_{\mathbb{R}^d} ||x||^2_2 \, d\eta(x) = 1. \tag{55}
\]
We want to bring the problem into an equivalent form, where the minimizer can be easier computed. First we have for \( \eta \in S_1 := \{ \eta \in \mathcal{P}_2(\mathbb{R}^d) : \int_{\mathbb{R}^d} ||x||^2_2 \, d\eta(x) = 1 \} \) and \( v_\eta \) as above that
\[
\int_{\mathbb{R}^d} ||x||^2_2 \, d(\text{Id} - v_\eta) \# \eta(x) = \int_{\mathbb{R}^d} ||x||^2_2 \, d\eta(x) - 2 \, v_\eta^T \int_{\mathbb{R}^d} x \, d\eta(x) + ||v_\eta||^2_2
\]
\[
= \int_{\mathbb{R}^d} ||x||^2_2 \, d\eta(x) - ||v_\eta||^2_2 = 1 - ||v_\eta||^2_2. \tag{56}
\]
In particular, we have \( ||v_\eta||^2_2 \leq 1 \) with equality if and only if \( \eta = \delta_{v_\eta} \). Now, we show that the set \( S_1 \) coincides with the set
\[
S_2 := \{ (\text{Id} + v_\eta) \# ((1 - ||v||^2)^{\frac{1}{2}} \text{Id}) \# \eta : (\eta, v) \in \mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d, \int_{\mathbb{R}^d} x \, d\eta(x) = 0, \int_{\mathbb{R}^d} ||x||^2_2 \, d\eta(x) = 1, ||v|| \leq 1 \}.
\]
Straightforward computation shows that \( S_2 \subseteq S_1 \). For the other direction, let \( \eta \in S_1 \) and \( v_\eta \) as above. In the case that \( ||v_\eta||^2_2 < 1 \) we consider \( \tilde{\eta} \) defined by
\[
\eta = (\text{Id} + v_\eta) \# ((1 - ||v_\eta||^2)^{\frac{1}{2}} \text{Id}) \# \eta \tag{57}
\]
Then we obtain by (56) that \( \int_{\mathbb{R}^d} ||x||^2_2 \, d\tilde{\eta}(x) = 1 \) and
\[
\int_{\mathbb{R}^d} x \, d\tilde{\eta}(x) = (1 - ||v_\eta||^2_2)^{-\frac{1}{2}} \int_{\mathbb{R}^d} x - v_\eta \, d\eta(x) = 0.
\]
Thus, \( \tilde{\eta} \) fulfills the constraints from \( S_2 \). For \( ||v_\eta||^2_2 = 1 \), we have by definition that \( \tilde{\eta} = U_{-v_\eta} \) fulfills the constraints from \( S_2 \) and formula (57) such that we obtain \( S_1 = S_2 \).

For \( r = 1 \), we have by Theorem 13 that \( H_{-\delta_p} \mathcal{E}_K(\delta_p) = \mathcal{E}_K(\eta) \) so that by the translational invariance of \( \mathcal{E}_K \) and since \( S_1 = S_2 \) problem (55) is equivalent to
\[
\min_{\eta \in \mathcal{P}_2(\mathbb{R}^d)} \min_{v \in \mathbb{R}^d} (1 - ||v||^2_2)^{\frac{1}{2}} \mathcal{E}_K(\eta) + \nabla V_{K,\nu}(p)^T v, \quad \text{s.t.} \quad \int_{\mathbb{R}^d} ||x||^2_2 \, d\eta(x) = 1, \int_{\mathbb{R}^d} x \, d\eta(x) = 0, \quad ||v||^2_2 \leq 1. \tag{58}
\]
Applying Cauchy–Schwarz’s inequality, we estimate the objective function by
\[
(1 - ||v||^2_2)^{\frac{1}{2}} \mathcal{E}_K(\eta) + \nabla V_{K,\nu}(p)^T v \geq (1 - ||v||^2_2)^{\frac{1}{2}} \mathcal{E}_K(\eta) - ||\nabla V_{K,\nu}(p)||_2 ||v||_2
\]
\[
= \left( \left( 1 - ||v||^2_2 \right)^{\frac{1}{2}}, \left( -||\nabla V_{K,\nu}(p)||_2 \right) \right)\]
with equality if and only if \( v = a \nabla V_{K, \nu}(p) \) for some \( a < 0 \). Applying Cauchy–Schwarz’s inequality once more, we obtain

\[
(1 - \|v\|_2^2)^{\frac{1}{4}} \mathcal{E}_K(\tilde{\eta}) + \nabla V_{K, \nu}(p)^T v \geq -\sqrt{\mathcal{E}_K(\tilde{\eta})^2 + \|\nabla V_{K, \nu}(p)\|_2^2}
\]

with equality if and only if

\[
(1 - \|v\|_2^2)^{\frac{1}{4}} = b (\|\nabla V_{K, \nu}(p)\|_2)\]

for some \( b > 0 \). Since the norm of the left-hand side is one, and due to the equality within the second component, equality can only hold if

\[
b = (\mathcal{E}_K(\tilde{\eta})^2 + \|\nabla V_{K, \nu}(p)\|_2^2)^{-\frac{1}{2}} = -a.
\]

Hence, for any fixed measure \( \tilde{\eta} \), the vector

\[
\hat{v} = -(\mathcal{E}_K(\tilde{\eta})^2 + \|\nabla V_{K, \nu}(p)\|_2^2)^{-\frac{1}{2}} \nabla V_{K, \nu}(p)
\]

minimizes the objective in (58), which then simplifies to

\[
\min_{\tilde{\eta} \in \mathcal{P}_2(\mathbb{R}^d)} - (\mathcal{E}_K(\tilde{\eta})^2 + \|\nabla V_{K, \nu}(p)\|_2^2)^{\frac{1}{2}}
\]

\[
s.t. \int_{\mathbb{R}^d} \|x\|^2 \, d\tilde{\eta}(x) = 1, \int_{\mathbb{R}^d} x \, d\tilde{\eta}(x) = 0.
\]

Due to the non-positiveness \( \mathcal{E}_K \), problem (59) is equivalent to (21) up to the additional condition \( \int_{\mathbb{R}^d} x \, d\tilde{\eta}(x) = 0 \). However, since by Proposition 15 every solution of (21) is orthogonally invariant, the solutions \( \eta^* \) of both problems coincide. Hence, any solution of (55) can be represented as

\[
\hat{\eta} = (\text{Id} - b^* \nabla V_{K, \nu}(p)) \# (b^* \mathcal{E}_K(\eta^*) \text{Id}) \# (b^* (\mathcal{E}_K(\eta^*) \text{Id} - \nabla V_{K, \nu}(p)) \# \eta^*)
\]

and

\[
b^* = (\mathcal{E}_K(\eta^*)^2 + \|\nabla V_{K, \nu}(p)\|_2^2)^{-\frac{1}{2}}.
\]

Since the minimum of (55) is \(-b^* \)^{-1} = \( H_{\delta_p \otimes \eta^*} F_{\nu}(\delta_p) \), we get the assertion.

For \( r \in (1, 2) \), we again apply Theorem 13 to conclude that (55) is equivalent to

\[
\min_{v \in \mathbb{R}^d} \nabla V_{K, \nu}(p)^T v \quad s.t. \quad \|v\|^2_2 \leq 1.
\]

Here the minimizer is given by \( \hat{v} = -\nabla V_{K, \nu}(p)/\|\nabla V_{K, \nu}(p)\|_2 \) such that it holds \( \hat{\eta} = \delta_{-\nabla V_{K, \nu}(p)/\|\nabla V_{K, \nu}(p)\|_2} \), and the minimum is given by \( H_{\delta_p \otimes \hat{\eta}} F_{\nu}(\delta_p) = -\|\nabla V_{K, \nu}(p)\|_2 \), which yields the assertion.

\[\Box\]

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