First-order Conditions for Optimization in the Wasserstein Space

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Abstract

We study first-order optimality conditions for constrained optimization in the Wasserstein space, whereby one seeks to minimize a real-valued function over the space of probability measures endowed with the Wasserstein distance. Our analysis combines recent insights on the geometry and the differential structure of the Wasserstein space with more classical calculus of variations. We show that simple rationales such as “setting the derivative to zero” and “gradients are aligned at optimality” carry over to the Wasserstein space. We deploy our tools to study and solve optimization problems in the setting of distributionally robust optimization and statistical inference. The generality of our methodology allows us to naturally deal with functionals, such as mean-variance, Kullback-Leibler divergence, and Wasserstein distance, which are traditionally difficult to study in a unified framework.

1 Introduction

Many problems in artificial intelligence, machine learning, and optimization under uncertainty can be cast as optimization problems over the space of probability measures of the form

$$\inf_{\mu \in \mathcal{P}(\mathbb{R}^d)} \{ J(\mu) : K(\mu) \leq 0 \},$$

(1)

where $\mathcal{P}(\mathbb{R}^d)$ is the space of Borel probability measures on $\mathbb{R}^d$, and $J : \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$ and $K : \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$ are real-valued functions over the probability space. Examples of interest include:

Example 1.1 (Distributionally robust optimization). In decision-making problems, one seeks a decision $w \in W \subseteq \mathbb{R}^n$ which minimizes the expected cost $\mathbb{E}^\mu[f(w, x)]$ of a function $f : W \times \mathbb{R}^d \to \mathbb{R}$, where the quantity $x$ is random with distribution $\mu \in \mathcal{P}(\mathbb{R}^d)$. Since the probability measure $\mu$ is rarely known in practice, distributionally robust optimization (DRO) aims to minimize the worst-case cost over the ambiguity set $\mathcal{P} \subset \mathcal{P}(\mathbb{R}^d)$:

$$\inf_{w \in W} \sup_{\mu \in \mathcal{P}} \mathbb{E}^\mu[f(w, x)].$$

Ambiguity sets are usually designed to ensure (statistical) performance guarantees and computational tractability; see [1, 2, 3, 4, 5] and references therein. A popular choice of ambiguity sets (also subject to study in this work, see Section 4) are Wasserstein balls, which include all probability measures within a given Wasserstein distance from a prescribed probability measure.

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Example 1.2 (Statistical inference). According to Kullback’s principle of minimum cross-entropy [6, 7, 8], the inference of a probability measure \( \mu \) given a prior estimate \( \bar{\mu} \) over a class of probability measures \( \mathcal{P} \) can be formulated as the minimization of the Kullback-Leibner (KL) divergence:

\[
\inf_{\mu \in \mathcal{P}} \text{KL}(\mu | \bar{\mu}) := \int_{\mathbb{R}^d} \log \left( \frac{\rho(x)}{\bar{\rho}(x)} \right) \bar{\rho}(x) \, dx,
\]

where \( \rho \) and \( \bar{\rho} \) are the densities of \( \mu \) and \( \bar{\mu} \). Here, \( \mathcal{P} \) usually encodes moment constraints, the class of the probability measure, or a ball around a prescribed probability measure. \( \triangle \)

Example 1.3 (Maximum likelihood deconvolution). Consider the problem of estimating an unknown probability measure \( \mu \in \mathcal{P}(\mathbb{R}^d) \) based on corrupted observations \( Y_1, \ldots, Y_n \), where \( Y_i = X_i + Z_i \), \( X_1, \ldots, X_n \) are independent copies of \( X \sim \mu \), and the errors \( Z_1, \ldots, Z_n \) are independent copies of \( Z \sim \bar{\mu} \) (with probability density \( \bar{\rho} \)) and independent of \( X_1, \ldots, X_n \). A natural candidate is the maximum-likelihood estimator

\[
\hat{\mu} := \operatorname{argmax}_{\mu \in \mathcal{P}} \sum_{i=1}^n \log \left( (\bar{\rho} \ast \mu)(Y_i) \right) := \sum_{i=1}^n \log \left( \int_{\mathbb{R}^d} \bar{\rho}(Y_i - x) \, d\mu(x) \right),
\]

(2)

where \( \mathcal{P} \subseteq \mathcal{P}(\mathbb{R}^d) \) is a class of probability measures. It is well known [9] that (2) can be reformulated as the (unconstrained) minimization the entropic optimal transport distance [10, 11, 12] from the empirical probability measure \( \frac{1}{n} \sum_{i=1}^n \delta_{Y_i} \). \( \triangle \)

In general, the optimization problem (1) can be formulated (or relaxed) as an infinite-dimensional optimization problem in the (vector) space of signed measures, whereby non-negativity and normalization are introduced as independent constraints. This augmentation permits to access the rich theory of optimization in Banach spaces; e.g., see [13, 14, 15, 16, 17] and references therein. For instance, when both \( J \) and \( K \) are restricted to be the expected value of some real-valued function, (1) culminates in the so-called problem of moments, a particular instance of conic linear problems in the space of signed measures for which powerful dual reformulations exist [18, 19, 20, 21]. Recent years also witnessed significant efforts in studying (1) in the context of DRO, whereby one seeks to evaluate the worst-case expected value of a real-valued function over an ambiguity set, oftentimes defined via moments, the KL divergence, or the Wasserstein distance [1, 2, 3, 4, 22, 23]. In many cases, DRO problems admit dual reformulations, which sometimes even reduce to a tractable finite-dimensional convex optimization problem. By using the expected value as a local linear approximation of a more general sufficiently well-behaved functional over the probability space, [24] develops a Frank-Wolfe algorithm in probability spaces for the unconstrained version of (1). In most cases, though, dual reformulations only hold when \( J \) is an expected value, and do not readily generalize to arbitrary constraints.

In this work, we adopt a different approach, and study (1) through the lens of optimal transport and its differential properties. The theory of optimal transport, dating back to the seminal works of Monge [25] and Kantorovich [26], provides us with a way to quantify the distance between probability measures, and thus to define a metric space (the so-called Wasserstein space) of probability measures [27, 28, 29]. Notably, this is sufficient to endow the probability space with a differential structure. This enlightening theory, pioneered by [30] and later formalized by [27], culminates in the rigorous formulation of gradient flows in probability spaces; see [31] for an introduction. While this theory has been widely used to study partial differential equations [32, 33, 34, 35], applications of Wasserstein gradient flows for optimization purposes remain largely unexplored.
Among the few approaches in this direction, [36] relies on Wasserstein gradients to devise computational methods to compute the “average” (so-called Wasserstein barycenter) of a collection of probability measures, implicitly defined as an unconstrained optimization problem over the probability space [37, 38]. Other applications in machine learning include the analysis of (over-parametrized) neural network [39, 40], approximate inference [41], variational inference [42], back-propagation of gradients through discrete random variables [43], and policy optimization in reinforcement learning [44]. In [45], Wasserstein gradient flows are used to design algorithms for the unconstrained version of (1).

The closest approach to ours is [46, 47, 48], which studies necessary conditions “à la Pontryagin” for optimality of control problems in the Wasserstein space. While our setting is different, we share some of the fundamentals of this work. The study of (1) in the probability space, and not in the space of signed measures, allows us to formulate simple, intuitive, and interpretable necessary and sufficient conditions for optimality, which oftentimes formally resemble their Euclidean counterparts (e.g., “set the gradient to zero”). In particular, we do not need to repeatedly deal with normalization and non-negativity of the signed measures.

Contributions More specifically, our contributions are as follows.

(i) We provide a concise and self-contained review of the Wasserstein space, its geometry, and its differential structure. Our review bases on both existing results as well as on various novel extensions, and it is geared towards solving (1). We do not content ourselves with enunciating the theoretic results, but present many examples of functionals over the Wasserstein space, and characterize their properties such as continuity and differentiability.

(ii) We derive novel necessary and sufficient KKT-type conditions for optimality of (1) in the case of equality constraints and specific inequality constraints. Our analysis combines recent advances in the geometry and the differential structure of the Wasserstein space with classical methods from calculus of variations.

(iii) We show that our methodology can be used to solve various problems (including unsolved ones) in DRO and statistical inference with the KL divergence, sometimes even in closed form. While not representing the core of this work, the study of these specific problems is of independent interest.

Organization This paper unfolds as follows. In Section 2, we recall and extend preliminaries in optimal transport and the Wasserstein space. In Section 3, we study necessary and sufficient conditions for optimality of (1). In Sections 4 and 5, we deploy our methodology to solve various optimization problems in the context of DRO and statistical inference with the KL divergence. Finally, Section 6 draws the conclusions of this paper.

Notation We will use several classes of real-valued continuous functions \( f : \mathbb{R}^d \to \mathbb{R} \), whereby \( \mathbb{R}^d \) is endowed with the Euclidean inner product \( \langle \cdot, \cdot \rangle \) and induced norm \( \| \cdot \| \). We denote by \( C^0(\mathbb{R}^d) \) the space of \( p \)-time continuously differentiable functions, by \( C_b(\mathbb{R}^d) \) the space of bounded continuous functions, by \( C^\infty_c(\mathbb{R}^d) \) the space of smooth (i.e., infinitely differentiable) functions with compact support, and by \( W^{1,1}_{\text{loc}}(\mathbb{R}^d; \mu) \) the (Sobolev) space of locally \( \mu \)-integrable functions whose gradient is locally \( \mu \)-integrable. A function \( f : \mathbb{R}^d \to \mathbb{R} \) is \( \alpha \)-convex (with \( \alpha \in \mathbb{R} \), possibly negative) if \( f - \alpha \| x \|^2 \) is convex. We denote
the gradient of \( f : \mathbb{R}^d \to \mathbb{R} \) by \( \nabla f \) and its Hessian by \( \nabla^2 f \). Similarly, we denote the Jacobian of \( g : \mathbb{R}^d \to \mathbb{R}^d \) at \( x \in \mathbb{R}^d \) by \( \nabla g \). We use the notation \( L^2(\mathbb{R}^d; \mu) \) to denote the space of real-valued \( \mu \)-measurable functions with bounded 2-norm (where integration is w.r.t. \( \mu \)) and the notation \( L^2(\mathbb{R}^d, \mathbb{R}^d; \mu) \) for functions \( f : \mathbb{R}^d \to \mathbb{R}^d \). We denote the identity function on \( \mathbb{R}^d \) by \( \text{Id} \) and canonical projections by \( \text{proj} \) (e.g., \( \text{proj}_1 : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d, (x, y) \mapsto x \)). We say \( f(x) = o(g(x)) \) for non-negative \( f \) and positive \( g \) if \( \lim_{x \to 0} \frac{f(x)}{g(x)} = 0 \); in particular, \( \lim_{x \to 0} \frac{\alpha(x)}{x} = 0 \). Finally, for a real number \( \alpha \in \mathbb{R} \), we define the negative part via \( \alpha^- := |\min\{\alpha, 0\}| \geq 0 \).

## 2 Optimal Transport and the Wasserstein Space

In this section, we review and extend various preliminaries in optimal transport and the Wasserstein space, including some background (Section 2.1), interpolation and geodesic convexity (Section 2.2), differential calculus (Section 2.3), and examples of smooth functionals (Section 2.4). The proofs of most of the statements of this section are deferred to Appendix B.

### 2.1 Background in Measure Theory, Optimal Transport, and Wasserstein Space

We start with basics in measure theory and optimal transport. We refer the reader to [27, 28, 29, 49] for a comprehensive review. We denote by \( \mathcal{P}(\mathbb{R}^d) \) the set of Borel probability measures on \( \mathbb{R}^d \), and by

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

the set of probability measures with finite second moment. We use the notation \( \mu \ll \nu \) to indicate that \( \mu \) is absolutely continuous with respect to \( \nu \). In particular, we denote by \( \mathcal{P}_2,\text{abs}(\mathbb{R}^d) \subset \mathcal{P}_2(\mathbb{R}^d) \) the space of absolutely continuous probability measures (with respect to the Lebesgue measure on \( \mathbb{R}^d \), denoted by \( \mathcal{L}^d \)). The pushforward of a measure \( \mu \in \mathcal{P}(\mathbb{R}^d) \) through a Borel map \( T : \mathbb{R}^d \to \mathbb{R}^d \), denoted by \( T_{\#}\mu \), is defined by \( (T_{\#}\mu)(A) := \mu(T^{-1}(A)) \) for all Borel sets \( A \subseteq \mathbb{R}^d \). We recall that for any \( f : \mathbb{R}^d \to \mathbb{R} \) \( T_{\#}\mu \)-integrable (or non-negative measurable/Borel bounded)

\[
\int_{\mathbb{R}^d} f(x) \, d(T_{\#}\mu)(x) = \int_{\mathbb{R}^d} f(T(x)) \, d\mu(x).
\]

Following [29], we define two notions of convergence in \( \mathcal{P}_2(\mathbb{R}^d) \):

- **narrow convergence**: \( (\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d) \) converges narrowly to \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) if

\[
\int_{\mathbb{R}^d} \phi(x) \, d\mu_n(x) \to \int_{\mathbb{R}^d} \phi(x) \, d\mu(x) \quad \forall \phi \in C_b(\mathbb{R}^d).
\]

- **weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \)**: \( (\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d) \) converges weakly in \( \mathcal{P}_2(\mathbb{R}^d) \) to \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \), denoted by \( \mu_n \rightharpoonup \mu \), if

\[
\int_{\mathbb{R}^d} \phi(x) \, d\mu_n(x) \to \int_{\mathbb{R}^d} \phi(x) \, d\mu(x) \quad \forall \phi \in C_b(\mathbb{R}^d) \quad \text{and} \quad \int_{\mathbb{R}^d} x^2 \, d\mu_n(x) \to \int_{\mathbb{R}^d} x^2 \, d\mu(x).
\]

Equivalently [29, Definition 6.8], \( \mu_n \rightharpoonup \mu \) if for all continuous functions \( \phi \in C^0(\mathbb{R}^d) \) with \( |\phi(x)| \leq C(1 + ||x||^2) \) for \( C \in \mathbb{R} \) we have

\[
\int_{\mathbb{R}^d} \phi(x) \, d\mu_n(x) \to \int_{\mathbb{R}^d} \phi(x) \, d\mu(x).
\]
Of course, weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$ implies narrow convergence. The converse, though, is not true, as $x \mapsto x^2 \notin C_b(\mathbb{R}^d)$.

**Example 2.1** (Narrow convergence $\not\Rightarrow$ weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$). Let $(\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}_2(\mathbb{R})$ be defined by $\mu_n := (1 - \frac{1}{n^2}) \delta_0 + \frac{1}{n^2} \delta_n$. Then, $\mu_n$ converges narrowly to $\delta_0$: for any $\phi \in C_b(\mathbb{R})$

$$
\int_{\mathbb{R}} \phi(x) d\mu_n(x) = \left(1 - \frac{1}{n^2}\right) \phi(0) + \frac{1}{n^2} \phi(n) \to \phi(0) = \int_{\mathbb{R}} \phi(x) d\delta_0(x),
$$

where we used that $\phi$ is bounded. However, $\mu_n \not\Rightarrow \delta_0$ as

$$
\int_{\mathbb{R}} x^2 d\mu_n(x) = \frac{1}{n^2} n^2 = 1 \nrightarrow 0 = \int_{\mathbb{R}} x^2 d\delta_0.
$$

△

Given $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ we say that $\gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d)$ is a plan (or coupling) between $\mu$ and $\nu$ if $(\text{proj}_1)\# \gamma = \mu$ and $(\text{proj}_2)\# \gamma = \nu$, where $\text{proj}_1, \text{proj}_2 : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ are the canonical projections; equivalently for all $\phi, \psi : \mathbb{R}^d \to \mathbb{R}$ integrable

$$
\int_{\mathbb{R}^d \times \mathbb{R}^d} \phi(x) d\gamma(x, y) = \int_{\mathbb{R}^d} \phi(x) d\mu(x) \quad \text{and} \quad \int_{\mathbb{R}^d \times \mathbb{R}^d} \psi(y) d\gamma(x, y) = \int_{\mathbb{R}^d} \psi(y) d\nu(y).
$$

We denote by $\Gamma(\mu, \nu) \subset \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ the set of couplings of $\mu$ and $\nu$. Since the product measure $\mu \times \nu$ has marginals $\mu$ and $\nu$, respectively, $\Gamma(\mu, \nu)$ is non-empty. We are now ready to define the Wasserstein distance:

**Definition 2.1** (Wasserstein distance [27, 28, 29, 49]). Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$. We define the (type 2) Wasserstein distance between $\mu$ and $\nu$ as

$$
W_2(\mu, \nu) := \left( \min_{\gamma \in \Gamma(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 d\gamma(x, y) \right)^{\frac{1}{2}}.
$$

(3)

We denote by $\Gamma_o(\mu, \nu)$ the set of couplings attaining the minimum in (3), and we call any $\gamma \in \Gamma_o(\mu, \nu)$ optimal transport plan between $\mu$ and $\nu$.

A compactness and lower semi-continuity argument (with respect to the topology induced by narrow convergence) shows that $\Gamma_o(\mu, \nu)$ is non-empty: The minimum in (3) is attained by some optimal transport plan $\gamma$ [29, Chapter 4]. If $\gamma \in \Gamma_o(\mu, \nu)$ is of the form $(\text{Id}, T^\nu_\mu)\# \mu$ for some measurable $T^\nu_\mu : \mathbb{R}^d \to \mathbb{R}^d$, we say that $\gamma$ is induced by an optimal transport map which pushes $\mu$ into $\nu$; i.e., $\nu = (T^\nu_\mu)\# \mu$, $T^\nu_\mu$ yields the minimum transportation cost, and $T^\nu_\mu$ is an optimal transport map between $\mu$ and $\nu$. The celebrated Brenier’s theorem sheds light on existence of optimal transport maps:

**Theorem 2.1** (Brenier’s theorem [27, 28, 29, 49]). Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, and assume that $\mu$ is absolutely continuous w.r.t. the Lebesgue measure. Then, there exists a unique optimal transport plan $\gamma$, induced by a unique optimal transport map $T^\nu_\mu$, and $T^\nu_\mu = \nabla \phi \mu$-a.e for some convex function $\phi : \mathbb{R}^d \to \mathbb{R}$.

Theorem 2.1 suggests that, whenever $\mu \ll \mathcal{L}^d$, it is safe to define the optimal transport map (inducing the optimal transport plan) between $\mu$ and $\nu$. Its inverse, if it exists, reveals the optimal transport map in “reverse direction”:

**Proposition 2.2** (Inverse of optimal transport maps). Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$. Assume an optimal transport map $T^\nu_\mu$ exists, and it is invertible $\mu$-almost everywhere. Then, $T^\nu_\mu$ exists, and it equals $(T^\nu_\mu)^{-1} \nu$-a.e.
Remark 2.1. Proposition 2.2 does not provide conditions for \((\mu\text{-a.e.})\) invertibility of \(T_\mu^\nu\), but it assumes it. A sufficient condition for \(\mu\text{-a.e.}\) invertibility is the absolutely continuity of \(\nu\). Then, by Brenier’s theorem (Theorem 2.1), \(T_\mu^\nu\) exists and \(T_\mu^\nu = (T_\mu^\nu)^{-1}\) \(\nu\text{-a.e.}\)

There is one final important setting where optimal transport maps exist:

**Proposition 2.3** (Pushforward via convex functions [28, Theorem 1.48]). Let \(\mu \in \mathcal{P}(\mathbb{R}^d)\) and \(T = \nabla \phi\) for some \(\phi : \mathbb{R}^d \to \mathbb{R}\) convex and differentiable \(\mu\text{-almost everywhere.}\) If \(\|T\|_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)} < +\infty\), then an optimal transport plan between \(\mu\) and \(T\#\mu \in \mathcal{P}(\mathbb{R}^d)\) is given by the optimal transport map \(T\).

Proposition 2.3 is non-obvious: There might exist another transport map \(\tilde{T}\) (or a transport plan) yielding a lower transport cost between \(\mu\) and \(T\#\mu\). We now exploit Proposition 2.3 to define a perturbation of measures, which will be a crucial building block for our variational analysis.

**Lemma 2.4** (Perturbation of probability measures). Let \(\mu \in \mathcal{P}_2(\mathbb{R}^d)\) and \(\psi \in C^\infty_0(\mathbb{R}^d)\). Then, there exists \(\bar{s} > 0\) such that \(\text{Id} + s\nabla \psi\) is an optimal transport map from \(\mu\) to \((\text{Id} + s\nabla \psi)\#\mu\) for all \(s \in (-\bar{s}, +\bar{s})\), i.e.,

\[
T_{\mu}^{(\text{Id} + s\nabla \psi)\#\mu} = \text{Id} + s\nabla \psi.
\]

Further, \((\text{Id} + s\nabla \psi)\#\mu \in \mathcal{P}_2(\mathbb{R}^d)\), and the Wasserstein distance between \(\mu\) and \((\text{Id} + s\nabla \psi)\#\mu\) is

\[
W_2(\mu, (\text{Id} + s\nabla \psi)\#\mu) = |s| \|\nabla \psi\|_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)}.
\]

**Proof.** By Proposition 2.3, it suffices to establish that \(\text{Id} + s\nabla \psi\) is the gradient of a convex function. Indeed, \(\text{Id} + s\nabla \psi\) is smooth, and so differentiable \(\mu\text{-a.e.}\), and

\[
\int_{\mathbb{R}^d} \|x + s\nabla \psi(x)\|^2 d\mu(x) \leq \int_{\mathbb{R}^d} (\|x\| + |s|\|\nabla \psi(x)\|)^2 d\mu(x)
\]

\[
\leq 2 \int_{\mathbb{R}^d} \|x\|^2 + |s|^2\|\nabla \psi(x)\|^2 d\mu(x)
\]

\[
\leq 2 \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + |s|^2 \max_{x \in \mathbb{R}^d} \|\nabla \psi(x)\|^2 < +\infty,
\]

where the maximum of \(\|\nabla \psi(x)\|^2\) exists and is bounded by (i) continuity of the gradient and the norm and (ii) due to compactness of the support of \(\psi\). So, by Proposition 2.3, if \(\text{Id} + s\nabla \psi\) is the gradient of a convex function, then it is an optimal transport map between \(\mu\) and \((\text{Id} + s\nabla \psi)\#\mu\). To prove convexity, by smoothness, it suffices to show that \(I + s\nabla^2 \psi(x)\) is positive definite for all \(x \in \mathbb{R}^d\). Without loss of generality, assume \(\nabla^2 \psi(x)\) is non-zero at least for some \(x \in \mathbb{R}^d\); else, the statement is trivial. Let \(\bar{s} := 1/\max_{x \in \mathbb{R}^d} \|\nabla^2 \psi(x)\| > 0\), where the maximum exists by compactness of the support of \(\psi\) and continuity of the norm. Then, \(I + s\nabla^2 \psi(x)\) is positive definite for all \(s \in (-\bar{s}, \bar{s})\), which implies \(\text{Id} + s\nabla \psi\) is the gradient of a convex function, and thus the statement follows. Finally, (4) shows that \((\text{Id} + s\nabla \psi)\#\mu \in \mathcal{P}_2(\mathbb{R}^d)\) and, by definition of Wasserstein distance and optimal transport map,

\[
W_2(\mu, (\text{Id} + s\nabla \psi)\#\mu) = \left(\int_{\mathbb{R}^d} \|x - (x - s\nabla \psi)\|^2 d\mu(x)\right)^{\frac{1}{2}} = |s|\|\nabla \psi\|_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)}.
\]

This concludes the proof. □
Finally, it is well known that the Wasserstein distance $W_2(\cdot, \cdot)$ defines a distance on $\mathcal{P}_2(\mathbb{R}^d)$ (but not on $\mathcal{P}(\mathbb{R}^d)$), so that $(\mathcal{P}_2(\mathbb{R}^d), W_2(\cdot, \cdot))$ is a metric space, often called the Wasserstein space [27, 28, 29]. We also recall that the Wasserstein distance metrizes weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$ [29, Theorem 6.9]; i.e., for $(\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d)$ and $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ we have $\lim_{n \to \infty} W_2(\mu_n, \mu) = 0$ if and only if $\mu_n \rightharpoonup \mu$.

**Example 2.2** (Example 2.1 revisited). In Example 2.1, $W_2(\mu_n, \delta_0) = 1$ for all $n$, so $W_2(\mu_n, \delta_0) \not\to 0$, and thus $\mu_n$ cannot converge weakly in $\mathcal{P}_2(\mathbb{R}^d)$ to $\delta_0$.

### 2.2 Interpolation and Geodesic Convexity

The theory of optimal transport naturally provides us with a notion of interpolation in the Wasserstein space: Let $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$ and $\gamma \in \Gamma_o(\mu_0, \mu_1)$, and consider the curve

$$
\mu_t := ((1 - t) \text{proj}_1 + t \text{proj}_2) \# \gamma.
$$

(5)

Then, $\mu_t$ interpolates between $\mu_0$ ($t = 0$) and $\mu_1$ ($t = 1$). Since multiple optimal transport plans might exist, the interpolation $\mu_t$ between $\mu_0$ and $\mu_1$ is generally not unique. Curves of the form (5) can be shown to be constant speed geodesics in $\mathcal{P}_2(\mathbb{R}^d)$ (i.e., $W_2(\mu_s, \mu_t) = (t - s)W_2(\mu_0, \mu_1)$ for all $0 \leq s \leq t \leq 1$), and all constant speed geodesics can be written as (5) [27, Theorem 7.2.2]. Accordingly, a functional $J : \mathcal{P}_2(\mathbb{R}^d) \to (\mathbb{R}, \infty]$ is $\alpha$-geodesically convex (with $\alpha \in \mathbb{R}$) if for all $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$ and all $t \in [0, 1]$ there exists $\mu_t$ as in (5) such that

$$
J(\mu_t) \leq (1 - t)J(\mu_0) + tJ(\mu_1) - \frac{\alpha}{2} t(1 - t)W_2(\mu_0, \mu_1)^2.
$$

(6)

We will sometimes need a stronger notion of geodesic convexity: geodesic convexity along generalized geodesics. A generalized geodesic joining $\mu_0$ and $\mu_1$ with base $\bar{\mu}$ is a curve

$$
\mu_t := ((1 - t) \text{proj}_2 + t \text{proj}_3) \# \gamma,
$$

(7)

where $\gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)$ is a coupling of $\bar{\mu}$, $\mu_0$, and $\mu_1$ which is optimal between $\bar{\mu}$ and $\mu_0$ (i.e., $(\text{proj}_{1,2}) \# \gamma \in \Gamma_o(\bar{\mu}, \mu_0)$) and between $\bar{\mu}$ and $\mu_1$ (i.e., $(\text{proj}_{1,3}) \# \gamma \in \Gamma_o(\bar{\mu}, \mu_2)$), but not necessarily optimal between $\mu_0$ and $\mu_1$. With the choice $\bar{\mu} = \mu_0$, we recover the geodesics (5). Accordingly, $J$ is $\alpha$-convex along generalized geodesics if for all $\bar{\mu}, \mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$ there exists $\mu_t$ as in (7) such that

$$
J(\mu_t) \leq (1 - t)J(\mu_0) + tJ(\mu_1) - \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} ||y - z||^2 d\gamma(x, y, z).
$$

Convexity along generalized geodesics is stronger than geodesic convexity. In particular, if $J$ is $\alpha$-convex along generalized geodesics, then it suffices to pick $\bar{\mu} = \mu_0$ to prove that $J$ is $\alpha$-geodesically convex. Finally, if $\alpha = 0$ we simply say that $J$ is geodesically convex (along generalized geodesics). Finally, if (6) holds for any $\gamma \in \Gamma(\mu, \nu)$ (not necessarily optimal) in (5), then $J$ is $\alpha$-convex along any interpolating curve. Clearly, this implies both geodesic convexity and convexity along generalized geodesics.

### 2.3 Differential Calculus in the Wasserstein Space

In this section, we equip, perhaps surprisingly, the Wasserstein space with a “differential structure”. Critically, $(\mathcal{P}_2(\mathbb{R}^d), W_2(\cdot, \cdot))$ does not enjoy a linear structure, so classical notions of differentials (e.g., Fréchet) do not apply. Henceforth, we will consider lower semi-continuous (w.r.t. to weak convergence
in $\mathcal{P}_2(\mathbb{R}^d)$) functionals of the form $J : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$. To ease the notation, we define the effective domain of $J$ as

$$D(J) := \{ \mu \in \mathcal{P}_2(\mathbb{R}^d) : J(\mu) < +\infty \}$$

and tacitly assume that $J$ is proper (i.e., $D(J) \neq \emptyset$). Inspired from classical definitions of sub- and super-differentiability in Euclidean settings, sub- and super-differentials are defined as follows:

**Definition 2.2** (Wasserstein sub- and super-differential [47]). Let $\mu \in D(J)$. We say that a map $\xi \in L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)$ belongs to the subdifferential $\partial^- J(\mu)$ of $J$ at $\mu$ if

$$J(\nu) - J(\mu) \geq \sup_{\gamma \in \Gamma_{\nu}(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x), y - x \rangle \, d\gamma(x, y) + o(W_2(\mu, \nu))$$

for all $\nu \in \mathcal{P}_2(\mathbb{R}^d)$. Similarly, $\xi \in L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)$ belongs to the superdifferential $\partial^+ J(\mu)$ of $J$ at $\mu$ if $(-\xi) \in \partial^- (-J)(\mu)$.

By Definition 2.2, sub- and super-differential are functions in $L^2$. Intuitively, $\xi(x)$, with $\xi \in \partial^- J(\mu)$, is the “(sub)gradient” experienced by the particles of $\mu$ located at $x \in \mathbb{R}^d$. It is now easy to define differentiability:

**Definition 2.3** (Differentiable functions [47]). A functional $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ is Wasserstein differentiable at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ if the intersection of sub- and superdifferential is non-empty; i.e., if $\partial^- J(\mu) \cap \partial^+ J(\mu) \neq \emptyset$. In this case, we say $\nabla \mu J(\mu) \in \partial^- J(\mu) \cap \partial^+ J(\mu)$ is a Wasserstein gradient of $J$ at $\mu$, satisfying

$$J(\nu) - J(\mu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \, d\gamma(x, y) + o(W_2(\mu, \nu))$$

for any $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ and any $\gamma \in \Gamma_{\alpha}(\mu, \nu)$.

Definition 2.3 states that Wasserstein gradients are general functions in $L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)$. As we shall see below, we can impose additional structure, and dictate that gradients belong the “Wasserstein tangent space”, which we define as follows.

**Definition 2.4** (Tangent space [27]). The tangent space at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ is the vector space

$$\text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) := \left\{ \nabla \psi : \psi \in \mathcal{C}^\infty_c(\mathbb{R}^d) \right\} \cap L^2(\mathbb{R}^d, \mathbb{R}^d; \mu),$$

where the closure is taken with respect to the $L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)$ topology.

**Remark 2.2.** Few remarks on Definitions 2.2–2.4 are in order. First, Definition 2.4 encapsulates the geometry of $(\mathcal{P}_2(\mathbb{R}^d), W_2(\cdot, \cdot))$: Gradients of functions $\psi \in \mathcal{C}^\infty_c(\mathbb{R}^d)$ generate optimal transport maps by perturbation of the identity via $(\text{Id} + \varepsilon \nabla \psi)\# \mu$ for $\varepsilon$ sufficiently small; see Lemma 2.4 above. Thus, they can be thought as tangent vectors to $(\mathcal{P}_2(\mathbb{R}^d), W_2(\cdot, \cdot))$. Second, an equivalent (more related to optimal transport) definition of tangent space is

$$\text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) = \left\{ \lambda (r - \text{Id}) : (\text{Id}, r)_{\#} \mu \in \Gamma_{\alpha}(\mu, r_{\#} \mu), \lambda > 0 \right\} \cap L^2(\mathbb{R}^d, \mathbb{R}^d; \mu).$$

We refer to [27, Theorem 8.5.1] for more details. Third, an alternative definitions of sub- and super-differentiability involves taking the *infimum* instead of the *supremum* in (8) [27, Definition 10.3.1]; yet, this definition is equivalent [50]. Fourth, it is straightforward to show linearity; i.e., for $\alpha, \beta \in \mathbb{R}$, $\nabla \mu (\alpha J_1 + \beta J_2)(\mu) = \alpha \nabla \mu J_1(\mu) + \beta \nabla \mu J_2(\mu)$, whenever $J_1$ and $J_2$ are Wasserstein differentiable at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. Fifth, we defined (sub)gradients for functions whose domain is $\mathcal{P}_2(\mathbb{R}^d)$. Yet, our definitions readily extends to any function whose domain is an open subset of $\mathcal{P}_2(\mathbb{R}^d)$ (e.g., $\mathcal{P}_{2, \text{abs}}(\mathbb{R}^d)$). $\triangle$
Definition 2.3 does not establish uniqueness of Wasserstein gradients. Indeed, the set \( \partial^- J(\mu) \cap \partial^+ J(\mu) \) generally contains multiple elements. Nonetheless, Wasserstein gradients are, if they exist, unique in \( L^2(\mathbb{R}^d, \mathbb{R}^d; \mu) \) modulo the equivalence relation induced by \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d)^+ \). That is, Wasserstein gradients are unique in \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \). In particular, since \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \) is a closed linear subspace of the Hilbert space \( L^2(\mathbb{R}^d, \mathbb{R}^d; \mu) \), the Hilbert decomposition theorem [51, Theorem 4.11] asserts that any element \( \xi \in L^2(\mathbb{R}^d, \mathbb{R}^d; \mu) \) can be uniquely decomposed as \( \xi = \xi^\parallel + \xi^\perp \), with \( \xi^\parallel \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \) and \( \xi^\perp \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d)^\perp \). The next proposition shows that

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi^\perp(x), y - x \rangle \, d\gamma(x, y) = 0
\]

for any \( \gamma \in \Gamma_o(\mu, \nu) \) and any \( \nu \in \mathcal{P}_2(\mathbb{R}^d) \), and thus

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x), y - x \rangle \, d\gamma(x, y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi^\parallel(x), y - x \rangle \, d\gamma(x, y).
\]

This, together with Definitions 2.2 and 2.3, suggests that we can always impose that Wasserstein sub- and super-differential belong to the tangent space \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \), and thus Wasserstein gradients, whenever they exist, are unique and also belong to \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \). Formally:

**Proposition 2.5** (Wasserstein gradients only act on tangent vectors). Let \( \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d) \), \( \gamma \in \Gamma_o(\mu, \nu) \), and \( \xi \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d)^\perp \). Then,

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x), y - x \rangle \, d\gamma(x, y) = 0.
\]  

In particular, we can without loss of generality impose that sub- and super-differential live in \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \). This way, also the Wasserstein gradient of \( J \) at \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) is, if it exists, the unique element \( \nabla_\mu J(\mu) \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \cap \partial^- J(\mu) \cap \partial^+ J(\mu) \).

Henceforth, we will therefore regard the Wasserstein gradient of \( J \) at \( \mu \), if it exists, as the unique element \( \nabla_\mu J(\mu) \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \cap \partial^- J(\mu) \cap \partial^+ J(\mu) \). While apparently of minor importance, imposing that Wasserstein gradients live in the tangent space \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \) (instead of in the more general \( L^2 \) space) will play a crucial role in later sections.

Next, we show that Wasserstein gradients provide a “linear approximation” even if perturbations are not induced by optimal transport plans. A similar, but less general, result for perturbations induced by transport maps is in [52, Proposition 4.2].

**Proposition 2.6** (Differentials are “strong”). Let \( \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d) \), \( \gamma \in \Gamma(\mu, \nu) \) (not necessarily optimal), and let \( J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R} \) be Wasserstein differentiable at \( \mu \) with Wasserstein gradient \( \nabla_\mu J(\mu) \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \). Then,

\[
J(\nu) - J(\mu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_\mu J(\mu)(x), y - x \rangle \, d\gamma(x, y) + o \left( \sqrt{\int_{\mathbb{R}^d \times \mathbb{R}^d} \| x - y \|^2 \, d\gamma(x, y)} \right).
\]

We now adapt three well-known facts on differentiable functions to the Wasserstein space. First, differentiability implies continuity (in the topology induced by the Wasserstein distance):

**Proposition 2.7** (Differentiability implies continuity). Let \( J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R} \) be Wasserstein differentiable at \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \). Then, \( J \) is continuous w.r.t. weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \) at \( \mu \).
As in the Euclidean case, we can further characterize Wasserstein gradients of geodesically convex functions (cf. [27, Theorem 10.3.6]):

**Proposition 2.8 (Gradients of geodesically convex functions).** Let $J$ be $\alpha$-geodesically convex with $\alpha \in \mathbb{R}$ and suppose that $J$ is Wasserstein differentiable at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. Then, for all $\nu \in \mathcal{P}_2(\mathbb{R}^d)$

$$J(\nu) - J(\mu) \geq \sup_{\gamma \in \Gamma_o(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_{\mu} J(\mu)(x), y - x \rangle \, d\gamma(x,y) + \frac{\alpha}{2} W_2(\mu,\nu)^2. \quad (10)$$

Moreover, Wasserstein gradients are “monotone”: If $J$ is differentiable at $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, then

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_{\mu} J(\nu)(y) - \nabla_{\mu} J(\mu)(x), y - x \rangle \, d\gamma(x,y) \geq \alpha W_2(\mu,\nu)^2 \quad (11)$$

for all $\gamma \in \Gamma_o(\mu,\nu)$.

Finally, we can prove the chain rule:

**Proposition 2.9 (Chain rule).** Let $g : \mathbb{R} \to \mathbb{R}$ be differentiable, $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be Wasserstein differentiable, and let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. Then, $g \circ J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ is Wasserstein differentiable at $\mu$, and

$$\nabla_{\mu} (g \circ J)(\mu) = g'(J(\mu)) \nabla_{\mu} J(\mu).$$

### 2.4 Examples of Smooth Functionals

After endowing the Wasserstein space with a differential structure, we study the topological and differential properties of five classes of important functionals:

- optimal transport discrepancies from a reference measure $\bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d)$:
  $$\mu \mapsto W_c(\mu,\bar{\mu}) := \min_{\gamma \in \Gamma(\mu,\bar{\mu})} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x,y) \, d\gamma(x,y),$$
  for some continuously differentiable transport cost $c : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \geq 0$, which also include the (squared) Wasserstein distance.

- expected value-type functionals:
  $$\mu \mapsto \mathbb{E}^{\mu} [V(x)] := \int_{\mathbb{R}^d} V(x) \, d\mu(x)$$
  for some twice continuously differentiable $V : \mathbb{R}^d \to \mathbb{R}$;

- interaction-type functionals:
  $$\mu \mapsto \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y) \, d(\mu \times \mu)(x,y),$$
  where $\mu \times \mu$ denotes the product measure, for some continuously differentiable $U : \mathbb{R}^d \to \mathbb{R} \geq 0$, related, among others, to the variance (see Corollary 2.14 below);

- internal-energy-type functionals:
  $$\mu \mapsto \begin{cases} \int_{\mathbb{R}^d} F(\rho(x)) \, dx & \text{if } \mu = \rho \mathcal{L}^d \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d), \\ +\infty & \text{else} \end{cases}$$
  for some continuously differentiable $F : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$, related, among others, to the entropy;
the divergences relative to a reference measure \( \bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d) \):

\[
\mu \mapsto \begin{cases} 
\int_{\mathbb{R}^d} F \left( \frac{d\mu}{d\bar{\mu}} \right) \, d\bar{\mu}(x) & \text{if } \mu \ll \bar{\mu}, \\
+\infty & \text{else},
\end{cases}
\]

where \( \frac{d\mu}{d\bar{\mu}} \) is the Radon-Nykodin derivative [51]; an example is the KL divergence.

We start with optimal transport discrepancies:

**Proposition 2.10 (Optimal transport discrepancy).** Let \( \bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d) \), \( c : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_{\geq 0} \), and consider the functional

\[
J(\mu) = W_c(\mu, \bar{\mu}) := \min_{\gamma \in \Gamma(\mu, \bar{\mu})} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) \, d\gamma(x, y).
\]

Assume that there exists \( C > 0 \) so that \( c(y, y) \leq C \) for all \( y \in \text{supp}(\bar{\mu}) \), \( c \) is twice continuously differentiable in the first argument, and there exists \( M > 0 \) so that \( \|\nabla_x^2 c(x, y)\| \leq M \) for all \( x \in \mathbb{R}^d, y \in \text{supp}(\bar{\mu}) \), and \( \|\nabla_x c(x, y)\|^2 \leq M(1 + \|x\|^2 + \|y\|^2) \). Then,

(i) \( J \) is proper and \( J(\mu) \geq 0 \) for all \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \);

(ii) \( J \) is lower semi-continuous w.r.t. weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \);

(iii) \( J \) is lower semi-continuous w.r.t. narrow convergence;

(iv) if \( -c(\cdot, y) \) is \( \alpha \)-convex (with \( \alpha \in \mathbb{R} \)) for all \( y \in \text{supp}(\bar{\mu}) \), then \( -J \) is \( \alpha \)-convex along any interpolating curve;

(v) if \( c \) is \( \alpha \)-convex, then \( J \) is \( \alpha \)-convex along the curve

\[
\mu_t = ((1 - t) \text{proj}_2 + t \text{proj}_3)\#\gamma;
\]

where \( \gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d) \), \( (\text{proj}_{12})\#\gamma \in \Gamma(\alpha, \mu, \bar{\mu}) \) and \( (\text{proj}_{13})\#\gamma \in \Gamma(\alpha, \nu, \bar{\mu}) \) (where optimality is intended w.r.t. the transport cost \( c \)), and \( \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d) \);

(vi) if \( \mu \in D(J) \) and \( \Gamma_\alpha(\mu, \bar{\mu}) \) contains a unique optimal transport plan induced an optimal transport map \( T_\mu^\bar{\mu} \in L^2(\mathbb{R}^d; \mu) \) (w.r.t. the cost \( c \)), \( J \) is Wasserstein differentiable at \( \mu \), and its Wasserstein gradient is

\[
\nabla_\mu J(\mu) = \nabla_x c(\cdot, T_\mu^\bar{\mu}(\cdot)).
\]

**Remark 2.3.** Two remarks are in order. First, Statement (iv) does not imply that \( J \) is convex along any interpolating curve, but only along the interpolating curves whose “base” is precisely \( \bar{\mu} \). Second, if \( c(x, y) = (x - y)^\top A(x - y) \) with \( A = A^\top \in \mathbb{R}^{d \times d} \) positive definite or \( c(x, y) = \ell(\|x - y\|) \) for \( \ell : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0} \) strictly convex which grows faster than linearly, then \( \mu \) being absolutely continuous is a sufficient condition for existence of a unique optimal transport plan induced by an optimal transport map; see [29, 53, 54] for details and generalizations.

As a corollary, we study the differentiability properties of the squared Wasserstein distance (cf. [27, Chapter 7.3] for similar results):

**Corollary 2.11 (Squared Wasserstein distance).** Let \( \bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d) \) and consider the functional

\[
J(\mu) = \frac{1}{2} W_2^2(\mu, \bar{\mu})^2.
\]

Then,
(i) $D(J) = \mathcal{P}_2(\mathbb{R}^d)$, $J$ is proper, and $J(\mu) \geq 0$ for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$;

(ii) $\mu \mapsto W_2(\mu, \bar{\mu})$ and $J$ are continuous w.r.t. weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$;

(iii) $\mu \mapsto W_2(\mu, \bar{\mu})$ and $J$ are lower semi-continuous w.r.t. to narrow convergence;

(iv) $-J$ is $(-1)$-convex and thus $J$ is $(-1)$-concave) along any interpolating curve;

(v) $J$ is $1$-convex along the curve

$$\mu_t = ((1-t) \text{proj}_2 + t \text{proj}_{3}) \gamma,$$

where $\gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)$, $(\text{proj}_{12}) \gamma \in \Gamma_o(\bar{\mu}, \mu)$ and $(\text{proj}_{13}) \gamma \in \Gamma_o(\bar{\mu}, \nu)$, and $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$;

(vi) if $\mu \in \mathcal{P}_2_{\text{abs}}(\mathbb{R}^d)$ is absolutely continuous, $J$ is Wasserstein differentiable at $\mu$ and its Wasserstein gradient is

$$\nabla_\mu J(\mu) = \text{Id} - T_{\bar{\mu}},$$

where $\text{Id} : \mathbb{R}^d \to \mathbb{R}^d$ is the identity map and $T_{\bar{\mu}} : \mathbb{R}^d \to \mathbb{R}^d$ is the (unique) optimal transport map from $\mu$ to $\bar{\mu}$.

Unlike in Euclidean (or more generally Hilbertian) settings, the distance function is not (geodesically) convex: It is in fact semiconcave. This makes the Wasserstein space a positively curved metric space; see [27]. This fact, among others, will complicate sufficient conditions for optimality, oftentimes intimately related to convexity. We later circumvent this technical difficulty in Theorem 3.8.

Next, we study expected values:

**Proposition 2.12** (Expected value). Let $V \in C^2(\mathbb{R}^d)$ with uniformly bounded Hessian (i.e., there exists $M > 0$ so that $\|\nabla^2_x V(x)\| \leq M$ for all $x \in \mathbb{R}^d$), and consider the functional

$$J(\mu) = E^\mu [V(x)] = \int_{\mathbb{R}^d} V(x) \text{d}\mu(x).$$

Then,

(i) $D(J) = \mathcal{P}_2(\mathbb{R}^d)$, $J$ is proper, and $J(\mu) > -\infty$ for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$;

(ii) $J$ is continuous w.r.t. weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$;

(iii) if $V^-(x) \leq C(1 + \|x\|^p)$ for $C \in \mathbb{R}$ and $p < 2$, then $J$ is lower semi-continuous w.r.t. narrow convergence;

(iv) $J$ is $\alpha$-convex along any interpolating curve if and only if $V$ is $\alpha$-convex;

(v) $J$ is Wasserstein differentiable and its Wasserstein gradient at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ is

$$\nabla_\mu J(\mu) = \nabla_x V.$$

We now consider interaction-type functionals:

**Proposition 2.13** (Derivative of interaction-type functionals). Let $U \in C^2(\mathbb{R}^d)$ with uniformly bounded Hessian (i.e., there exists $M > 0$ so that $\|\nabla^2_x U(z)\| \leq M$ for all $z \in \mathbb{R}^d$), and consider the functional

$$J(\mu) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y) \text{d}(\mu \times \mu)(x, y).$$

Then,
(i) \( D(J) = \mathcal{P}_2(\mathbb{R}^d) \), \( J \) is proper, and \( J(\mu) > -\infty \) for all \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \);

(ii) \( J \) is continuous w.r.t. weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \);

(iii) if \( U^-(z) \leq C(1 + \|z\|^p) \) for \( C \in \mathbb{R} \) and \( p < 2 \), then \( J \) is lower semi-continuous w.r.t. narrow convergence;

(iv) if \( U \) is convex, then \( J \) is convex along any interpolating curve;

(v) \( J \) is Wasserstein differentiable and its Wasserstein gradient at \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) is

\[
\nabla_{\mu} J(\mu) = \nabla U * \mu,
\]

provided that \( \nabla_{\mu} J(\mu) \in L^2(\mathbb{R}^d, \mathbb{R}^d; \mu) \), where the convolution is defined as

\[
\nabla_{\mu} J(\mu)(x) = (\nabla U * \mu)(x) := \int_{\mathbb{R}^d} \nabla U(x - y) d\mu(y).
\]

Remark 2.4. If \( U \) is \( \alpha \)-geodesically convex, then \( J \) is not necessarily \( \alpha \)-geodesically convex; e.g., see Lemma 4.5. Nonetheless, if \( \alpha \geq 0 \), then \( J \) is (0-)geodesically convex.

We now instantiate Proposition 2.13 to the study the variance:

Corollary 2.14 (Variance). Let \( a \in \mathbb{R}^d \) and \( J(\mu) = \operatorname{Var}^\mu [\langle a, x \rangle] \). Then, \( J \) is continuous w.r.t. to weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \), convex along any interpolating curve, and its Wasserstein gradient at \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) is

\[
\nabla_{\mu} J(\mu)(x) = 2a \langle a, x - E^\mu [x] \rangle.
\]

Remak 2.5. If \( d = 1 \) and \( a = 1 \), the Wasserstein gradient reduces to the natural expression \( \nabla_{\mu} \operatorname{Var}^\mu [x] = 2(\operatorname{Id} - E^\mu [x]) \). The gradient evaluates to zero when all probability mass is concentrated at the expected value and the variance achieves its global minimum; see Section 3. Moreover, Corollary 2.14 also follows from the chain rule (Proposition 2.9): Since \( \operatorname{Var}^\mu [\langle a, x \rangle] = E^\mu [\langle a, x \rangle^2] - E^\mu [\langle a, x \rangle]^2 \), we conclude

\[
\nabla_{\mu} J(\mu) = 2a \langle a, \operatorname{Id} \rangle - 2a E^\mu [\langle a, x \rangle] = 2a \langle a, \operatorname{Id} - E^\mu [x] \rangle.
\]

We can now recall the properties internal energy-type functionals:

Proposition 2.15 (Derivative of internal energy-type functionals). Let \( F : \mathbb{R}_{\geq 0} \to \mathbb{R} \) be convex, differentiable, with superlinear growth at infinity, and satisfy \( F(0) = 0 \). Consider the functional

\[
J(\mu) = \begin{cases} 
\int_{\mathbb{R}^d} F(\rho(x)) dx & \text{if } \mu = \rho \mathcal{L}^d \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d), \\
+\infty & \text{else}.
\end{cases}
\]

Then,

(i) \( D(J) \subset \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d) \) and \( J \) is proper;

(ii) \( J \) is lower semi-continuous w.r.t. weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \);

(iii) \( J \) is lower semi-continuous w.r.t. narrow convergence.

Moreover, if \( s \mapsto s^d F(s^{-d}) \) is convex and non-increasing on \((0, +\infty)\), then
(iv) \( J \) is convex along generalized geodesics;

If additionally there exists \( C > 0 \) s.t. \( F(z + w) \leq C(1 + F(z) + F(w)) \) for all \( z, w \in \mathbb{R}^d \), then

(v) \( J \) is Wasserstein differentiable at \( \mu = \rho \mathcal{L}^d \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d) \) with Wasserstein gradient

\[
\nabla_{\mu}J(\mu) = \frac{\nabla(\rho F'(\rho) - F(\rho))}{\rho},
\]

provided that all terms are well defined (i.e., \( \rho F'(\rho) + \rho \in W^{1,1}_{\text{loc}}(\mathbb{R}^d; \mu) \) and \( \nabla_{\mu}J(\mu) \in L^2(\mathbb{R}^d; \mu) \).

As an example, we consider the entropy:

**Example 2.3** (Entropy). Consider the entropy \( J = \int_{\mathbb{R}^d} \rho \log(\rho)dx \); i.e., \( F(z) = z \log(z) \) (with \( F(0) = 0 \)). Clearly, \( F \) is convex, differentiable, and has superlinear growth. Moreover, \( s^d s^{-d} \log(s^{-d}) = -d \log(s) \) is convex and non-increasing, and

\[
(z + w) \log(z + w) \leq 2(1 + z \log(z) + w \log(w)).
\]

So, if \( \mu = \rho \mathcal{L}^d \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d) \), the Wasserstein gradient is

\[
\nabla_{\mu}J(\mu) = \frac{\nabla(\rho + \rho \log(\rho) - \rho \log(\rho))}{\rho} = \frac{\nabla \rho}{\rho}.
\]

To conclude, we compute the derivative of divergences:

**Proposition 2.16** (Derivative of the divergences). Let \( F : \mathbb{R}_{\geq 0} \to \mathbb{R} \) be convex, differentiable, with superlinear growth at infinity, and satisfy \( F(0) = 0 \). Let \( \bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d) \). Consider the functional

\[
J(\mu) = \begin{cases} 
\int_{\mathbb{R}^d} F\left( \frac{d\mu}{d\bar{\mu}}(x) \right) d\bar{\mu}(x) & \text{if } \mu \ll \bar{\mu}, \\
+\infty & \text{else},
\end{cases}
\]

where \( \frac{d\mu}{d\bar{\mu}} \) is the Radon-Nikodym derivative. Then,

(i) \( D(J) \subset \{ \mu \in \mathcal{P}_2(\mathbb{R}^d) : \mu \ll \bar{\mu} \} \) and \( J \) is proper;

(ii) \( J \) is lower semi-continuous w.r.t. weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \);

(iii) \( J \) is lower semi-continuous w.r.t. narrow convergence.

Moreover, if \( s \mapsto s^d F(s^{-d}) \) is convex and non-increasing on \( (0, +\infty) \) and \( \bar{\mu} \) is log-concave, then

(iv) \( J \) is convex along generalized geodesics.

Additionally, if there exists \( C > 0 \) such that \( F(z + w) \leq C(1 + F(z) + F(w)) \) for all \( z, w \in \mathbb{R}^d \) and \( \bar{\mu} = e^{-V} \mathcal{L}^d \) with \( V : \mathbb{R}^d \to \mathbb{R} \) convex and continuously differentiable, then

(v) \( J \) is Wasserstein differentiable at \( \mu = \rho \mathcal{L}^d \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d) \) with Wasserstein gradient

\[
\nabla_{\mu}J(\mu) = \frac{\nabla(\rho/e^{-V} F'(\rho/e^{-V}) - F(\rho/e^{-V}))}{\rho} e^{-V},
\]

provided that all terms are well defined (i.e., \( \rho/e^{-V} F'(\rho/e^{-V}) + \rho/e^{-V} \in W^{1,1}_{\text{loc}}(\mathbb{R}^d; \mu) \) and \( \nabla_{\mu}J(\mu) \in L^2(\mathbb{R}^d; \mu) \)).
A prominent example is the KL divergence:

**Example 2.4 (KL divergence).** Let $\tilde{\mu} = e^{-V}L^d$ with $V$ convex and continuously differentiable. Consider the KL divergence, defined as

$$\text{KL}(\mu|\tilde{\mu}) = \begin{cases} \int_{\mathbb{R}^d} \log \left( \frac{\rho(x)}{e^{-V}(x)} \right) \frac{\rho(x)}{e^{-V}(x)} e^{-V(x)} dx & \text{if } \mu = \rho L^d \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d), \\ +\infty & \text{else.} \end{cases}$$

We can proceed as in Example 2.3 and use Proposition 2.16 to obtain

$$\nabla_\mu J(\mu) = \frac{\nabla(\rho/e^{-V} + \rho/e^{V} \log(\rho/e^{-V}) - \rho/e^{-V} \log(\rho/e^{-V}))}{\rho/e^{-V}} = \nabla \rho + \nabla V. \quad \triangle$$

We summarize these functionals, together with their Wasserstein gradients, in Table 1.

| Functional | Wasserstein gradient | Notes |
|------------|---------------------|-------|
| $E[\mu | f]$ | $\nabla f$ | cond. on $f$ |
| $\min_{\gamma \in \Gamma(\mu, \rho)} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x,y) d\gamma(x,y)$ | $\nabla_x c(\cdot, T^\rho_\mu(\cdot))$ | cond. on $c$, $T^\rho_\mu$ exists |
| $\frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} (x-y)d(\mu \times \mu)(x,y)$ | $\nabla U * \mu$ | cond. on $U$ |
| $\int_{\mathbb{R}^d} F(\rho(x)) dx$ | $\nabla (\rho F'(\rho/e^{-V}) - F(\rho/e^{-V})) / \rho/e^{-V}$ | $\mu = \rho L^d$, cond. on $F$ |
| $\int_{\mathbb{R}^d} F(\rho(x)/e^{-V(x)}) e^{-V(x)} dx$ | $\nabla (\rho F'(\rho/e^{-V}) - F(\rho/e^{-V})) / \rho/e^{-V}$ | $\mu = \rho L^d$, $\tilde{\mu} = e^{-V}L^d$, cond. on $F, V$ |

Table 1: Wasserstein gradients of real-valued functions over the Wasserstein space.

### 3 Optimality conditions

Consider a lower semi-continuous (w.r.t. weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$) functional $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$. For ease of notation, we denote (open) Wasserstein balls of radius $r > 0$ centered at $\tilde{\mu} \in \mathcal{P}_2(\mathbb{R}^d)$ by

$$B_r(\tilde{\mu}) := \{ \mu \in \mathcal{P}_2(\mathbb{R}^d) : W_2(\mu, \tilde{\mu}) < r \}.$$

#### 3.1 Unconstrained Optimization

In the setting of unconstrained optimization, minimizers are defined as usual:

**Definition 3.1 (Local, global, and strict minimizers for unconstrained optimization).** A probability measure $\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ is a local minimizer of $J$ if there exists $r > 0$ such that $J(\mu) \geq J(\mu^*)$ for all $\mu \in B_r(\mu^*)$. If this holds for any $r > 0$, then $\mu^*$ is a global minimizer. If $J(\mu) > J(\mu^*)$ for all $\mu \in \mathcal{P}_2(\mathbb{R}^d), \mu \neq \mu^*$, then $\mu^*$ is the strict minimizer of $J$.

Similarly to Euclidean settings, local minimality and derivatives are intimately related:

**Theorem 3.1 (First-order necessary conditions).** Let $\mu^*$ be a local minimizer of $J$ and assume $J$ is Wasserstein differentiable at $\mu^*$. Then, the Wasserstein gradient of $J$ vanishes at $\mu^*$:

$$\nabla_\mu J(\mu^*)(x) = 0 \quad \mu^* \text{-a.e.},$$

i.e., $\nabla_\mu J(\mu^*) = 0$ in $L^2(\mathbb{R}^d, \mathbb{R}^d; \mu^*)$. 

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Surprisingly, the proof of Theorem 3.1 is not elementary. In particular, we first need a revisited version of fundamental lemma of calculus of variations:

**Lemma 3.2** (Fundamental lemma of calculus of variations, revisited). Let \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) and \( H \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \). Assume that for all \( \psi \in C^\infty_c(\mathbb{R}^d) \)

\[
\int_{\mathbb{R}^d} \langle H(x), \nabla \psi(x) \rangle \, d\mu(x) = 0.
\]

Then, \( H \equiv 0 \) in \( L^2(\mathbb{R}^d, \mathbb{R}^d; \mu) \).

**Proof.** Let \( \varepsilon > 0 \). Then, by definition of \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \), there exists \( \varphi_\varepsilon \in C^\infty_c(\mathbb{R}^d) \) such that

\[
\| H - \nabla \varphi_\varepsilon \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)} < \varepsilon.
\]

Consider (12) with \( \psi = \varphi_\varepsilon \), then

\[
0 = -2 \int_{\mathbb{R}^d} \langle H, \nabla \varphi_\varepsilon \rangle \, d\mu(x) = \int_{\mathbb{R}^d} \| H - \nabla \varphi_\varepsilon \|^2 - \| H \|^2 - \| \nabla \varphi_\varepsilon \|^2 \, d\mu(x)
\]

\[
= \| H - \nabla \varphi_\varepsilon \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)} - \| H \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)} - \| \nabla \varphi_\varepsilon \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)},
\]

and thus

\[
\| H \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)} \leq \| H - \nabla \varphi_\varepsilon \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)} - \| \nabla \varphi_\varepsilon \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu)} < \varepsilon.
\]

Let \( \varepsilon \to 0 \) to get \( H \equiv 0 \). \( \square \)

**Proof of Theorem 3.1.** Let \( T = \nabla \psi \) for some \( \psi \in C^\infty_c(\mathbb{R}^d) \). By Lemma 2.4, there exists \( \bar{s} > 0 \) such that \( \text{Id} + \varepsilon T \) are the optimal transport maps between \( \mu^* \) and \( \mu := (\text{Id} + \varepsilon T)_\# \mu^* \) for all \( \varepsilon \in (-\bar{s}, \bar{s}) \).

Moreover, observe that \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) and

\[
W_2(\mu^*, \mu) = |\varepsilon| \| T \|^2_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu^*)}.
\]

Thus, by local minimality of \( \mu^* \), for \( \varepsilon \) sufficiently small it holds \( J(\mu) - J(\mu^*) \geq 0 \). So, for all \( \varepsilon > 0 \), differentiability gives

\[
0 \leq \frac{J((\text{Id} + \varepsilon T)_\# \mu^*) - J(\mu^*)}{\varepsilon} = \int_{\mathbb{R}^d} \langle \nabla \mu J(\mu^*) (x), T(x) \rangle \, d\mu^*(x) + \frac{o(\varepsilon)}{\varepsilon}.
\]

Letting \( \varepsilon \to 0 \) we get

\[
\int_{\mathbb{R}^d} \langle \nabla \mu J(\mu^*) (x), T(x) \rangle \, d\mu^*(x) \geq 0.
\]

Similarly, for \( \varepsilon < 0 \), we get

\[
\int_{\mathbb{R}^d} \langle \nabla \mu J(\mu^*) (x), T(x) \rangle \, d\mu^*(x) \leq 0,
\]

and thus

\[
\int_{\mathbb{R}^d} \langle \nabla \mu J(\mu^*) (x), T(x) \rangle \, d\mu^*(x) = 0.
\]

Finally, by Lemma 3.2, we conclude \( \nabla \mu J(\mu^*) (x) = 0 \), for \( \mu^* \)-almost all \( x \in \mathbb{R}^d \). \( \square \)

Under an additional convexity assumption, we get sufficient conditions:
Theorem 3.3 (First-order sufficient conditions). Assume that \( J \) is \( \alpha \)-geodesically convex with \( \alpha \geq 0 \). Suppose there exists \( \mu^* \in \mathcal{P}_2(\mathbb{R}^d) \) such that \( J \) is Wasserstein differentiable at \( \mu^* \) and the Wasserstein gradient of \( J \) vanishes at \( \mu^* \), i.e., \( \nabla_\mu J(\mu^*)(x) = 0 \) \( \mu^* \)-a.e.. Then, \( \mu^* \) is a global minimizer of \( J \). If \( \alpha > 0 \), \( \mu^* \) is the strict minimizer of \( J \).

Proof. Consider a competitor \( \nu \in \mathcal{P}_2(\mathbb{R}^d), \nu \neq \mu \). Then, by Proposition 2.8,

\[
J(\nu) - J(\mu) \geq \frac{\alpha}{2} W_2(\mu, \nu)^2.
\]

By non-negativity of \( \alpha \), \( J(\nu) \geq J(\mu) \); if additionally \( \alpha > 0 \), \( J(\nu) > J(\mu) \). Since \( \nu \) is arbitrary, we conclude the proof. \( \square \)

Example 3.1. Consider \( J(\mu) = \mathbb{E}^\mu \left[ \frac{1}{2} x^2 \right] \). Then, by Proposition 2.12, \( \nabla_\mu J(\mu^*) = \text{Id} \). Thus, by Theorem 3.1, a necessary condition for optimality is \( \nabla_\mu J(\mu^*)(x) = 0 \) \( \mu^* \)-a.e., which holds if and only if \( \mu^* = \delta_0 \). By Proposition 2.12, \( J \) is 1-geodesically convex, and so \( \mu^* \) is the strict minimizer of \( J \), by Theorem 3.3. \( \triangle \)

3.2 Constrained Optimization

Consider now the constrained optimization problem

\[
\inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \{ J(\mu) : K(\mu) = 0 \}, \tag{14}
\]

for some lower semi-continuous (w.r.t. weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \)) functional \( K : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R} \). To start, we adapt Definition 3.1 to the constrained setting:

Definition 3.2 (Local, global, and strict minimizers for constrained optimization). A probability measure \( \mu^* \in \mathcal{P}_2(\mathbb{R}^d) \) is a local minimizer of (14) if there exists \( r > 0 \) such that \( J(\mu) \geq J(\mu^*) \) for all \( \mu \in B_r(\mu^*) \cap \{ \mu \in \mathcal{P}_2(\mathbb{R}^d) : K(\mu) = 0 \} \). If this holds for any \( r > 0 \), then \( \mu^* \) is a global minimizer. If \( J(\mu) > J(\mu^*) \) for all \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \cap \{ \mu \in \mathcal{P}_2(\mathbb{R}^d) : K(\mu) = 0 \} \), \( \mu \neq \mu^* \), then \( \mu^* \) is the strict minimizer of (14).

The definition of (local, global, strict) minimality for inequality-constrained optimization problems is analogous. Then, similarly to Euclidean settings, necessary conditions for optimality take the form of Lagrange multipliers:

Theorem 3.4 (Lagrange multipliers in the Wasserstein space). Let \( \mu^* \) be a local minimizer of (14) and assume that \( J \) and \( K \) are Wasserstein differentiable at \( \mu^* \). Assume that \( \nabla_\mu K(\mu^*) \) is non-vanishing at \( \mu^* \), that is, there exists \( H = \nabla \varphi \) for some \( \varphi \in C^\infty_c(\mathbb{R}^d) \) such that

\[
\int_{\mathbb{R}^d} \langle \nabla_\mu K(\mu^*)(x), H(x) \rangle \, d\mu^*(x) \neq 0.
\]

Then, there exists a unique \( \lambda \in \mathbb{R} \) (called multiplier) such that

\[
\nabla_\mu J(\mu^*)(x) = \lambda \nabla_\mu K(\mu^*)(x)
\]

for \( \mu^* \)-almost every \( x \in \mathbb{R}^d \).

To prove the theorem we need the following preliminary lemma, which will later be instrumental in “making arbitrary variations admissible”:

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Lemma 3.5. Let $\mu^*$ and $H$ as in Theorem 3.4. Let $T = \nabla \psi$ for some $\psi \in C_0^\infty(\mathbb{R}^d)$. Then, there exists $\varepsilon > 0$ and a continuously differentiable function $\sigma_\varepsilon \in C^1 : (-\varepsilon, \varepsilon) \to \mathbb{R}$ with $\sigma(0) = 0$ such that for all $\varepsilon \in (-\varepsilon, \varepsilon)$

$$K((\text{Id} + \varepsilon T + \sigma(\varepsilon)H)\#\mu) = 0.$$ 

Proof. Define the function

$$\chi : \mathbb{R} \times \mathbb{R} \to \mathbb{R}
\quad (\varepsilon, \delta) \mapsto K((\text{Id} + \varepsilon T + \delta H)\#\mu^*).$$

Trivially, $\chi(0,0) = K(\mu^*) = 0$, by feasibility of $\mu^*$. We are interested in studying the derivative with respect to $\delta$. To do so, we first need to establish differentiability. Let $\delta > 0$. Since $H$ is the gradient of a smooth compactly supported function, we know, by Lemma 2.4, that for $\delta$ sufficiently small $\text{Id} + \delta H$ is an optimal transport map from $\mu^*$ to $(\text{Id} + \delta H)\#\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ and

$$W_2((\text{Id} + \delta H)\#\mu^*, \mu^*) = \delta \|H\|_{L^2(\mathbb{R}^d, \mu^*)}.$$ 

Without loss of generality, assume $H$ is normalized; i.e., $\|H\|_{L^2(\mathbb{R}^d, \mu^*)} = 1$. Then, by Wasserstein differentiability (cf. Definition 2.3) we have

$$K((\text{Id} + \delta H)\#\mu^*) - K(\mu^*) = \frac{1}{\delta} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_{\mu} K(\mu^*)(x), y - x \rangle \, d\gamma(x,y) + o(\delta)$$

for $\gamma \in \Gamma_\mu(\mu^*, (\text{Id} + \delta H)\#\mu^*)$. As $\text{Id} + \delta H$ is an optimal transport map, we choose $\gamma = (\text{Id}, \text{Id} + \delta H)\#\mu^*$ to get

$$\frac{K((\text{Id} + \delta H)\#\mu^*) - K(\mu^*)}{\delta} = \int_{\mathbb{R}} \langle \nabla_{\mu} K(\mu^*)(x), H(x) \rangle \, d\mu^*(x) + \frac{o(\delta)}{\delta},$$

which proves that the limit $\delta \to 0$ exists (and, by definition, equals the derivative). Hence,

$$\frac{d\chi}{d\delta}(0,0) = \lim_{\delta \to 0} \int_{\mathbb{R}} \langle \nabla_{\mu} K(\mu^*)(x), H(x) \rangle \, d\mu^*(x) + \frac{o(\delta)}{\delta}$$

$$= \int_{\mathbb{R}} \langle \nabla_{\mu} K(\mu^*)(x), H(x) \rangle \, d\mu^*(x).$$

Analogously, we obtain that

$$\frac{d\chi}{d\varepsilon}(0,0) = \int_{\mathbb{R}} \langle \nabla_{\mu} K(\mu^*)(x), T(x) \rangle \, d\mu^*(x),$$

which is well defined since $T$ has compact support. Thus, by the implicit function theorem [55, Theorem 1.3.1], there exists $\bar{\varepsilon} > 0$ and a continuously differentiable function $\sigma : (-\bar{\varepsilon}, \bar{\varepsilon}) \to \mathbb{R}$ such that $\sigma(0) = 0$ and

$$K((\text{Id} + \varepsilon T + \sigma(\varepsilon)H)\#\mu^*) = 0$$

for all $\varepsilon \in (-\bar{\varepsilon}, \bar{\varepsilon})$. \qed

Proof of Theorem 3.4. The proof goes by variations. As in the proof of Theorem 3.1, we will consider variations via gradients of compactly supported smooth functions; we will then deploy Lemma 3.5 to make sure that variations are admissible (i.e., they satisfy the constraint). More specifically, let $T = \nabla \psi$ for some $\psi \in C_0^\infty(\mathbb{R}^d)$. The variation $(\text{Id} + \varepsilon T)\#\mu^*$ is not admissible, as generally $K((\text{Id} + \varepsilon T)\#\mu^*) \neq 0$. Yet, we can use Lemma 3.5 to make the variation admissible. In particular, there exists $\bar{\varepsilon} > 0$ and $\sigma \in C^1((-\bar{\varepsilon}, \bar{\varepsilon}))$ such that the variation $(\text{Id} + \varepsilon T + \sigma(\varepsilon)H)\#\mu^*$ is admissible for
all \( \varepsilon \in (-\varepsilon, \varepsilon) \). As \( \sigma(\varepsilon) = \sigma'(0)\varepsilon + o(\varepsilon) \), Lemma 2.4 gives that, for \( \varepsilon \) sufficiently small, \( \text{Id} + \varepsilon T + \sigma(\varepsilon)H \) is an optimal transport map from \( \mu^* \) to \( (\text{Id} + \varepsilon T + \sigma(\varepsilon)H)\# \mu^* \). So,

\[
W_2((\text{Id} + \varepsilon T + \sigma(\varepsilon)H)_\# \mu^*, \mu^*) = \| \varepsilon T + \sigma(\varepsilon)H \|_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu^*)} \\
\leq \| \varepsilon \|_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu^*)} + \| \sigma(\varepsilon) \|_{L^2(\mathbb{R}^d, \mathbb{R}^d; \mu^*)}.
\]

As \( \sigma(\varepsilon) \to 0 \) as \( \varepsilon \to 0 \), local minimality of \( \mu^* \) with \( \varepsilon > 0 \), together with differentiability, gives

\[
0 \leq \frac{J((\text{Id} + \varepsilon T + \sigma(\varepsilon)H)_\# \mu^*) - J(\mu^*)}{\varepsilon} = \frac{1}{\varepsilon} \int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*)(x), x + \varepsilon T(x) + \sigma(\varepsilon)H(x) - x \rangle \, d\mu^*(x) + \frac{o(\varepsilon)}{\varepsilon}.
\]

Let \( \varepsilon \to 0 \) to conclude

\[
\int_{\mathbb{R}} \langle \nabla_\mu J(\mu^*), T + \sigma'(0)H \rangle \, d\mu^* \geq 0.
\]

If we repeat the argument with \( \varepsilon < 0 \), we get

\[
\int_{\mathbb{R}} \langle \nabla_\mu J(\mu^*), T + \sigma'(0)H \rangle \, d\mu^* \leq 0,
\]

and thus

\[
0 = \int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*), T + \sigma'(0)H \rangle \, d\mu^*(x)
= \int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*), T \rangle \, d\mu^* + \sigma'(0) \int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*), H \rangle \, d\mu^*.
\]

Moreover, for all \( \varepsilon \in (-\varepsilon, \varepsilon) \) the function \( \varepsilon \mapsto K((\text{Id} + \varepsilon T + \sigma(\varepsilon)H)_\# \mu) \) is zero. Hence, proceeding as above, we get

\[
\int_{\mathbb{R}} \langle \nabla_\mu K(\mu^*), T \rangle \, d\mu^* + \sigma'(0) \int_{\mathbb{R}} \langle \nabla_\mu K(\mu^*), H \rangle \, d\mu^* = 0,
\]

which leads, as by assumption \( \int_{\mathbb{R}} \langle \nabla_\mu K(\mu^*), H \rangle \, d\mu^* \neq 0 \), to

\[
\sigma'(0) = -\frac{\int_{\mathbb{R}} \langle \nabla_\mu K(\mu^*), T \rangle \, d\mu^*}{\int_{\mathbb{R}} \langle \nabla_\mu K(\mu^*), H \rangle \, d\mu^*} \in \mathbb{R}.
\]

So, (15) reads

\[
\int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*), T \rangle \, d\mu^* - \frac{\int_{\mathbb{R}} \langle \nabla_\mu K(\mu^*), T \rangle \, d\mu^*}{\int_{\mathbb{R}} \langle \nabla_\mu K(\mu^*), H \rangle \, d\mu^*} \int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*), H \rangle \, d\mu^* = 0.
\]

Define the multiplier as

\[
\lambda := \frac{\int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*), H \rangle \, d\mu^*}{\int_{\mathbb{R}^d} \langle \nabla_\mu K(\mu^*), H \rangle \, d\mu^*} \in \mathbb{R}.
\]

Then, (16) becomes

\[
\int_{\mathbb{R}^d} \langle \nabla_\mu J(\mu^*) - \lambda \nabla_\mu K(\mu^*), T \rangle \, d\mu^* = 0.
\]

As \( T \) is arbitrary, Lemma 3.2 gives

\[
\nabla_\mu J(\mu^*) - \lambda \nabla_\mu K(\mu^*) \equiv 0,
\]

or equivalently \( \nabla_\mu J(\mu^*)(x) = \lambda \nabla_\mu K(\mu^*)(x) \) for \( \mu^* \)-almost all \( x \in \mathbb{R}^d \). Finally, to show uniqueness, assume that there exists another \( \lambda' \in \mathbb{R} \) so that

\[
\nabla_\mu J(\mu^*) = \lambda' \nabla_\mu K(\mu^*)(x).
\]
for $\mu^*$-almost every $x \in \mathbb{R}^d$. Then, $\lambda' \nabla \mu K(\mu^*) = \lambda \nabla \mu K(\mu^*)$, and
\[
\lambda' \int_{\mathbb{R}^d} (\nabla \mu K(\mu^*) (x), H(x)) \, d\mu^*(x) = \lambda \int_{\mathbb{R}^d} (\nabla \mu K(\mu^*) (x), H(x)) \, d\mu^*(x).
\]
Since, by assumption $\int_{\mathbb{R}^d} (\nabla \mu K(\mu^*) (x), H(x)) \, d\mu^*(x) \neq 0$, we conclude $\lambda' = \lambda$. \hfill $\square$

**Remark 3.1.** Few remarks are in order. First, Theorems 3.1 and 3.4 provide necessary conditions for optimality. In particular, they do not provide conditions for existence of minimizers for $J$ or (14). Second, Theorem 3.4 readily extends to multidimensional constraints of the form $K : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$, with $l \in \mathbb{N}_{\geq 1}$, which we deliberately omitted to ease the exposition. Third, Theorems 3.1 and 3.4 apply to maximization problems with no changes. One simply considers upper semi-continuous (w.r.t. weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$) functional $J : \mathcal{P}_2(\mathbb{R}^d) \to [−\infty, +\infty)$ with the effective domain $D(J) := \{\mu \in \mathcal{P}_2(\mathbb{R}^d) : J(\mu) > −\infty\} \neq \emptyset$. We will tacitly use this fact throughout the next sections. \hfill $\triangle$

Under a convexity assumption, we can study sufficient conditions in the more general setting of inequality-constrained optimization. The first result is an application of Theorem 3.3:

**Theorem 3.6** (First-order sufficient conditions for constrained optimization). Let $J, K : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be convex along geodesics. Consider
\[
\inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \{J(\mu) : K(\mu) \leq 0\}. \quad (17)
\]
Suppose there exists (finite) $\lambda \geq 0$ and $\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ such that $J$ and $K$ are Wasserstein differentiable at $\mu^*$ and
\[
\nabla_{\mu} J(\mu^*) + \lambda \nabla_{\mu} K(\mu^*) = 0,
\]
\[
K(\mu^*) = 0.
\]
Then, $\mu^*$ is a global minimizer of (17). Moreover, if $J$ is $\alpha_J$-convex along geodesics, $K$ is $\alpha_K$-convex along geodesics, and $\alpha_J + \lambda \alpha_K > 0$, then $\mu^*$ is the strict minimizer.

**Proof.** Without loss of generality, $\lambda > 0$; else, the result follows directly from Theorem 3.3. Let $\alpha_J \geq 0$ be the convexity parameter of $J$ and $\alpha_K$ be the convexity parameter of $K$, then $J + \lambda K$ is $(\alpha_J + \lambda \alpha_K)$-geodesically convex. By Theorem 3.3, $\mu^*$ is a (global) minimizer of $\mu \mapsto J(\mu) + \lambda K(\mu)$. Then, let $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ such that $\nu \neq \mu^*$ and $K(\nu) \leq 0$:
\[
J(\nu) \geq J(\nu) + \lambda K(\nu) \\
\geq J(\mu^*) + \lambda K(\mu^*) + \frac{\alpha_J + \lambda \alpha_K}{2} W_2(\mu^*, \nu)^2 \\
= J(\mu^*) + \frac{\alpha_J + \lambda \alpha_K}{2} W_2(\mu^*, \nu)^2.
\]
Since $\nu$ is arbitrary, $\mu^*$ is a global minimizer of (17). If additionally $\alpha_J + \lambda \alpha_K > 0$, $\mu^*$ is the strict minimizer. \hfill $\square$

If the constraint is “linear” (i.e., both geodesically convex and concave) we can further strengthen the result:

**Corollary 3.7** (“Linear” constraints). Let $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be geodesically convex, and $K : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be both geodesically convex and geodesically concave. Consider
\[
\inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \{J(\mu) : K(\mu) = 0\}. \quad (18)
\]
Suppose there exists (finite) $\lambda \in \mathbb{R}$ and $\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ such that $J$ and $K$ are Wasserstein differentiable at $\mu^*$ and

$$\nabla_\mu J(\mu^*) + \lambda \nabla_\mu K(\mu^*) = 0,$$

$$K(\mu^*) = 0.$$

Then, $\mu^*$ is a global minimizer of (18). Moreover, if $J$ is $\alpha_J$-geodesically convex with $\alpha_J > 0$, then $\mu^*$ is the strict minimizer.

**Proof.** The proof leverages Theorem 3.6 with $\mu \mapsto K(\mu)$ and $\mu \mapsto -K(\mu)$. \qed

Unfortunately, the Wasserstein distance is not convex along geodesics, which prevents us from deploying Theorem 3.6 whenever $K$ is defined in terms of the Wasserstein distance (e.g., $K(\mu) = W_2(\mu, \bar{\mu}) - \varepsilon$ for some $\bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d)$ and $\varepsilon > 0$). We resolve this issue in greater generality by studying optimal transport discrepancies:

**Theorem 3.8** (First-order sufficient conditions for constrained optimization, revisited). Let $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be convex along any interpolation curve with convexity parameter $\alpha_J \in \mathbb{R}$ and suppose $c : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_{\geq 0}$ satisfies the assumptions of Proposition 2.10. Let $\bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d)$, and suppose that $c(\cdot, y)$ is $\alpha_c$-convex for all $y \in \text{supp}(\bar{\mu})$. Consider

$$\inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \{ J(\mu) : W_c(\mu, \bar{\mu}) \leq \varepsilon \}. \quad (19)$$

Suppose there exist finite $\lambda \geq \frac{\alpha_J}{\alpha_c}$ and $\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ such that $J$ and $W_c(\mu, \bar{\mu})$ are Wasserstein differentiable at $\mu^*$ and

$$\nabla_\mu J(\mu) + \lambda \nabla_\mu W_c(\mu, \bar{\mu}) = 0,$$

$$W_c(\mu, \bar{\mu}) = \varepsilon.$$

Then, $\mu^*$ is the global minimizer of (19). If additionally $\alpha_J > 0$ or $\lambda > \frac{\alpha_J}{\alpha_c}$, then $\mu^*$ is the strict minimizer.

**Proof.** By Proposition 2.10 and convexity along interpolation curves of $J$, the function $\mathcal{L}(\mu) = J(\mu) + \lambda W_c(\bar{\mu}, \mu)$ is $(\lambda \alpha_c + \alpha_J)$-convex along the interpolation curve between $\mu^*$ and $\nu$ “centered” at $\bar{\mu}$, defined by

$$\mu_t := ((1 - t) \text{proj}_2 + t \text{proj}_3)_\# \gamma,$$

where

$$\gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d), \quad (\text{proj}_{12})_\# \gamma \in \Gamma_o(\bar{\mu}, \mu^*), \quad (\text{proj}_{13})_\# \gamma \in \Gamma_o(\bar{\mu}, \nu),$$

where optimality is intended w.r.t. transport cost $c$. Note that $(\text{proj}_{23})_\# \gamma \in \Gamma(\mu^*, \nu)$ and

$$(\text{proj}_2, (1 - t) \text{proj}_2 + t \text{proj}_3)_\# \gamma \in \Gamma(\mu^*, \mu_t),$$

where both plans are generally not optimal. In particular,

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_\mu \mathcal{L}(\mu^*)(x), y - x \rangle d((\text{proj}_2, (1 - t) \text{proj}_2 + t \text{proj}_3)_\# \gamma)(x, y)$$

$$= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_\mu \mathcal{L}(\mu^*)(x), (1 - t)x + ty - x \rangle d((\text{proj}_2, \text{proj}_3)_\# \gamma)(x, y) \quad (20)$$

$$= t \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_\mu \mathcal{L}(\mu^*)(x), y - x \rangle d((\text{proj}_2, \text{proj}_3)_\# \gamma)(x, y)$$
\[
\begin{align*}
\int_{\mathbb{R}^d \times \mathbb{R}^d} \|y - x\|^2 \text{d}((\text{proj}_2, (1-t) \text{proj}_2 + t \text{proj}_3)\# \gamma)(x, y) \\
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \|(1-t)x + ty - x\|^2 \text{d}((\text{proj}_2, \text{proj}_3)\# \gamma)(x, y) \\
= t^2 \int_{\mathbb{R}^d \times \mathbb{R}^d} \|y - x\|^2 \text{d}((\text{proj}_2, \text{proj}_3)\# \gamma)(x, y).
\end{align*}
\]

Then, Proposition 2.6 gives
\[
\mathcal{L}(\mu_t) - \mathcal{L}(\mu^*) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \left< \nabla_\mu \mathcal{L}(\mu^*) (x), y - x \right> \text{d}((\text{proj}_2, (1-t) \text{proj}_2 + t \text{proj}_3)\# \gamma)(x, y) \\
+ o \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|y - x\|^2 \text{d}((\text{proj}_2, (1-t) \text{proj}_2 + t \text{proj}_3)\# \gamma)(x, y) \right)^{(20),(21)} \leq t \int_{\mathbb{R}^d \times \mathbb{R}^d} \left< \nabla_\mu \mathcal{L}(\mu^*) , y - x \right> \text{d}((\text{proj}_2, \text{proj}_3)\# \gamma)(x, y) + o(t).
\]

Since $\mathcal{L}$ is $(\lambda \alpha_c + \alpha_f)$-convex the interpolation curve $\mu_t$, for all $t \in (0, 1)$ we have
\[
\mathcal{L}(\mu_t) \leq (1-t)\mathcal{L}(\mu^*) + t \mathcal{L}(\nu) - \frac{\lambda \alpha_c + \alpha_f}{2} t (1-t)\int_{\mathbb{R}^d \times \mathbb{R}^d} \|y - x\|^2 \text{d}((\text{proj}_2, \text{proj}_3)\# \gamma)(x, y) \\
\leq (1-t)\mathcal{L}(\mu^*) + t \mathcal{L}(\nu) - \frac{\lambda \alpha_c + \alpha_f}{2} t (1-t)W_2(\mu^*, \nu)^2,
\]
where the second inequality follows from $\lambda \geq \frac{\alpha_f}{\alpha_c}$ and suboptimality of the plan $(\text{proj}_2, \text{proj}_3)\# \gamma \in \Gamma(\mu^*, \nu)$. Thus,
\[
\frac{\mathcal{L}(\mu_t) - \mathcal{L}(\mu^*)}{t} \leq \mathcal{L}(\nu) - \mathcal{L}(\mu^*) - \frac{\lambda \alpha_c + \alpha_f}{2} (1-t)W_2(\mu^*, \nu)^2. \quad (23)
\]
Thus, using (strong) Wasserstein differentiability (Proposition 2.6)
\[
\mathcal{L}(\nu) - \mathcal{L}(\mu^*) - \frac{\lambda \alpha_c + \alpha_f}{2} W_2(\mu^*, \nu)^2 \\
= \lim_{t \downarrow 0} \mathcal{L}(\nu) - \mathcal{L}(\mu^*) - \frac{\lambda \alpha_c + \alpha_f}{2} (1-t)W_2(\mu^*, \nu)^2 \\
\geq \lim_{t \downarrow 0} \frac{\mathcal{L}(\mu_t) - \mathcal{L}(\mu^*)}{t} \quad (23) \\
\geq \lim_{t \downarrow 0} \frac{t \int_{\mathbb{R}^d \times \mathbb{R}^d} \left< \nabla_\mu \mathcal{L}(\mu^*) , y - x \right> \text{d}((\text{proj}_2, \text{proj}_3)\# \gamma)(x, y) + o(t)}{t} \quad (22) \\
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \left< \nabla_\mu \mathcal{L}(\mu^*) , y - x \right> \text{d}((\text{proj}_2, \text{proj}_3)\# \gamma)(x, y).
\]

Since, by assumption, $\nabla_\mu \mathcal{L}(\mu^*) = 0$, we conclude
\[
\mathcal{L}(\nu) - \mathcal{L}(\mu^*) \geq \frac{\lambda \alpha_c + \alpha_f}{2} W_2(\mu^*, \nu)^2.
\]
Suppose now that $\nu$ is feasible; i.e., $W_c(\gamma, \bar{\nu}) \leq \varepsilon$. Then,
\[
J(\nu) \geq J(\nu) + \lambda (W_c(\nu, \bar{\nu}) - \varepsilon) \\
\geq J(\mu^*) + \lambda (W_c(\mu^*, \bar{\nu}) - \varepsilon) + \frac{\lambda \alpha_c + \alpha_f}{2} W_2(\mu^*, \nu)^2 \\
= J(\mu^*) + \frac{\lambda \alpha_c + \alpha_f}{2} W_2(\mu^*, \nu)^2.
\]
Since $\nu$ is arbitrary, $\mu^*$ is a global minimizer. If $\alpha_f > 0$ or $\lambda > \frac{\alpha_f}{\alpha_c}$, then $\mu^*$ is the strict minimizer. \qed
The special case of the Wasserstein distance is then obtained as a corollary. In this case, convexity along generalized geodesics (instead of general interpolation curves) suffices:

**Corollary 3.9** (First-order sufficient conditions for constrained optimization, revisited). Let $J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ be convex along generalized geodesics with convexity parameter $\alpha \in \mathbb{R}$. Let $\bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d)$, and consider

$$\inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \{ J(\mu) : W_2(\mu, \bar{\mu}) \leq \varepsilon \} \equiv \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \{ J(\mu) : W_2(\mu, \bar{\mu})^2 \leq \varepsilon^2 \}. \quad (24)$$

Suppose there exist $\lambda \geq \frac{\alpha}{2}$ and $\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ such that $J$ and $W_2(\mu, \bar{\mu})^2$ are Wasserstein differentiable at $\mu^*$ and

$$\nabla_{\mu} J(\mu) + \lambda W_2(\mu, \bar{\mu})^2 = 0,$$

$$W_2(\mu, \bar{\mu}) = \varepsilon.$$

Then, $\mu^*$ is the a global minimizer of (24). If additionally $\alpha > 0$ or $\lambda > \frac{\alpha}{2}$, then $\mu^*$ is the strict minimizer.

**Proof.** In the case of the squared Wasserstein distance, we have $c(x, y) = \|x - y\|^2$, and thus $\alpha_e = 2$. By Corollary 2.11 and convexity along generalized geodesics of $J$, the function $L(\mu) = J(\mu) + \lambda W_2(\bar{\mu}, \mu)^2$ is $(2\lambda + \alpha)$-convex along the generalized geodesic curve between $\mu^*$ and $\nu$ “centered” at $\bar{\mu}$. Then, proof is identical to the proof of Theorem 3.8. \qed

**Remark 3.2.** For the special case $\lambda > \frac{\alpha}{2}$, existence of a unique minimizer for $L$ is in good agreement with [27, Theorem 4.1.2]. Specifically, [27, Theorem 4.1.2] requires coercitivity; i.e., existence $\bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d)$ and $r > 0$ such that $\inf_{\mu \in B_r(\bar{\mu})} J(\mu) > -\infty$. Indeed, by Proposition 2.8, for $\mu \in \mathcal{P}_2(\mathbb{R}^d)$

$$J(\mu) \geq J(\mu^*) + \sup_{\gamma \in \Gamma_{\mu}(\mu^*, \mu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_{\mu} J(\mu)(x), y - x \rangle \, d\gamma(x, y) + \frac{\alpha}{2} W_2(\mu^*, \mu)^2.$$

Hölder’s inequality gives

$$J(\mu) \geq J(\mu^*) - \|\nabla_{\mu} J(\mu^*)\|_{L^2(\mathbb{R}^d \times \mathbb{R}^d), \mu^*} W_2(\mu^*, \mu^*) + \frac{\alpha}{2} W_2(\mu^*, \mu^*)^2,$$

which is bounded whenever $W_2(\mu^*, \mu)$ is bounded. Thus, $J$ is coercive. By [27, Theorem 4.1.2], for all $\lambda > \frac{\alpha}{2}$, the function $\mu \mapsto \lambda W_2(\mu, \bar{\mu})^2 + J(\mu)$ has a unique (global) minimizer. \hfill \Box

**Example 3.2.** Consider the optimization problem

$$\inf_{\mu \in \mathcal{P}_2(\mathbb{R})} \left\{ J(\mu) := \mathbb{E}^\mu \left[ \frac{1}{2} x^2 \right] : K(\mu) := \mathbb{E}^\mu [x] - 1 = 0 \right\}.$$

Let us assume that a minimizer exists; we will later use sufficient conditions to prove its optimality. As $\nabla_{\mu} K(\mu) = 1$ for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, it is straightforward to construct $\varphi$ so that $\int_{\mathbb{R}^d} (1, \nabla \varphi(x)) \, d\mu^*(x) = 0$. Hence, by Theorem 3.4, at optimality it necessarily holds $\nabla_{\mu} J(\mu) = \text{Id} = \lambda \mu^*$-almost everywhere. Thus, $\int_{\mathbb{R}^d} |x - \lambda| d\mu^*(x) = 0$, and so $\mu^* = \delta_\lambda$. As $\mathbb{E}^{\delta_\lambda} [x] = 1$, we conclude $\mu^* = \delta_1$ and $\lambda = 1$. By Proposition 2.12, $J$ and $K$ are convex along geodesics with $\alpha_J = 1$ and $\alpha_K = 0$. Thus, $\mu^*$ the strict minimizer, by Theorem 3.6 or Corollary 3.7. \hfill \Box
4 Application to the Evaluation of Worst-case Risk over Wasserstein Ambiguity Sets

Consider the problem of evaluating the worst-case risk of a real-valued function over an ambiguity set defined in terms of the Wasserstein distance, intimately related to DRO (cf. Example 1.1). It is well known that when the risk is the expected value of an (integrable) real-valued function \( f : \mathbb{R}^d \to \mathbb{R} \), then the worst-case risk admits the following dual reformulation [3, 4]:

\[
\sup_{\mu \in B_{\varepsilon}(\hat{\mu})} \mathbb{E}^\mu [f] = \inf_{\lambda \geq 0} \lambda \varepsilon^2 - \mathbb{E}^{\hat{\mu}} \left[ \inf_{y \in \mathbb{R}^d} \lambda \|x - y\|^2 - f(y) \right],
\]

(25)

where \( \bar{B}_{\varepsilon}(\hat{\mu}) \) denotes the closed Wasserstein ball of radius \( \varepsilon \) centered at \( \hat{\mu} \in \mathcal{P}_2(\mathbb{R}^d) \):

\[
\bar{B}_{\varepsilon}(\hat{\mu}) := \{ \mu \in \mathcal{P}_2(\mathbb{R}^d) : W_2(\mu, \hat{\mu}) \leq \varepsilon \}.
\]

In this section, we use necessary and sufficient conditions for optimality in the Wasserstein space to study the more general setting

\[
J^* := \sup_{\mu \in B_{\varepsilon}(\hat{\mu})} J(\mu)
\]

(26)

for several cost functionals \( J : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R} \) which are not necessarily representable as expected values. We start by showing that, up to arbitrarily small perturbations of the radius of the Wasserstein ball, one can always assume that \( \hat{\mu} \) is absolutely continuous:

**Proposition 4.1** (Absolute continuity of the center). Let \( \delta > 0 \) and \( \hat{\mu} \in \mathcal{P}_2(\mathbb{R}^d) \). Then, there exists \( \hat{\mu}'_{\delta} \in \bar{B}_{\delta}(\hat{\mu}) \) absolutely continuous w.r.t. the Lebesgue measure such that

\[
\sup_{\mu \in \bar{B}_{\varepsilon - 2\delta}(\hat{\mu}'_{\delta})} J(\mu) \leq \sup_{\mu \in \bar{B}_{\varepsilon - \delta}(\hat{\mu})} J(\mu) \leq \sup_{\mu \in \bar{B}_{\varepsilon}(\hat{\mu}')} J(\mu) \leq \sup_{\mu \in \bar{B}_{\varepsilon + \delta}(\hat{\mu}')} J(\mu).
\]

**Proof.** Existence of \( \hat{\mu}'_{\delta} \) is ensured by density (with respect to the Wasserstein distance) of \( \mathcal{P}_2(\mathbb{R}^d) \) in \( \mathcal{P}_2(\mathbb{R}^d) \) [38, Theorem 2.2.7]. Then, the result follows from triangle inequality.

Second, we recall a well-known compactness result for Wasserstein balls. Its proof, included for completeness, is relegated to Appendix B.

**Proposition 4.2** (Properties of Wasserstein balls). Let \( \hat{\mu} \in \mathcal{P}_2(\mathbb{R}^d) \) and \( \varepsilon > 0 \). Then,

(i) \( \bar{B}_{\varepsilon}(\hat{\mu}) \) is closed, but not compact w.r.t. weak convergence;

(ii) \( \bar{B}_{\varepsilon}(\hat{\mu}) \) is compact w.r.t. narrow convergence.

4.1 Pedagogical Example

As a pedagogical example, consider

\[
J(\mu) = \mathbb{E}^\mu [(w, x)]
\]

(27)

for some non-zero \( w \in \mathbb{R}^d \). In this case, the solution of (26) is easily found via (25). Yet, as an illustrative example, we study (26) through necessary and sufficient conditions for optimality in the Wasserstein space. To do so, we first show that maxima are attained at the boundary of the Wasserstein ball, and so we can replace the inequality \( W_2(\mu, \hat{\mu}) \leq \varepsilon \) with an equality:

Here, the closure is intended with respect to the topology induced by the Wasserstein distance.
Lemma 4.3 (Existence of a maximum at the boundary). There exists a worst-case probability measure \( \mu^* \) attaining the supremum (26) such that \( W_2(\hat{\mu}, \mu^*) = \varepsilon \).

Proof. Existence of a solution follows directly by Weierstrass’ extreme value theorem (e.g., see the proof of [29, Theorem 4.1]): (i) by Proposition 2.12, \(-J\) is lower semi-continuous w.r.t. narrow convergence and (ii) by Proposition 4.2 Wasserstein balls are compact w.r.t. narrow convergence. So, there exists \( \mu^* \in \bar{B}_\varepsilon(\hat{\mu}) \); i.e., \( W_2(\mu^*, \hat{\mu}) \leq \varepsilon \). Now, assume for the sake of contradiction that \( W_2(\hat{\mu}, \mu^*) < \varepsilon \). By Proposition 2.12, \( \mathbb{E}^\mu [\langle w, x \rangle] \) is Wasserstein differentiable at each \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \) and its Wasserstein gradient reads

\[ \nabla_\mu \mathbb{E}^\mu [\langle w, x \rangle] = \nabla \langle w, x \rangle = w. \]

By Theorem 3.1, at optimality the Wasserstein gradient must vanish (in \( L^2 \) sense). However, the Wasserstein gradient \( \nabla_\mu \mathbb{E}^\mu [\langle w, x \rangle] \) equals the zero function if and only if \( w = 0 \), which leads to a contradiction.

We can now attack (26) via Theorems 3.4 and 3.8. Without loss of generality, we assume that \( \hat{\mu} \) is absolutely continuous; see Proposition 4.1. The proof strategy is conceptually simple: We assume enough regularity to use necessary conditions for optimality (Theorem 3.4) to construct candidates for optimality, and then leverage sufficient conditions for optimality (Theorem 3.8) to prove that one candidate solution is indeed optimal.

Proposition 4.4 (Optimal solution). Consider problem (26) with cost functional (27). Assume \( \hat{\mu} \in \mathcal{P}_{2, \text{abs}}(\mathbb{R}^d) \) is absolutely continuous with respect to the Lebesgue measure. Then, the unique worst-case probability measure is \( \mu^* = T\#\hat{\mu} \), where

\[ T(x) = x + \varepsilon \frac{w}{\|w\|}, \]

and the corresponding worst-case cost is

\[ J^* = \mathbb{E}^{\hat{\mu}} [\langle w, x \rangle] + \varepsilon \|w\|. \quad (28) \]

Proof. By Lemma 4.3, we can restrict ourselves to probability measures such that \( W_2(\hat{\mu}, \mu^*)^2 = \varepsilon^2 \). Then, the proof consists of two parts. First, we assume absolute continuity of \( \mu^* \) to ensure differentiability of the Wasserstein distance, and use the necessary conditions for optimality (Theorem 3.4) to construct candidates for optimality. We then prove its optimality via sufficient conditions. Assume \( \mu^* \) is absolutely continuous. By Corollary 2.11, together with absolutely continuity of \( \mu^* \), the Wasserstein gradient of \( K \) reads

\[ \nabla_\mu K(\mu) = 2 \left( T_{\mu^*}^\mu - \text{Id} \right). \]

We can assume that there exists \( \varphi \in C_0^\infty(\mathbb{R}^d) \) such that

\[ 2 \int_{\mathbb{R}^d} \left\langle T_{\mu^*}^\mu - \text{Id}, \nabla \varphi \right\rangle \, d\mu^* \neq 0. \]

Indeed, if

\[ \int_{\mathbb{R}^d} \left\langle T_{\mu^*}^\mu - \text{Id}, \nabla \varphi \right\rangle \, d\mu^* = 0 \quad (29) \]

for all \( \varphi \in C_0^\infty(\mathbb{R}^d) \), then, by Lemma 3.2, \( T_{\mu^*}^\mu = \text{Id} \). In this case, however, the optimal transport map from \( \mu^* \) to \( \hat{\mu} \) would coincide with the identity map, which contradicts Lemma 4.3 showing that
$W_2(\mu^*, \hat{\mu}) = \varepsilon > 0$. Thus, we can deploy Theorem 3.4 to conclude that at optimality there exists $\lambda \in \mathbb{R}$ such that for $\mu^*$-almost all $x \in \mathbb{R}^d$

$$w = 2\lambda \left( x - T_{\mu^*}^\hat{\mu}(x) \right).$$

As $w \neq 0$, $\lambda = 0$ is certainly not a solution. Thus, we have

$$T_{\mu^*}^\hat{\mu}(x) = x - \frac{1}{2\lambda}w.$$  

As $T_{\mu^*}^\hat{\mu}$ is invertible, Proposition 2.2 suggests that the optimal transport map from $\hat{\mu}$ to $\mu^*$ reads

$$T_{\mu^*}^\hat{\mu}(x) = x + \frac{1}{2\lambda}w.$$  

Note that, as a consequence, $\mu^*$ is absolutely continuous whenever $\hat{\mu}$ is absolutely continuous. Moreover,

$$\varepsilon^2 = W_2(\hat{\mu}, \mu^*)^2 = \int_{x \in \mathbb{R}^d} \left\| x - T_{\mu^*}^\hat{\mu}(x) \right\|^2 d\hat{\mu}(x) = \frac{1}{4\lambda^2} \|w\|^2.$$  

Hence, the Wasserstein ball constraint reduces to

$$\frac{1}{2\lambda} = \pm \frac{\varepsilon}{\|w\|},$$

and thus $T_{\mu^*}^\hat{\mu}(x) = x \pm \varepsilon \frac{w}{\|w\|}$. Overall, this gives

$$\mathbb{E}^\mu^* [\langle w, x \rangle] = \int_{x \in \mathbb{R}^d} \left\langle w, x \pm \frac{1}{2\lambda}w \right\rangle d\hat{\mu}(x) = \mathbb{E}^\hat{\mu} [\langle w, x \rangle] \pm \frac{1}{2\lambda} \|w\|^2.$$  

It is clearly optimal to pick $1/(2\lambda) = +\varepsilon/\|w\|$, which gives

$$T_{\mu^*}^\hat{\mu}(x) = x + \varepsilon \frac{w}{\|w\|}$$

and

$$J^* = \mathbb{E}^{\mu^*} [\langle w, x \rangle] = \mathbb{E}^\hat{\mu} [\langle w, x \rangle] + \varepsilon \|w\|.$$  

We can now use Corollary 3.9 to prove optimality of $\mu^* = (T_{\mu^*}^\hat{\mu}) \# \hat{\mu}$. Since $\lambda > 0$, $\mu^*$ is absolutely continuous (since $T_{\mu^*}^\hat{\mu}$ is invertible and $\hat{\mu}$ is absolutely continuous), and $-J$ is 0-convex along generalized geodesics (by Proposition 2.12), we directly have optimality and uniqueness of $\mu^*$.

In particular, (28) suggests that the DRO problem is equivalent to an explicit regularization scheme of the nominal cost $J(\hat{\mu})$. We refer to [56, 57, 58] for details on the interplay between DRO and explicit regularization.

### 4.2 Mean-Variance

Consider now the mean-variance functional

$$J(\mu) = \mathbb{E}^\mu [\langle w, x \rangle] + \rho \text{Var}^\mu [\langle w, x \rangle]$$

for some non-zero $w \in \mathbb{R}^d$ and finite $\rho > 0$. Among others, the risk measure (30) is widely used in portfolio selection problems [59, 60]. Being a non-linear functional of the measure, the duality result (25) does not apply and the mean-variance functional has received little attention in the context of DRO [61, 62]. We start by studying the properties of $J$:
Lemma 4.5 (Properties of $J$). The mean-variance functional $-J$ is continuous with respect to weak convergence and $(-2\rho\|w\|^2)$-convex along any interpolating curve.

**Proof.** Continuity w.r.t. weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$ follows from Proposition 2.12 and Corollary 2.14. For geodesic convexity, consider $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, $\gamma \in \Gamma(\mu_0, \mu_1)$, and $\mu_t = ((1-t)\text{proj}_1 + t \text{proj}_2)_\# \gamma$. Then,

$$-\text{Var}^{\mu_t}[\langle w, x \rangle]$$

$$= -\frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\langle w, x - y \rangle\|^2 d(\mu_t \times d\mu_t)(x, y)$$

$$= -\frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\langle w, (1-t)x + tx' - (1-t)y - ty' \rangle\|^2 d\gamma(x, x')d\gamma(y, y')$$

$$= -\frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} (1-t)\|\langle w, x - y \rangle\|^2 + t\|\langle w, x' - y' \rangle\|^2 d\gamma(x, x')d\gamma(y, y')$$

$$+ \frac{1}{2} t(1-t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\langle w, x - x' - y + y' \rangle\|^2 d\gamma(x, x')d\gamma(y, y')$$

$$= - (1-t) \text{Var}^{\mu_0}[\langle w, x \rangle] - t \text{Var}^{\mu_1}[\langle w, x \rangle]$$

$$+ \frac{1}{2} t(1-t) \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\langle w, x - x' \rangle\|^2 d\gamma(x, x') + \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\langle w, y - y' \rangle\|^2 d\gamma(y, y') \right)$$

$$- \frac{1}{2} t(1-t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} 2\langle w, x - x' \rangle \langle w, y - y' \rangle d\gamma(x, x')d\gamma(y, y')$$

$$\leq - (1-t) \text{Var}^{\mu_0}[\langle w, x \rangle] - t \text{Var}^{\mu_1}[\langle w, x \rangle] + t(1-t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\langle w, x - x \rangle\|^2 d\gamma(x, x')$$

$$\geq - (1-t) \text{Var}^{\mu_0}[\langle w, x \rangle] - t \text{Var}^{\mu_1}[\langle w, x \rangle] + \|w\|^2 t(1-t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - x'\|^2 d\gamma(x, x'),$$

where in $\Diamond$ we used

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle w, x - x' \rangle \langle w, y - y' \rangle d\gamma(x, x')d\gamma(y, y') = \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle w, x - x' \rangle d\gamma(x, x') \right)^2 \geq 0,$$

and in $\heartsuit$ we used the Cauchy-Schwarz inequality [51, Theorem 4.2]. Since $\mathbb{P}^\mu[\langle w, x \rangle]$ is 0-convex (by Proposition 2.12), $-J$ is $(-2\rho\|w\|^2)$-convex along any interpolating curve. $\square$

**Remark 4.1.** In this case, we cannot resort to lower semi-continuity and compactness w.r.t. narrow convergence to prove existence of maximizers. Indeed, $-J$ is not lower semi-continuous w.r.t. narrow convergence. Consider $d = 1$, $w = 1$, and $\rho = 1$. Let $\mu_n := (1 - \frac{1}{n})\delta_0 + \frac{1}{n}\delta_n$, narrowly converging to $\delta_0$. Then, $\liminf_{n \to \infty} -J(\mu_n) = \liminf_{n \to \infty} -1 - (n - 1)^2 = -\infty$, but $-J(\delta_0) = 0$. So, $\liminf_{n \to \infty} -J(\mu_n) \nleq -J(\delta_0)$. $\triangle$

Second, we show that, if they exist, worst-case probability measures lie at the boundary:

**Lemma 4.6** (Existence of a maximizer at the boundary). Assume that there exists a worst-case probability measure $\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ attaining the supremum (26). Then, $\mu^*$ lies on the boundary of the Wasserstein ball; i.e., $W_2(\hat{\mu}, \mu^*) = \varepsilon$.

**Proof.** Assume, for the sake of contradiction, that there exists a locally optimal $\mu^* \in \mathcal{P}_2(\mathbb{R}^d)$ which is strictly feasible; i.e., $W_2(\mu^*, \hat{\mu}) < \varepsilon$. We start by computing gradients, to then apply Theorem 3.1. By Proposition 2.12 and Corollary 2.14, we have

$$\nabla_{\mu}J(\mu) = w + 2\rho w \left( \langle w, x - \mathbb{E}^{\mu^*} [x] \rangle \right) = w \left( 1 + 2\rho \left( \langle w, x - \mathbb{E}^{\mu^*} [x] \rangle \right) \right).$$
Then, by Theorem 3.1, \( \nabla_{\mu} J(\mu^*) \) must vanish at optimality; i.e., it necessarily holds

\[
\langle w, x \rangle = -\frac{1}{2\rho} + \mathbb{E}^{\mu^*}[\langle w, x \rangle]
\]  
(31)

for \( \mu^* \)-almost all \( x \in \mathbb{R}^d \). This is a contradiction: If (31) holds \( \mu^* \)-a.e., then \( \langle w, x \rangle \) is constant \( \mu^* \)-a.e.; say, \( \langle w, x \rangle = \alpha \in \mathbb{R} \) for \( \mu^* \)-almost all \( x \in \mathbb{R}^d \). Then, (31) reads

\[
\alpha = -\frac{1}{2\rho} + \int_{\mathbb{R}^d} \langle w, x \rangle \, d\mu^*(x) = -\frac{1}{2\rho} + \int_{\mathbb{R}^d} \alpha d\mu^*(x) = -\frac{1}{2\rho} + \alpha,
\]

which is a contradiction. Hence, the maximum (if it exists) lies at the boundary. \( \square \)

Armed with these lemmas, we can now deploy Theorems 3.4 and 3.8 to characterize optimal solutions. More specifically, we will now show that the evaluation of the worst-case probability measure amounts to computing the roots of a fourth-order polynomial:

**Proposition 4.7 (Optimal solution of mean-variance DRO).** Consider problem (25) with the mean-variance cost functional (30). Assume \( \hat{\mu} \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d) \) is absolutely continuous with respect to the Lebesgue measure. Then, the worst-case probability measure is unique, and it is given by \( \mu^* = T_\# \hat{\mu} \), where

\[
T(x) = \left( I + \frac{\rho}{1 - \frac{\rho}{\lambda^*} \|w\|^2} w w^\top \right) x + \left( \frac{1}{2\lambda^*} - \frac{\rho}{1 - \frac{\rho}{\lambda^*} \|w\|^2} \mathbb{E}^\hat{\mu}[\langle w, x \rangle] \right) w,
\]

where \( \lambda^* \) is the unique real root strictly larger than \( \rho \|w\|^2 \) of the fourth-order polynomial

\[
\lambda^4 - 2\rho \|w\|^2 \lambda^3 + \left( \frac{\rho^2 \|w\|^2}{\varepsilon^2} \text{Var}^\hat{\mu}[\langle w, x \rangle] - \|w\|^2 \frac{4\varepsilon^2}{\rho^2} + \rho^2 \|w\|^4 \right) \lambda^2 + \rho \|w\|^4 \frac{2\varepsilon^2}{\rho^2} - \frac{\rho^2 \|w\|^6}{4\varepsilon^2}.
\]

The resulting worst-case cost reads

\[
J^* = \mathbb{E}^\hat{\mu}[\langle w, x \rangle] + \frac{1}{2\lambda^*} \|w\|^2 + \rho \left( \frac{1}{1 - \frac{\rho}{\lambda^*} \|w\|^2} \right)^2 \text{Var}^\hat{\mu}[\langle w, x \rangle].
\]

**Proof.** We split the proof in two parts. First, we assume enough regularity (in particular, absolute continuity of \( \mu^* \)) to use the necessary conditions for optimality to construct candidate solutions. Second, we use sufficient conditions for optimality to show that the probability measure built before is indeed optimal.

Let us assume that \( \mu^* \) exists and that it is absolutely continuous with respect to the Lebesgue measure. By Theorem 3.4, there exists \( \lambda \in \mathbb{R} \) such that

\[
w + 2\rho w \left( w, \text{Id} - \mathbb{E}^{\mu^*}[x] \right) = 2\lambda \left( \text{Id} - T_{\#}^{\mu^*} \right),
\]

where the gradient of \( J \) is computed as the in proof of Lemma 4.6, and the gradient of the Wasserstein distance stems from Corollary 2.11. In particular, (32) yields the affine optimal transport map

\[
T_{\#}^{\mu^*} = \left( \text{Id} + \frac{\rho}{\lambda} \frac{w w^\top}{\|w\|^2} \right) x - \frac{w}{2\lambda} + \frac{\rho}{\lambda} \mathbb{E}^{\mu^*}[\langle w, x \rangle] w,
\]

where \( A = A^\top \) and \( \text{spec}(A) = \{1, \ldots, 1, 1 - \frac{\rho}{\lambda} \|w\|^2 \} \). Since \( \mu^* \) is, by assumption, absolutely continuous, the optimal transport map \( T_{\#}^{\mu^*} \) is the gradient of a convex function, which implies \( \text{det}(A) \geq 0 \), and so \( \lambda \geq \rho \|w\|^2 \). Moreover, if \( \lambda = \rho \|w\|^2 \), then \( A \) is not invertible, which contradicts \( \hat{\mu} \) being absolutely
continuous (since all probability mass would be concentrated on a linear subspace, which has measure 0). Thus, \( \lambda > \rho \|w\|^2 \), \( A \) is invertible, and by Proposition 2.2:

\[
T_{\hat{\mu}}(x) = (T_{\hat{\mu}}^*)^{-1}(x) = A^{-1}x - A^{-1}b. \tag{33}
\]

It readily verified that

\[
A^{-1} = I + \frac{\rho}{\lambda} \|w\|^2 w w^T,
\]

well defined since \( 1 - \rho \|w\|^2 / \lambda > 0 \). By definition, \( A + \frac{\rho}{\lambda} w w^T = I \), so

\[
A^{-1}w = \left(1 + \frac{\rho}{\lambda} \|w\|^2\right) w = \frac{1}{1 - \frac{\rho}{\lambda} \|w\|^2} w. \tag{34}
\]

By definition of \( b \), we have

\[
b = -\frac{w}{2\lambda} + \frac{\rho}{\lambda} E_{\hat{\mu}}^* [\langle w, x \rangle] w
\]

\[
= -\frac{w}{2\lambda} + \frac{\rho}{\lambda} E_{\hat{\mu}}^* \left[\langle w, T_{\hat{\mu}}^*(x) \rangle\right] w
\]

\[
= -\frac{w}{2\lambda} + \frac{\rho}{\lambda} \left( E_{\hat{\mu}}^* [\langle w, A^{-1}x \rangle] - \langle w, A^{-1}b \rangle \right) w,
\]

\[
= -\frac{w}{2\lambda} + \frac{\rho}{\lambda} \left( E_{\hat{\mu}}^* [\langle A^{-1}w, x \rangle] - \langle A^{-1}w, b \rangle \right) w
\]

\[
= -\frac{w}{2\lambda} + \frac{\rho}{\lambda} \left( w w^T A^{-1}w \right) w - \frac{\rho}{\lambda} w w^T A^{-1}b
\]

\[
\triangleq -\frac{w}{2\lambda} + \frac{\rho}{1 - \frac{\rho}{\lambda} \|w\|^2} E_{\hat{\mu}}^* [\langle w, x \rangle] w + b - A^{-1}b,
\]

where in \( \diamond \) we used

\[
\frac{\rho}{\lambda} w w^T A^{-1} = \frac{\rho}{\lambda} w (A^{-1}w)^T = \frac{\rho}{1 - \frac{\rho}{\lambda} \|w\|^2} w w^T = I - A^{-1}.
\]

Thus,

\[
A^{-1}b = -\frac{w}{2\lambda} + \frac{\rho}{1 - \frac{\rho}{\lambda} \|w\|^2} E_{\hat{\mu}}^* [\langle w, x \rangle] w. \tag{35}
\]

Thus,

\[
\varepsilon^2 = W_2(\hat{\mu}, \mu^*)^2
\]

\[
= \int_{\mathbb{R}^d} \|x - (A^{-1}x - A^{-1}b)\|^2 d\hat{\mu}(x)
\]

\[
= \int_{\mathbb{R}^d} \| (I - A^{-1})x + A^{-1}b\|^2 d\hat{\mu}(x)
\]

\[
= \int_{\mathbb{R}^d} \left\| -\frac{\rho}{\lambda} w w^T A^{-1}x + A^{-1}b \right\|^2 d\hat{\mu}(x)
\]

\[
= \int_{\mathbb{R}^d} \left\| \frac{\rho}{1 - \frac{\rho}{\lambda} \|w\|^2} \langle w, x \rangle w + A^{-1}b \right\|^2 d\hat{\mu}(x) \tag{36}
\]

\[
= \int_{\mathbb{R}^d} \left( \frac{\rho}{1 - \frac{\rho}{\lambda} \|w\|^2} \right)^2 \text{Var}^\hat{\mu} [\langle w, x \rangle] + \frac{\rho}{1 - \frac{\rho}{\lambda} \|w\|^2} \left( \int_{\mathbb{R}^d} \langle w, x \rangle d\hat{\mu}(x) - E_{\hat{\mu}}^* [\langle w, x \rangle] \right)^2 + \|w\|^2 / 4\lambda^2
\]

\[
= \left( \frac{\rho \|w\|^2}{1 - \frac{\rho}{\lambda} \|w\|^2} \right)^2 \text{Var}^\hat{\mu} [\langle w, x \rangle] + \|w\|^2 / 4\lambda^2.
\]

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Finally, we multiply (36) by $\lambda^2 (1 - \frac{x}{\lambda} ||w||^2)^2/\varepsilon^2$ and rearrange to obtain the fourth-order polynomial equation $f(\lambda) = 0$ with

$$f(\lambda) := \lambda^4 - 2\rho ||w||^2 \lambda^2 + \left( -\frac{\rho^2 ||w||^2}{\varepsilon^2} \Var^\mu [(w, x)] - \frac{||w||^2}{4\varepsilon^2} + \rho^2 ||w||^4 \right) \lambda^2 + \frac{\rho ||w||^4}{2\varepsilon^2} - \lambda - \frac{\rho^2 ||w||^6}{4\varepsilon^2}.$$ 

To ease the notation, let

$$\Lambda := \{ \lambda \in \mathbb{R} \setminus [0, \rho ||w||^2] : f(\lambda) = 0 \}.$$ 

The set $\Lambda$ contains all real roots of $f$ such that $1 - \rho ||w||^2/\lambda > 0$. Values of $\lambda \in [0, \rho ||w||^2]$ would contradict the optimality of the transport map. Clearly, $|\Lambda| \leq 4$: we will now prove $\Lambda$ is non-empty. First, $f(\lambda) \to +\infty$ as $\lambda \to +\infty$. Second, $f(\lambda) \to -\rho^2 ||w||^6/(4\varepsilon^2) < 0$ for $\lambda \uparrow 0$. Third, $f(\lambda) \to -||w||^6 \rho^4 \Var^\mu [(w, x)]/\varepsilon^2 < 0$ (since $\hat{\mu}$ is absolutely continuous, $\Var^\hat{\mu} [(w, x)] > 0$) for $\lambda \downarrow \rho ||w||^2 > 0$. So, by the intermediate value theorem, $\Lambda$ is non-empty and $|\Lambda| \geq 2$: one strictly negative root and one root strictly larger than $\rho ||w||^2$. The resulting cost is

$$J^* = J^*(\mu^*) = \mathbb{E}^\mu^* [(w, x)] + \rho \Var^\mu^* [(w, x)]$$

$$= \mathbb{E}^\mu \left[ (w, A^{-1} x - A^{-1} b) \right] + \rho \Var^\hat{\mu} \left[ (w, A^{-1} x - A^{-1} b) \right]$$

$$= \mathbb{E}^\mu \left[ (w, A^{-1} x) \right] - \langle w, A^{-1} b \rangle + \rho \int_{\mathbb{R}^d} \left( w, A^{-1} x - A^{-1} b - A^{-1} \mathbb{E}^\mu \left[ x \right] + A^{-1} b \right)^2 d\hat{\mu}(x)$$

$$= \mathbb{E}^\mu \left[ (w, A^{-1} x) \right] + \frac{||w||^2}{2\lambda} - \frac{\rho^2 ||w||^2}{1 - \frac{\rho}{\lambda} ||w||^2} \Var^\mu \left[ (w, x) \right] + \rho \int_{\mathbb{R}^d} \left( A^{-1} w - \mathbb{E}^\mu \left[ x \right] \right)^2 d\hat{\mu}(x)$$

$$= \mathbb{E}^\mu \left[ (w, x) \right] + \frac{||w||^2}{2\lambda} + \rho \left( \frac{1}{1 - \frac{\rho}{\lambda} ||w||^2} \right)^2 \Var^\mu \left[ (w, x) \right].$$

By inspection, any negative $\lambda \in \Lambda$ cannot be optimal, as strictly outperformed by $\lambda > \rho ||w||^2$. In particular, our candidate for optimality is $\lambda^* = \max \Lambda$. To show that $\lambda^* > \rho ||w||^2$ is indeed optimal, we will use sufficient conditions. From above, there exists $\mu^*$ absolutely continuous and $\lambda > \rho ||w||^2$ such that

$$-\nabla_{\mu} J^*(\mu^*) = \lambda \nabla_{\mu} W_2(\mu^*, \hat{\mu})^2.$$ 

Thanks to Lemma 4.5 and Theorem 3.8, $\mu^*$ is the unique global minimizer. In particular, this also proves that $\Lambda$ contains at most one root strictly larger than $\rho ||w||^2$; else, we would contradict uniqueness. \qed

Remark 4.2. When $\rho \to 0$, $\lambda^* = 1/(2\varepsilon)$ and we recover the results of Section 4.1. Conversely, when $\rho \to \infty$, $\lambda^*/\rho = ||w||^2 \pm ||w|| \std^\hat{\mu} [(w, x)]/\varepsilon$, and

$$\frac{J^*}{\rho} = \left( \std^\hat{\mu} [(w, x)] + \varepsilon ||w|| \right)^2,$$ 

where $\std^\hat{\mu} [(w, x)] := \sqrt{\Var^\hat{\mu} [(w, x)]}$ is the standard deviation of $(w, x)$. This is again a form of explicit regularization. \triangle

Our results are in agreement with [61, Appendix C], and additionally fully characterize the worst-case probability measure and prove its uniqueness. Differently from [61], we do not base our analysis
on structural ambiguity sets consisting of all semidefinite affine pushforwards of the center \( \hat{\mu} [61, \text{Definitions 6}] \), but we work in the “full” probability space \( \mathcal{P}_2(\mathbb{R}^d) \). Accordingly, the fact that here and below worst-case probability measures sometimes happen to be positive semidefinite affine pushforward of \( \hat{\mu} \) is not stipulated ex ante, but emerges naturally from our optimality conditions. In [62], instead, the mean-variance functional is replaced the variance and a lower bound on the worst-case mean.

### 4.3 Mean-Standard Deviation

Consider now the mean-standard deviation functional

\[
J(\mu) = \mathbb{E}^\mu [\langle w, x \rangle] + \rho \text{std}^\mu [\langle w, x \rangle] = \mathbb{E}^\mu [\langle w, x \rangle] + \rho \sqrt{\text{Var}^\mu [\langle w, x \rangle]}
\]

for some non-zero \( w \in \mathbb{R}^d \) and \( \rho > 0 \). Also this risk measure found application in portfolio theory [63]. Due to its nonlinearity, the mean-standard deviation functional has not been studied in the context of DRO, with the exception of [61] which provides an upper bound (so-called Gelbrich risk) on the worst-case cost. First, we study properties of \( J \):

**Lemma 4.8** (Properties of \( J \)). The mean-standard deviation cost functional \(-J\) is continuous with respect to weak convergence. Moreover, for all \( \mu \in \hat{B}_c(\hat{\mu}) \)

\[
J(\mu) \leq J(\hat{\mu}) + \varepsilon \|w\| \sqrt{1 + \rho^2}.
\]

**Proof.** Continuity follows from Proposition 2.12 and Corollary 2.14, together with continuity of \( x \mapsto -\sqrt{x} \). To prove the upper bound, let \( \mu \in \hat{B}_c(\hat{\mu}) \) be arbitrary. Then,

\[
\begin{align*}
J(\mu) &= \mathbb{E}^\mu [\langle w, x \rangle] + \rho \text{std}^\mu [\langle w, x \rangle] \\
&= \langle w, \mathbb{E}^\mu [x] \rangle + \rho \sqrt{\mathbb{E}^\mu [\text{Var}^\mu [x]] w} \\
&\leq \langle w, \mathbb{E}^{\hat{\mu}} [x] \rangle + \|w\| \|\mathbb{E}^\mu [x] - \mathbb{E}^{\hat{\mu}} [x]\| \\
&\quad + \rho \|\text{Var}^\mu [x]^{1/2} w\| + \rho \|w\| \|\text{Var}^{\hat{\mu}} [x]^{1/2} - \text{Var}^{\hat{\mu}} [x]^{1/2}\| \\
&\leq J(\hat{\mu}) + \|w\| \left( \|\mathbb{E}^\mu [x] - \mathbb{E}^{\hat{\mu}} [x]\| + \rho \|\text{Var}^\mu [x]^{1/2} - \text{Var}^{\hat{\mu}} [x]^{1/2}\| \right) \\
&= J(\hat{\mu}) + \|w\| \left( \|\mathbb{E}^\mu [x] - \mathbb{E}^{\hat{\mu}} [x]\| + \rho \|\text{Var}^\mu [x]^{1/2} - \text{Var}^{\hat{\mu}} [x]^{1/2}\| \right) \\
&\leq J(\hat{\mu}) + \|w\| \sqrt{1 + \rho^2} \sqrt{\|\mathbb{E}^\mu [x] - \mathbb{E}^{\hat{\mu}} [x]\|^2 + \|\text{Var}^\mu [x]^{1/2} - \text{Var}^{\hat{\mu}} [x]^{1/2}\|^2} \\
&\leq J(\hat{\mu}) + \|w\| \sqrt{1 + \rho^2} W_2(\mu, \hat{\mu}) \\
&\leq J(\hat{\mu}) + \varepsilon \|w\| \sqrt{1 + \rho^2},
\end{align*}
\]

where

- in \( \triangle \) we use Cauchy-Schwarz inequality [51, Theorem 4.2];
- in \( \square \) we use that the Frobenius norm \( \|\|_\text{Fro} \) of a matrix upper bounds its induced norm \( \|\| \) [64];
- in \( \heartsuit \) we use that \( \sqrt{a^2 + b^2} \geq \frac{a + c b}{\sqrt{1 + c^2}} \) for all non-negative \( a, b, c \in \mathbb{R}_{\geq 0} \).

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• in ◊ we use Gelbrich bound [65]: If \( \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d) \) with mean \( m_1, m_2 \in \mathbb{R}^d \) and covariance matrix \( \Sigma_1, \Sigma_2 \in \mathbb{R}^d \times \mathbb{R}^d \), with \( \Sigma_1, \Sigma_2 \) symmetric and positive semi-definite, then,

\[
W_2(\mu, \nu) \geq \sqrt{\|m_1 - m_2\|^2 + \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_{\text{Fro}}}.
\]

where \( \Sigma_1^{1/2} \in \mathbb{R}^{d \times d} \) is the unique matrix such that \( (\Sigma_1^{1/2})^2 = \Sigma \) and \( \|\cdot\|_{\text{Fro}} \) is the Frobenius norm.

\[\square\]

\textbf{Remark 4.3.} Again, \(-J\) is not lower semi-continuous w.r.t. narrow convergence. The proof (by counter-example) is identical the one of the mean-variance functional (Remark 4.1). \(\triangle\)

Second, we show that, if they exist, worst-case probability measures lie at the boundary:

\textbf{Lemma 4.9 (Existence of a maximizer at the boundary).} Assume that there exists a worst-case probability measure \( \mu^* \) attaining the supremum (26). Then, \( \mu^* \) lies on the boundary of the Wasserstein ball; i.e., \( W_2(\hat{\mu}, \mu^*) = \varepsilon \).

\textbf{Proof.} The proof is identical to the proof of Lemma 4.6. \(\square\)

Armed with these results, we can now study optimal solutions:

\textbf{Proposition 4.10 (Optimal solution of mean-standard deviation DRO).} Consider problem (25) with the mean-standard deviation cost functional (38). Assume that \( \hat{\mu} \in \mathcal{P}_{2,\text{abs}}(\mathbb{R}^d) \) is absolutely continuous with respect to the Lebesgue measure. Then, the worst-case probability measure is given by \( \mu^* = T_{\#}\hat{\mu} \), where

\[
T(x) = \left( I + \frac{\rho \varepsilon}{\|w\|\sqrt{1 + \rho^2 \text{std}^2 \mu^* \langle w, x \rangle}} \right) x + \left( 1 - \frac{\rho \hat{\mu} \langle w, x \rangle}{\text{std}^2 \mu^* \langle w, x \rangle} \right) \frac{\varepsilon}{\sqrt{1 + \rho^2 \|w\|^2}} w,
\]

and the resulting worst-case cost reads

\[
J^* = \mathbb{E}^{\hat{\mu}} \langle w, x \rangle + \rho \text{std}^2 \mu^* \langle w, x \rangle + \varepsilon \|w\| \sqrt{1 + \rho^2} = J(\hat{\mu}) + \varepsilon \|w\| \sqrt{1 + \rho^2}.
\]

\textbf{Proof.} Again, we assume sufficient regularity to use necessary conditions for optimality to construct a solution. We will then prove that this solution is indeed optimal.

Let us assume that \( \mu^* \) exists and that it is absolutely continuous. By Theorem 3.4, there exists \( \lambda \in \mathbb{R} \) such that

\[
w + \frac{\rho}{\text{std}^2 \mu^* \langle w, x \rangle} w  \left( w, \mathbb{E}^{\mu^*} \langle w, x \rangle \right) = 2\lambda \left( \text{Id} - T_{\#}^\mu \right),
\]

where we used Proposition 2.12 and Corollaries 2.11 and 2.14, together with the chain rule of Proposition 2.9, to compute gradients. By assumption, \( \mu^* \) is absolutely continuous, and so \( \text{std}^2 \mu^* \langle w, x \rangle > 0 \). In particular, (41) yields the optimal transport map

\[
T_{\#}^\mu(x) = \left( \text{Id} - \alpha w w^\top \right) x - \frac{w}{2\lambda} + \alpha \mathbb{E}^{\mu^*} \langle w, x \rangle w,
\]

where \( \alpha := \frac{\rho}{2\lambda \text{std}^2 \mu^* \langle w, x \rangle} \) and \( A = A^\top \) and spec(\( A \)) = \{1, \ldots, 1, 1 - \alpha \|w\|^2 \}. Since \( \mu^* \) is, by assumption, absolutely continuous, the optimal transport map \( T_{\#}^\mu \) is the gradient of a convex function, and \( 1 - \alpha \|w\|^2 \geq 0 \). Moreover, if \( 1 - \alpha \|w\|^2 = 0 \), then \( A \) is not invertible, which contradicts \( \hat{\mu} \) being absolutely
continuous (since all probability mass would be concentrated on a linear subspace, which has measure 0). Thus, by Proposition 2.2,

$$T^{\mu^*}(x) = (T^{\hat{\mu}})^{-1}(x) = A^{-1}x - A^{-1}b.$$  \hfill (43)

It is readily verified that

$$A^{-1} = I + \frac{\alpha}{1 - \alpha\|w\|^2}ww^\top,$$

well defined since $1 - \alpha\|w\|^2 > 0$. Thus,

$$A^{-1}w = \left(1 + \frac{\alpha\|w\|^2}{1 - \alpha\|w\|^2}\right)w = \frac{1}{1 - \alpha\|w\|^2}w$$  \hfill (44)

and

$$\text{std}^{\mu^*}[\langle w, x \rangle] = \sqrt{w^\top A^{-1} \text{Var} \hat{\mu} [x] A^{-1}w} = \frac{1}{1 - \alpha\|w\|^2} \text{std} \hat{\mu} [\langle w, x \rangle]$$  \hfill (45)

Thus, the definition and (45) yield

$$\alpha = \frac{\rho}{2\lambda \text{std}^\mu [\langle w, x \rangle]} = \frac{\rho}{2\lambda \text{std} \hat{\mu} [\langle w, x \rangle]}(1 - \alpha\|w\|^2),$$

which gives

$$\alpha = \frac{\rho}{2\lambda \text{std} \hat{\mu} [\langle w, x \rangle] + \rho\|w\|^2}$$  \hfill (46)

and

$$1 - \alpha\|w\|^2 = \frac{2\lambda \text{std} \hat{\mu} [\langle w, x \rangle]}{2\lambda \text{std}^\mu [\langle w, x \rangle] + \rho\|w\|^2} > 0.$$

Thus,

$$A = I - \frac{\rho}{2\lambda \text{std} \hat{\mu} [\langle w, x \rangle] + \rho\|w\|^2}ww^\top.$$  

Similarly,

$$b = \frac{w}{2\lambda} + \alpha \text{E}^{\mu^*}[\langle w, x \rangle]w$$

$$= \frac{w}{2\lambda} + \alpha \left(\text{E}^{\hat{\mu}}[\langle w, A^{-1}x \rangle] - \langle w, A^{-1}b \rangle\right)w$$

$$= \frac{w}{2\lambda} + \alpha \left(\text{E}^{\hat{\mu}}[\langle A^{-1}w, x \rangle] - \langle A^{-1}w, b \rangle\right)w$$

$$= \frac{w}{2\lambda} + \alpha \frac{1 - \alpha\|w\|^2}{\text{E}^{\hat{\mu}}[\langle w, x \rangle]}w - \alpha ww^\top A^{-1}b$$

$$= \frac{w}{2\lambda} + \alpha \frac{1 - \alpha\|w\|^2}{\text{E}^{\hat{\mu}}[\langle w, x \rangle]}w + b - A^{-1}b,$$

and so

$$A^{-1}b = -\frac{w}{2\lambda} + \frac{\alpha}{1 - \alpha\|w\|^2} \text{E}^{\hat{\mu}}[\langle w, x \rangle]w$$

$$= -\frac{w}{2\lambda} + \frac{\rho}{2\lambda \text{std} \hat{\mu} [\langle w, x \rangle]} \text{E}^{\hat{\mu}}[\langle w, x \rangle]w.$$  

We can now evaluate the constraint $W_2(\hat{\mu}, \mu^*)$ to find an expression for $\lambda$. We can proceed as in (36) to obtain

$$\epsilon^2 = W_2(\hat{\mu}, \mu^*)^2 = \frac{1}{4\lambda^2}\|w\|^2(1 + \rho^2),$$

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and so $\lambda^* = \pm \frac{1}{2\varepsilon} \|w\| \sqrt{1 + \rho^2}$. The resulting worst-case cost reads

$$J^* = J(\mu^*) = E^\mu^* [(w, x)] + \rho \text{std}^\mu^* [(w, x)]$$

$$= E^\hat{\mu} [(w, A^{-1}x - A^{-1}b)] + \rho \text{std}^\mu [(w, x)]$$

$$= E^\hat{\mu} [(w, A^{-1}x)] - (w, A^{-1}b) + \frac{2\lambda^* \text{std}^\hat{\mu} [(w, x)] + \rho^2 \|w\|^2}{2\lambda^*}$$

$$= \frac{2\lambda^* \text{std}^\hat{\mu} [(w, x)] + \rho^2 \|w\|^2}{2\lambda^*}$$

$$+ \frac{\|w\|^2}{2\lambda^*} - \frac{\rho \|w\|^2}{2\lambda^* \text{std}^\hat{\mu} [(w, x)]} E^\mu [(w, x)] + \frac{2\lambda^* \text{std}^\hat{\mu} [(w, x)] + \rho^2 \|w\|^2}{2\lambda^*}$$

$$= E^\mu [(w, x)] + \text{std}^\mu [(w, x)] + \frac{1}{2\lambda^*} \|w\|^2(1 + \rho^2).$$

It is clearly optimal to select $\lambda^* = \pm \frac{1}{2\varepsilon} \|w\| \sqrt{1 + \rho^2}$. The resulting worst-case cost reads

$$J^* = J(\mu^*) = E^\mu^* [(w, x)] + \text{std}^\mu [(w, x)] + \varepsilon \|w\| \sqrt{1 + \rho^2}.$$

To prove that $\mu^*$ is indeed optimal, it suffices to observe that it attains the (a priori) upper bound (39).

As in Section 4.1, (40) suggests that (26) coincides with an explicit regularization scheme.

## 5 Minimum Entropy on Wasserstein Balls

Consider the optimization problem

$$\inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \{ \text{KL}(\mu | \mu_p) : W_2(\mu, \mu_r) \leq \varepsilon \},$$

with prior probability measure $\mu_p \in \mathcal{P}_2(\mathbb{R}^d)$ and reference probability measure $\mu_r \in \mathcal{P}_2(\mathbb{R}^d)$. The optimization problem (47) combines the well-known Kullback’s principle of minimum cross-entropy [6, 7, 8] in statistical inference with additional side information, encoded in the probability measure $\mu_r$ [66]. For instance, in [66], $\mu_r$ is chosen to be the empirical probability measure $\hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i}$ constructed with $N$ data points $\{(x_i)\}_{i=1}^{N}$, while $\mu_p$ is a strictly positive probability measure on a compact subset of $\mathbb{R}^d$. Here, we study optimality conditions for (47). We assume that $\mu_p = e^{-V_p \mathcal{L}^d}$ and $\mu_r = e^{-V_r \mathcal{L}^d}$ for some $V_p : \mathbb{R}^d \rightarrow \mathbb{R}$ and $V_r : \mathbb{R}^d \rightarrow \mathbb{R}$ convex and continuously differentiable. To start, we show that a minimizer exists:

**Lemma 5.1 (Existence).** The optimization problem (47) has a solution. Moreover, any minimizer $\mu^*$ is absolutely continuous.

**Proof.** The proof follows by lower semi-continuity of the KL divergence (Proposition 2.16) and compactness of Wasserstein balls (Proposition 4.2) w.r.t. narrow convergence. Since the KL divergence evaluates to infinity for non-absolutely continuous measures, the minimizer is necessarily absolutely continuous. 

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Without loss of generality, we assume that the minimizer lies on the boundary; else, we trivially have \( \mu^* = \mu_p \). Then, Theorem 3.1 leads to the following optimality condition, which yields to an (almost) closed-form solution when \( \mu_p \) and \( \mu_t \) are Gaussian:

**Proposition 5.2 (Conditions for optimality).** Consider problem (47), and let \( \mu^* = \rho^* \mathcal{L}^d \in \mathcal{P}_{2,\text{als}}(\mathbb{R}^d) \) be an optimal solution of (47). Then, there exists \( \lambda \in \mathbb{R} \) such that

\[
\nabla V_p - \nabla T_{\mu^*}^{\mu^*}(\nabla V_t \circ T_{\mu^*}^{\mu^*}) + \text{tr} \left( (\nabla T_{\mu^*}^{\mu^*})^{-1} \sum_{i=1}^d \frac{\partial}{\partial x_i} \nabla T_{\mu^*}^{\mu^*} \right) = 2\lambda (\text{Id} - T_{\mu^*}^{\mu^*}),
\]

provided all terms are well defined almost everywhere. In particular, if \( V_p(x) \) and \( V_t(x) \) are convex quadratic of the form \( V_p(x) = \frac{1}{2} x^T \Sigma_p^{-1} x - \langle \Sigma_p^{-1} m_p, x \rangle + C_p \) and \( V_t(x) = \frac{1}{2} x^T \Sigma_t^{-1} x - \langle \Sigma_t^{-1} m_t, x \rangle + C_t \), where \( \Sigma_t, \Sigma_p \in \mathbb{R}^{d \times d} \) symmetric and positive definite, \( m_p, m_t \in \mathbb{R}^d \), and \( C_p, C_t \) chosen so that \( \mu_t \) and \( \mu_p \) are valid probability measures (that is, \( \mu_p, \mu_t \) are Gaussian with mean \( \mu_p, m_t \) and variance \( \Sigma_p, \Sigma_t \), respectively), then

\[
\mu^* = (A^{-1} x - (\Sigma_p^{-1} - 2\lambda^* I)^{-1}(\Sigma_p^{-1} m_p - A \Sigma_t^{-1} m_t))_{\#} \mu_t,
\]

where \( A \in \mathbb{R}^{n \times n} \) symmetric and positive definite and \( \lambda^* \leq 0 \) are the unique solutions of

\[
e^2 = \text{tr} \left( (I - A^2)^{-1}(\Sigma_t + m_t m_t^T) \right) + 2 \langle (I - A^{-1})(\Sigma_p^{-1} - 2\lambda^* I)^{-1}(\Sigma_p^{-1} m_p - A \Sigma_t^{-1} m_t), m_t \rangle \\
+ \| (\Sigma_p^{-1} - 2\lambda^* I)^{-1}(\Sigma_p^{-1} m_p - A \Sigma_t^{-1} m_t) \|^2,
\]

\[
0 = 2\lambda A - A \Sigma_t^{-1} A + \Sigma_p^{-1} - 2\lambda I.
\]

Moreover, \( \mu^* \) is unique and Gaussian.

**Proof.** By Proposition 2.16 (and Example 2.4), with \( \mu^* = \rho^* \mathcal{L}^d \), we have

\[
\nabla_\mu \text{KL}(\mu^*|\mu_p) = \frac{\nabla \rho^*}{\rho^*} + \nabla V_p.
\]

Since both \( \mu_t \) and \( \mu^* \) are absolutely continuous, [27, Proposition 6.2.12] gives \( \nabla T_{\mu^*}^{\mu^*}(x) > 0 \) \( \mu^* \)-a.e.. Thus, the usual change of variables for integrals [27, Lemma 5.3.3] yields

\[
\det \nabla T_{\mu^*}^{\mu^*}(x) = \frac{\rho^*(x)}{\rho_t(T_{\mu^*}^{\mu^*}(x))}.
\]

Then,

\[
\frac{\nabla \rho^*(x)}{\rho^*(x)} = \frac{\nabla \left( \det \nabla T_{\mu^*}^{\mu^*}(x)\rho_t(T_{\mu^*}^{\mu^*}(x)) \right)}{\det \nabla T_{\mu^*}^{\mu^*}(x)\rho_t(T_{\mu^*}^{\mu^*}(x))} = \frac{\nabla \det \nabla T_{\mu^*}^{\mu^*}(x)}{\det \nabla T_{\mu^*}^{\mu^*}(x)} + \frac{\nabla (\rho_t(T_{\mu^*}^{\mu^*}(x)))}{\rho_t(T_{\mu^*}^{\mu^*}(x))} = \sum_{i=1}^d \text{tr} \left( (\nabla T_{\mu^*}^{\mu^*}(x))^{-1} \frac{\partial}{\partial x_i} \nabla T_{\mu^*}^{\mu^*}(x) \right) e_i - \nabla T_{\mu^*}^{\mu^*}(x) \nabla V_t(T_{\mu^*}^{\mu^*}(x)),
\]

where we used Jacobi’s formula [67] for the derivative of the determinant and

\[
\nabla \rho_t(T_{\mu^*}^{\mu^*}(x)) = \nabla \left( \rho_t(T_{\mu^*}^{\mu^*}(x)) \right) = -\nabla T_{\mu^*}^{\mu^*}(x) \nabla V_t(T_{\mu^*}^{\mu^*}(x)) \rho_t(T_{\mu^*}^{\mu^*}(x)) = -\nabla T_{\mu^*}^{\mu^*}(x) \nabla V_t(T_{\mu^*}^{\mu^*}(x)) \rho_t(T_{\mu^*}^{\mu^*}(x)).
\]
To deploy Theorem 3.1, we first need to prove there exists \( \varphi \in C^\infty_c(\mathbb{R}^d) \) such that
\[
2 \int_{\mathbb{R}^d} \left< T^{\mu^*}_{\mu^*} - \text{Id}, \nabla \varphi \right> \, d\mu^* \neq 0.
\]
As in Proposition 4.4, existence of such \( \varphi \) is easily proved by contradiction. Thus, since the derivative of the Wasserstein distance exists (by absolute continuity of \( \mu^* \)) and it reads as \( 2(\text{Id} - T^{\mu^*}_{\mu^*}) \), we get (48).

In the case of Gaussian probability measures, we first show that (48) admits a solution of the form \( T^{\mu^*}_{\mu^*}(x) = Ax + b \) for \( A \in \mathbb{R}^{d \times d} \) symmetric and positive definite and \( b \in \mathbb{R}^d \). In this case, by Proposition 2.3, the optimal transport from \( \mu_r \) to \( \mu^* \) is
\[
T^{\mu^*}_{\mu^*}(x) = (T^{\mu^*}_{\mu^*})^{-1}(x) = A^{-1}x - A^{-1}b. 
\]
Finally, we will use Corollary 3.9 to prove optimality. Since \( \nabla T^{\mu^*}_{\mu^*} = A \), (48) reduces to
\[
\Sigma_p^{-1}x - \Sigma_p^{-1}m_p - A(\Sigma_t^{-1}(Ax + b) - \Sigma_t^{-1}m_t) = 2\lambda(x - (Ax + b)) \quad \mu^*\text{-a.e.,}
\]
which, by the absolute continuity of \( \mu^* \), gives
\[
\Sigma_p^{-1} - A\Sigma_t^{-1}A = 2\lambda(I - A)
\]
\[
-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}b - A\Sigma_t^{-1}m_t = -2\lambda b.
\]
Basic algebraic manipulations then lead to
\[
0 = 2\lambda A - A\Sigma_t^{-1}A + \Sigma_p^{-1} - 2\lambda I, \quad (50a)
\]
\[
b = A(\Sigma_p^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t). \quad (50b)
\]
For any fixed \( \lambda \leq 0 \), the system of equations (50) fully characterizes \( A \) and \( b \). Indeed, (50a) is a continuous-time algebraic Riccati equation (with \( A = \lambda I \), \( N = \Sigma_t \), \( B = I \), and \( C = (\Sigma_p - 2\lambda I)^{1/2} \) in the notation in [68]). Thus, since \( (A, B) \) is stabilizable and \( (C, A) \) observable, there exists a unique positive definite solution \( A \in \mathbb{R}^{d \times d} \) for any \( \lambda \leq 0 \) [68, Theorem 4.1]. Moreover, for any \( \lambda \leq 0 \), \( \Sigma_p^{-1} - 2\lambda I \) is positive definite and thus invertible, and \( b \) is well defined by (50b). The Lagrange multiplier \( \lambda \) is then found by imposing \( W_2(\mu^*, \mu_t) = \varepsilon \):
\[
\int_{\mathbb{R}^d} \|x - (A^{-1}x - A^{-1}b)\|^2 \, d\mu_t(x) \\
= \int_{\mathbb{R}^d} \|(I - A^{-1})x + (\Sigma_p^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t)\|^2 \, d\mu_t(x) \\
= \text{tr} \left( (I - A^{-1})(\Sigma_t + m_tm_t^\top)(I - A^{-1}) \right) \]
\[
+ 2 \langle (\Sigma_p^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t), (I - A^{-1})m_t \rangle \\
+ \|((\Sigma_p^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t))\|^2 \\
= \text{tr} \left( (I - A^{-1})^2(\Sigma_t + m_tm_t^\top) \right) \]
\[
+ 2 \langle (I - A^{-1})(\Sigma_p^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t), m_t \rangle \\
+ \|((\Sigma_p^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t))\|^2 \\
= \varepsilon^2,
\]
where we used (49) to express the optimal transport map between $\mu_\tau$ and $\mu^*$. Equivalently, we look for the non-positive roots of

$$f(\lambda) := \int_{\mathbb{R}^d} \|x - (A^{-1}x - A^{-1}b)\|^2 d\mu_\tau(x) - \epsilon^2$$

$$= \text{tr} \left( (I - A^{-1})(\Sigma_\tau + m_\tau m_\tau^T) \right) + 2\langle (I - A^{-1})(\Sigma_t^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t), m_t \rangle$$

$$+ \|A\Sigma_t^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t)\|^2 - \epsilon^2. $$

We now prove that at least one negative root exists using the intermediate value theorem. Note that $f$ is continuous in $\lambda$, since $A$ is continuous $\lambda$, by (50a) and (50b). In particular, for $\lambda \to -\infty$ we have $A \to I$. Thus, $\lim_{\lambda \to -\infty} f(\lambda) = -\epsilon^2 < 0$. Conversely, for $\lambda = 0$, (50a) reads

$$A\Sigma_t^{-1}A = \Sigma_p^{-1}, \tag{51}$$

which has the unique positive definite solution

$$A = \Sigma_t^{1/2}(\Sigma_t^{-1/2}\Sigma_p\Sigma_t^{-1/2})^{1/2}\Sigma_t^{1/2} = \Sigma_t^{1/2}(\Sigma_t^{-1/2}\Sigma_p\Sigma_t^{-1/2})^{1/2}\Sigma_t^{1/2}. \tag{52}$$

Overall,

$$T_{\mu_\tau}^{\mu^*}(x) = (T_{\mu_\tau}^{\mu^*})^{-1}(x) \overset{(49)}{=} A^{-1}x - A^{-1}b$$

$$\overset{(50b)}{=} A^{-1}x - \Sigma_p(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t)$$

$$\overset{(51)}{=} A^{-1}x - \Sigma_p(-\Sigma_p^{-1}m_p + \Sigma_t^{-1}A^{-1}m_t)$$

$$= A^{-1}(x - m_t) + m_p$$

$$\overset{(52)}{=} \Sigma_t^{-1/2}(\Sigma_t^{1/2}\Sigma_p\Sigma_t^{1/2})^{1/2}\Sigma_t^{-1/2}(x - m_t) + m_p. $$

It is readily verified [38, Chapter 1.6.3] that $T_{\mu_\tau}^{\mu^*}$ coincides with the optimal transport map from $\mu_\tau$ to $\mu_p$. Thus, $\mu^* = \mu_p$. Since by assumption $W_2(\mu^*, \mu_p) > \epsilon$, we get

$$f(0) = W_2(\mu^*, \mu_\tau)^2 - \epsilon^2 = W_2(\mu_\tau, \mu_\tau)^2 - \epsilon^2 > 0.$$

Hence, the intermediate value theorem establishes the existence of $\lambda^* < 0$ so that $f(\lambda^*) = 0$. A candidate solution for optimality is therefore

$$\mu^* = (A^{-1}x - A^{-1}b)_{#\mu_\tau} \overset{(50b)}{=} (A^{-1}x - (\Sigma_p^{-1} - 2\lambda I)^{-1}(-\Sigma_p^{-1}m_p + A\Sigma_t^{-1}m_t))_{#\mu_\tau},$$

where $A$ and $b$ result from (50a) and (50b) with $\lambda = \lambda^*$, respectively. We can now deploy Corollary 3.9 to prove optimality. Since $\mu^*$ is absolutely continuous and the KL divergence is convex along generalized geodesics of (by Proposition 2.16), $\mu^*$ is indeed the unique globally optimal solution. As a byproduct of the uniqueness of $\mu^*$, we obtain uniqueness of $A$ and, by (50a), of $\lambda$. \hfill \Box

6 Conclusions

We studied first-order conditions for optimization in the Wasserstein space. We combined the geometric and differential properties of the Wasserstein space with classical calculus of variations to formulate first-order necessary and sufficient conditions for optimality, showing that simple and interpretable rationales (e.g., “set the gradient to zero” and “gradients are aligned at optimality”) carry over to the Wasserstein space. With our tools we can study and solve, sometimes in closed form, optimization problems in distributionally robust optimization and statistical inference. We hope our results will pave the way for future research on optimization in probability spaces through the lens of optimal transport.
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A Technical Preliminaries in Measure Theory

In this section, we provide some technical background in measure theory. We start with tightness:

**Definition A.1 (Tight).** A set of probability measures $\mathcal{K} \subset \mathcal{P}(\mathbb{R}^d)$ is tight if for all $\varepsilon > 0$ there exists a compact set $K_\varepsilon \subset \mathbb{R}^d$ such that $\mu(\mathbb{R}^d \setminus K_\varepsilon) \leq \varepsilon$ for all $\mu \in \mathcal{K}$.

A simple criterion for tightness is the following:

**Lemma A.1 (Criterion for tightness).** Let $\mathcal{K} \subset \mathcal{P}(\mathbb{R}^d)$. Suppose there exists $\Phi : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$ with compact level sets (i.e., $\{x \in \mathbb{R}^d : \Phi(x) \leq \lambda\}$ is compact for all $\lambda \in \mathbb{R}$) so that

$$\sup_{\mu \in \mathcal{K}} \int_{\mathbb{R}^d} \Phi(x) d\mu(x) < +\infty.$$  

Then, $\mathcal{K}$ is tight.

**Proof.** The statement can be found in [27, Remark 5.1.5]; we prove it for completeness. Let $\varepsilon > 0$, and let

$$C := \sup_{\mu \in \mathcal{K}} \int_{\mathbb{R}^d} \Phi(x) d\mu(x) < +\infty.$$  

Define $K_\varepsilon := \{x \in \mathbb{R}^d : \Phi(x) \leq C/\varepsilon\}$. Since $\Phi$ has compact level sets, $K_\varepsilon$ is compact. Then, for $\mu \in \mathcal{K}$

$$\mu(\mathbb{R}^d \setminus K_\varepsilon) = \int_{\mathbb{R}^d \setminus K_\varepsilon} d\mu(x)$$

$$\leq \int_{\mathbb{R}^d \setminus K_\varepsilon} \Phi(x) d\mu(x)$$

$$\leq \frac{\varepsilon}{C} \int_{\mathbb{R}^d} \Phi(x) d\mu(x)$$

$$\leq \varepsilon.$$

Since $\mu$ is arbitrary, we conclude. □

Tightness of a set is intimately related to its compactness (under narrow convergence):

**Theorem A.2 (Prokhorov [27, Theorem 5.1.3]).** A set $\mathcal{K} \subset \mathcal{P}(\mathbb{R}^d)$ is tight if and only if it is relatively compact for the narrow convergence.

As a consequence of Prokhorov theorem, if $(\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}(\mathbb{R}^d)$ is so that $\{\mu_n\}_{n \in \mathbb{N}}$ is tight, then $\mu_n$ admits a subsequence converging to some $\mu \in \mathcal{P}(\mathbb{R}^d)$.

Next, we focus on the narrow convergence of transport plans $\gamma_n \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$. In particular, we show convergence for the inner product $(x, y) \mapsto (x, y)$. Since this is unbounded functional, the statement does not follow directly from the definition of narrow convergence, and requires adequate assumptions:
Proposition A.3 ([27, Lemma 5.2.4]). Let \((\gamma_n)_{n \in \mathbb{N}} \subset \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)\) be narrowly converging to \(\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)\). Suppose that

\[
\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 \, d\gamma_n(x, y) < +\infty,
\]

and that either \((\text{proj}_1)_\# \gamma_n\) or \((\text{proj}_2)_\# \gamma_n\) have uniformly integrable second moment. Then,

\[
\lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle x, y \rangle \, d\gamma_n(x, y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle x, y \rangle \, d\gamma(x, y).
\]

Finally, we recall the celebrated Gluing Lemma:

Proposition A.4 (Gluing lemma [27, Lemma 5.3.2]). Let \(\gamma_{12}, \gamma_{13} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)\) so that \((\text{proj}_1)_\# \gamma_{12} = (\text{proj}_1)_\# \gamma_{13} = \mu_1 \in \mathcal{P}(\mathbb{R}^d)\). Then, there exists \(\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)\) such that

\[
(\text{proj}_{12})_\# \gamma = \gamma_{12},
\]

\[
(\text{proj}_{13})_\# \gamma = \gamma_{13}.
\]

Moreover, if \(\gamma_{12}\) or \(\gamma_{13}\) are induced by a transport, then \(\gamma\) is unique.

B Proofs

B.1 Proofs of the Statements

Proof of Proposition 2.2. By symmetry of the Wasserstein distance, it suffices to show

\[
W_2(\mu, \nu)^2 = \int_{\mathbb{R}^d} \| (T_\mu^\nu)^{-1}(y) - y \|^2 \, d\nu(y).
\]

Indeed,

\[
W_2(\mu, \nu)^2 = \int_{\mathbb{R}^d} \| x - T_\mu^\nu(x) \|^2 \, d\mu(x)
\]

\[
= \int_{\mathbb{R}^d} \| (T_\mu^\nu)^{-1}(T_\mu^\nu(x)) - T_\mu^\nu(x) \|^2 \, d\mu(x)
\]

\[
= \int_{\mathbb{R}^d} \| (T_\mu^\nu)^{-1}(y) - y \|^2 \, d((T_\mu^\nu)_\# \mu)(y)
\]

\[
= \int_{\mathbb{R}^d} \| (T_\mu^\nu)^{-1}(y) - y \|^2 \, d\nu(y).
\]

This concludes the proof.

Proof of Proposition 2.5. The proof of (9) follows from [27, Proposition 8.5.4, Eq. (8.4.4)]. Note that when \(\gamma\) is induced by a transport map, (9) also follows from \(T_\mu^\nu - \text{Id} \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d)\) (cf. Remark 2.2) and the definition of \(L^2\) inner product. Indeed, since \(\xi \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d)\) and \(T_\mu^\nu - \text{Id} \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d)\), by definition of the orthogonal complement we have

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x), y - x \rangle \, d((\text{Id}, T_\mu^\nu)_\# \mu)(x, y) = \int_{\mathbb{R}^d} \langle \xi(x), T_\mu^\nu(x) - x \rangle \, d\mu(x)
\]

\[
= \langle \xi, T_\mu^\nu - \text{Id} \rangle_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)}
\]

\[
= 0.
\]

To show uniqueness of Wasserstein gradients it suffices to show that \(\partial^- J(\mu) \cap \partial^+ J(\mu)\) contains at most one element in \(\text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d)\). Without loss of generality, assume \(\partial^- J(\mu) \cap \partial^+ J(\mu)\) is non-empty.
Let \( \xi, \xi' \in \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \cap \partial^- J(\mu) \cap \partial^+ J(\mu) \), and let \( \varepsilon > 0 \). Then, there exist \( \varphi_\varepsilon, \varphi'_\varepsilon \in C^\infty_c(\mathbb{R}^d) \) such that
\[
\|\xi - \nabla \varphi_\varepsilon\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)} < \frac{\varepsilon}{2}, \quad \|\xi' - \nabla \varphi'_\varepsilon\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)} < \frac{\varepsilon}{2}.
\]

Then, let \( \sigma := (\text{Id} + s \nabla \varphi_\varepsilon)_# \mu \) and \( \sigma' := (\text{Id} + s \nabla \varphi'_\varepsilon)_# \mu \). By Lemma 2.4, there is \( s > 0 \) sufficiently small such that \( \text{Id} + s \nabla \varphi_\varepsilon \) is an optimal transport map between \( \mu \) and \( \sigma \), and \( \text{Id} + s \nabla \varphi'_\varepsilon \) is an optimal transport map between \( \mu \) and \( \sigma' \). Thus, by definition of sub- and super-differentials
\[
J(\sigma) - J(\mu) \geq \int_{\mathbb{R}^d} \langle \xi, s \nabla \varphi_\varepsilon \rangle \, d\mu(x) + o(s)
\]
\[
-J(\sigma') + J(\mu) \geq \int_{\mathbb{R}^d} \langle -\xi, s \nabla \varphi'_\varepsilon \rangle \, d\mu(x) + o(s)
\]
\[
J(\sigma') - J(\mu) \geq \int_{\mathbb{R}^d} \langle \xi', s \nabla \varphi'_\varepsilon \rangle \, d\mu(x) + o(s)
\]
\[
-J(\sigma) + J(\mu) \geq \int_{\mathbb{R}^d} \langle -\xi', s \nabla \varphi_\varepsilon \rangle \, d\mu(x) + o(s).
\]

We can divide all inequalities by \( s \), sum them up, and let \( s \to 0 \) to get
\[
0 \geq \int_{\mathbb{R}^d} \langle \xi, \nabla \varphi_\varepsilon \rangle + \langle \xi', \nabla \varphi'_\varepsilon \rangle - \langle \xi, \nabla \varphi'_\varepsilon \rangle - \langle \xi', \nabla \varphi_\varepsilon \rangle \, d\mu(x) = \int_{\mathbb{R}^d} \langle \xi - \xi', \nabla \varphi_\varepsilon - \nabla \varphi'_\varepsilon \rangle \, d\mu(x). \tag{53}
\]

Thus,
\[
\|\xi - \xi'\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)} \leq \left( \|\xi - \xi'\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)}^2 - 2 \int_{\mathbb{R}^d} \langle \xi - \xi', \nabla \varphi_\varepsilon - \nabla \varphi'_\varepsilon \rangle \, d\mu(x) + \|\nabla \varphi_\varepsilon - \nabla \varphi'_\varepsilon\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)}^2 \right)^{\frac{1}{2}}
\]
\[
= \|\xi - \xi' - (\nabla \varphi_\varepsilon - \nabla \varphi'_\varepsilon)\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)}
\]
\[
\leq \|\xi - \nabla \varphi_\varepsilon\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)} + \|\xi' - \nabla \varphi'_\varepsilon\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)} < \varepsilon.
\]

Let \( \varepsilon \to 0 \) to conclude \( \xi = \xi' \). \hfill \Box

**Proof of Proposition 2.7.** Let \( (\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d) \) such that \( \mu_n \to \mu \), and let \( \gamma_n \in \Gamma_o(\mu, \mu_n) \). By differentiability,
\[
\limsup_{n \to \infty} |J(\mu_n) - J(\mu)| \leq \limsup_{n \to \infty} \left| \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \, d\gamma_n(x, y) \right| + |o(W_2(\mu_n, \mu))|
\]
\[
\leq \limsup_{n \to \infty} \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\nabla \mu J(\mu)(x)\|^2 \, d\gamma_n(x, y) \right)^{\frac{1}{2}} \left( \int_{\mathbb{R}^d} \|y - x\|^2 \, d\gamma_n(x, y) \right)^{\frac{1}{2}}
\]
\[
\leq \limsup_{n \to \infty} \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\nabla \mu J(\mu)(x)\|^2 \, d\mu(x) \right)^{\frac{1}{2}} W_2(\mu, \mu_n)
\]
\[
= \|\nabla \mu J(\mu)\|_{L^2(\mathbb{R}^d, \mathbb{R}^d, \mu)} \limsup_{n \to \infty} W_2(\mu_n, \mu),
\]
where the first inequality from Cauchy-Schwarz inequality in the Hilbert space \( L^2(\mathbb{R}^d, \mathbb{R}^d; \gamma_n) \) [51, Theorem 4.2]. Since the Wasserstein distance metrizes weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \), \( W_2(\mu_n, \mu) \to 0 \). Thus, we conclude \( \lim_{n \to \infty} J(\mu_n) = J(\mu) \), and thus continuity w.r.t. weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \). \hfill \Box
Proof of Proposition 2.6. We prove subdifferentiability; the proofs of superdifferentiability and thus differentiability are analogous. We conduct the proof by contradiction. Assume that there is $\delta > 0$ and a sequence $(\nu_n)_{n \in \mathbb{N}} \subset P_2(\mathbb{R}^d)$ and $\gamma_n \in \Gamma(\mu, \nu_n)$ so that

\[
\varepsilon_n := \sqrt{\int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 \, d\gamma_n(x, y)} \to 0
\]

and

\[
J(\nu_n) - J(\mu) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \, d\gamma_n(x, y) \leq -\delta \varepsilon_n. \tag{54}
\]

Then, let $\beta_n \in \Gamma_o(\mu, \nu_n)$ be an optimal transport plan between $\mu$ and $\nu_n$. By definition, $W_2(\mu, \nu_n) \leq \varepsilon_n \to 0$. By definition of subdifferential, there exists $N$ so that for all $n > N$ we have

\[
J(\nu_n) - J(\mu) \geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \, d\beta_n(x, y) - \frac{\delta}{2} \varepsilon_n. \tag{55}
\]

We can combine (54) and (55) to get

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \, d\beta_n(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \, d\gamma_n(x, y) \leq -\frac{\delta}{2} \varepsilon_n \tag{56}
\]

for all $n > N$. Let us now introduce the “rescaled” plans

\[
\hat{\gamma}_n := \left(\text{proj}_1, \frac{\text{proj}_2 - \text{proj}_1}{\varepsilon_n}\right)_\# \gamma_n,
\]

\[
\hat{\beta}_n := \left(\text{proj}_1, \frac{\text{proj}_2 - \text{proj}_1}{\varepsilon_n}\right)_\# \beta_n. \tag{57}
\]

Then, (56) can be rewritten to

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\hat{\beta}_n(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\hat{\gamma}_n(x, y) \leq -\frac{\delta}{2} \tag{58}
\]

for all $n > N$. We now claim that $\hat{\mu}_n$ and $\hat{\beta}_n$ converge narrowly (up to subsequences) to some $\hat{\mu}$ and $\hat{\beta}$ with finite second moment:

- Narrow convergence: We equivalently show that the sets $\{\hat{\gamma}_n\}_{n \in \mathbb{N}}$ and $\{\hat{\beta}_n\}_{n \in \mathbb{N}}$ are tight, which automatically establishes convergence to some $\hat{\gamma}$ and $\hat{\beta}$ by Prokhorov’s Theorem (Theorem A.2 in Appendix A). To show tightness it suffices to prove that

\[
\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 \, d\hat{\gamma}_n(x, y) < +\infty,
\]

by Lemma A.1 in Appendix A. In particular,

\[
\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 \, d\hat{\gamma}_n(x, y) = \sup_n \int_{\mathbb{R}^d} \|x\|^2 \, d\mu(x) + \int_{\mathbb{R}^d} \left\|\frac{y - x}{\varepsilon_n}\right\|^2 \, d\gamma_n(x, y) \]

\[
= \sup_n \int_{\mathbb{R}^d} \|x\|^2 \, d\mu(x) + \frac{\varepsilon_n}{\varepsilon_n^2} \]

\[
= \int_{\mathbb{R}^d} \|x\|^2 \, d\mu(x) + 1 \]

\[
< +\infty,
\]

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where we used that the first marginal of $\gamma_n$ is $\mu$, and $\mu$ has finite second moment. Similarly, the set $\{\beta_n\}_{n \in \mathbb{N}}$ is tight since

$$\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 d\hat{\beta}_n(x,y) = \sup_n \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + \int_{\mathbb{R}^d} \frac{\|y - x\|^2}{\varepsilon_n} d\beta_n(x,y)$$

$$= \sup_n \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + \frac{W_2(\mu, \nu_n)^2}{\varepsilon_n^2}$$

(60)

$$\leq \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + 1$$

$$< +\infty.$$  

Thus, $\gamma_n$ and $\beta_n$ converge narrowly (up to subsequences) to $\hat{\mu}$ and $\hat{\beta}$.

- **Finite second moment:** Since $(x,y) \mapsto \|x\|^2 + \|y\|^2$ is non-negative and lower semi-continuous, $\gamma \mapsto \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 d\gamma(x,y)$ is lower semi-continuous w.r.t. narrow convergence (see Proposition 2.12 below or [27, Lemma 5.1.7]). Thus,

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 d\hat{\gamma}(x,y) \leq \liminf_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 d\gamma_n(x,y) \leq \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + 1,$$

which implies that $\hat{\gamma}$ has finite second moment. Analogously, $\hat{\beta}$ has finite second moment.

We now seek to prove that

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla J_\mu(\mu)(x), y \rangle d\hat{\beta}_n(x,y) \to \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla J_\mu(\mu)(x), y \rangle d\hat{\beta}(x,y).$$

(61)

Note that this does not follow from narrow convergence, since the inner product is not a bounded function. Let $\eta > 0$, and define $\zeta_\eta \in C^{\infty}_c(\mathbb{R}^d)$ so that $\|\nabla J_\mu(\mu) - \nabla J_\eta\|_{L^2(\mathbb{R}^d \times \mathbb{R}^d, \mu)} < \eta$, which exists by density of gradients of compactly supported functions in $\text{Tan}_\mu P_2(\mathbb{R}^d)$. Then,

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \zeta_\eta(x), y \rangle d\hat{\beta}_n(x,y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle x, y \rangle d(\zeta_\eta \times \text{Id}) \# \hat{\beta}_n(x,y).$$

By continuity of $\zeta_\eta \# (\zeta_\eta \times \text{Id}) \# \hat{\beta}_n$ converges narrowly to $(\zeta_\eta \times \text{Id}) \# \hat{\beta}$. Moreover, we have that (i) $\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 d(\zeta_\eta \times \text{Id}) \# \hat{\beta}_n(x,y) = \sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \|\zeta_\eta(x)\|^2 d\mu(x) + \int_{\mathbb{R}^d \times \mathbb{R}^d} \|y\|^2 d\hat{\beta}_n(x,y) < +\infty$ by the compact support of $\zeta_\eta$ and (60), and (ii) $(\text{proj}_{1\#}(\zeta_\eta \times \text{Id}) \# \hat{\beta}_n = (\zeta_\eta) \# \mu$ has trivially uniformly integrable second moment (since it does not depend on $n$). Thus, Proposition A.3 gives

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \zeta_\eta(x), y \rangle d\hat{\beta}_n(x,y) \to \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \zeta_\eta(x), y \rangle d\hat{\beta}(x,y).$$

Thus,

$$\limsup_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla J_\mu(\mu)(x), y \rangle d\hat{\beta}_n(x,y)$$

$$= \limsup_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \zeta_\eta(x), y \rangle d\hat{\beta}_n(x,y) + \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla J_\mu(\mu)(x) - \zeta_\eta(x), y \rangle d\hat{\beta}_n(x,y)$$

$$\leq \lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \zeta_\eta(x), y \rangle d\hat{\beta}_n(x,y) + \eta \sup_n \|y\|_{L^2(\mathbb{R}^d \times \mathbb{R}^d, \hat{\beta}_n)}$$

(60)

$$\leq \lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \zeta_\eta(x), y \rangle d\hat{\beta}_n(x,y) + \eta \left( \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + 1 \right)$$

$$= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \zeta_\eta(x), y \rangle d\hat{\beta}(x,y) + \eta \left( \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + 1 \right)$$

$$\leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla J_\mu(\mu)(x), y \rangle d\hat{\beta}(x,y) + 2\eta \left( \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + 1 \right),$$

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where the first inequality results from Cauchy-Schwarz inequality \([51, \text{Theorem 4.2}]\). Similarly,

\[
\liminf_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\beta_n(x, y) \\
\geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\beta(x, y) - 2\eta \left( \int_{\mathbb{R}^d} \|x\|^2 \, d\mu(x) + 1 \right).
\]

Let \(\eta \to 0\) to establish \((61)\). An analogous argument gives

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\tilde{\gamma}_n(x, y) \to \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\tilde{\gamma}(x, y),
\]

and so, by \((58)\),

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\beta(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\tilde{\gamma}(x, y) \leq -\frac{\delta}{2} < 0. \tag{62}
\]

We will show that the left-hand side of \((62)\) is at the same time non-negative, which yields contradiction. Consider \(\zeta \in C_c^\infty(\mathbb{R}^d)\), and \(x, y \in \mathbb{R}^d\). Then, by the Taylor’s expansion, there exists \(z \in \mathbb{R}^d\) so that

\[
\zeta(y) = \zeta(x) + \langle \zeta(x), y - x \rangle + \frac{1}{2} \langle (y - x), \nabla^2 \zeta(z)(y - x) \rangle. \tag{63}
\]

Thus, with \(M = \sup_{x \in \mathbb{R}^d} \|\nabla^2 \zeta\|\), we have

\[
\zeta(y) - \zeta(x) \leq \langle \nabla \zeta(x), y - x \rangle + \frac{M}{2} \|x - y\|^2. \tag{64}
\]

The same bound applied to \(-\zeta\) yields

\[
-\zeta(y) + \zeta(x) \leq \langle \nabla \zeta(x), x - y \rangle + \frac{M}{2} \|x - y\|^2.
\]

Thus, for all \(x, y_1, y_2 \in \mathbb{R}^d\) we have

\[
\zeta(y_1) - \zeta(y_2) \leq \langle \nabla \zeta(x), y_1 - y_2 \rangle + \frac{M}{2} \|x - y_1\|^2 + \frac{M}{2} \|x - y_2\|^2.
\]

Since \((\text{proj}_1)_\# \beta_n = (\text{proj}_1)_\# \gamma_n = \mu\), we can deploy Gluing Lemma (Proposition A.4 in Appendix A) to construct \(\tilde{\gamma}_n \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)\) so that

\[
(\text{proj}_{12})_\# \tilde{\gamma}_n = \beta_n \quad \text{and} \quad (\text{proj}_{13})_\# \tilde{\gamma}_n = \gamma_n.
\]

Then, we have

\[
0 = \int_{\mathbb{R}^d} \zeta(y_1) \, d\nu_n(y_1) - \int_{\mathbb{R}^d} \zeta(y_2) \, d\nu_n(y_2)
= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \zeta(y_1) - \zeta(y_2) \, d\tilde{\gamma}_n(x, y_1, y_2)
\leq \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y_1 - y_2 \rangle \, d\tilde{\gamma}_n(x, y_1, y_2) + \frac{M}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|y_1 - x\|^2 + \|y_2 - x\|^2 \, d\tilde{\gamma}_n(x, y_1, y_2)
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y_1 - x - (y_2 - x) \rangle \, d\tilde{\gamma}_n(x, y_1, y_2)
\leq \frac{-\delta}{2} + \frac{\delta}{2} + M \epsilon^2_n = \epsilon_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\beta_n(x, y) - \epsilon_n \langle \nabla \zeta(x), y \rangle \, d\gamma_n(x, y) + M \epsilon^2_n.
\]
Overall, this can be re-expressed as
\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\tilde{\beta}_n(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\hat{\gamma}_n(x, y) + M \epsilon_n \geq 0.
\]
Again by Proposition A.3 (see the proof of (61) above), we let \( n \to \infty \) and conclude
\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\tilde{\beta}(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\hat{\gamma}(x, y) \geq 0. \tag{65}
\]
We will now use the density of gradients of smooth compactly supported functions in \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \) to obtain the desired contradiction. Specifically, let \( \zeta \in C^\infty_c(\mathbb{R}) \) so that \( ||\nabla \zeta - \nabla \mu J(\mu)|| \leq \frac{\delta}{6} (\int_{\mathbb{R}^d} ||x||^2 d\mu(x) + 1)^{-1} \). The existence of \( \zeta \) is ensured by the density of gradients of smooth compactly supported functions in \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^d) \). Then,
\[
0 > -\frac{\delta}{2} \geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\tilde{\beta}(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y \rangle \, d\hat{\gamma}(x, y)
\]
\[
\geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\tilde{\beta}(x, y) + \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x) - \nabla \zeta(x), y \rangle \, d\tilde{\beta}(x, y)
\]
\[
- \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\hat{\gamma}(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x) - \nabla \zeta(x), y \rangle \, d\hat{\gamma}(x, y)
\]
\[
\geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\tilde{\beta}(x, y) - \|\nabla \mu J(\mu) - \nabla \zeta\|_{L^2(\mathbb{R}^d, d\beta)}\|y\|_{L^2(\mathbb{R}^d, d\beta)}
\]
\[
- \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\hat{\gamma}(x, y) - \|\nabla \mu J(\mu) - \nabla \zeta\|_{L^2(\mathbb{R}^d, d\hat{\gamma})}\|y\|_{L^2(\mathbb{R}^d, d\hat{\gamma})}
\]
\[
\geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\tilde{\beta}(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\hat{\gamma}(x, y) - \|\nabla \mu J(\mu) - \nabla \zeta\|_{L^2(\mathbb{R}^d, d\hat{\gamma})}\|y\|_{L^2(\mathbb{R}^d, d\hat{\gamma})}
\]
\[
\geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\tilde{\beta}(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\hat{\gamma}(x, y) - \frac{\delta}{3}.
\]
which gives
\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\tilde{\beta}(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \zeta(x), y \rangle \, d\hat{\gamma}(x, y) \leq -\frac{\delta}{6} < 0.
\]
This contradicts (65), and concludes the proof. \( \square \)

**Proof of Proposition 2.8.** Let \( \gamma \in \Gamma_o(\mu, \nu) \) and set \( \mu_t := (1 - t) \text{proj}_1 + t \text{proj}_2 \# \gamma \). By definition of geodesic convexity
\[
J(\mu_t) \leq (1 - t)J(\mu) + tJ(\nu) - \frac{\alpha}{2} t(1 - t)W_2(\mu, \nu)^2
\]
for all \( t \in (0, 1) \) and so
\[
\frac{J(\mu_t) - J(\mu)}{t} \leq J(\nu) - J(\mu) - \frac{\alpha}{2} (1 - t)W_2(\mu, \nu)^2. \tag{66}
\]
Also, by definition of a geodesic, \( W_2(\mu, \mu_t) = tW_2(\mu, \nu) \). Let \( \gamma_t = (\text{proj}_1, (1 - t) \text{proj}_1 + t \text{proj}_2) \# \gamma \). We claim \( \gamma_t \in \Gamma_o(\mu, \mu_t) \). Indeed,
\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} ||x - y||^2 d\gamma_t = \int_{\mathbb{R}^d \times \mathbb{R}^d} ||x - ((1 - t)x + ty)||^2 d\gamma(x, y) = t^2W_2(\mu, \nu)^2 = W_2(\mu, \mu_t)^2.
\]
Thus, by Wasserstein differentiability,
\[ J(\nu) - J(\mu) - \frac{\alpha}{2} W_2(\mu, \nu)^2 = \liminf_{t \downarrow 0} J(\nu) - J(\mu) - \frac{\alpha}{2} (1 - t) W_2(\mu, \nu)^2 \]
\[
\geq \liminf_{t \downarrow 0} \frac{J(\mu_t) - J(\mu)}{t}
= \liminf_{t \downarrow 0} \frac{\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \ d\gamma(x, y) + o(t)}{t}
= \liminf_{t \downarrow 0} \frac{\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), (1 - t)x + ty - x \rangle \ d\gamma(x, y) + o(t)}{t}
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \ d\gamma(x, y).
\]

In particular, the inequality holds for the supremum over \( \gamma \in \Gamma(\mu, \nu) \). For the second inequality, observe that \((\text{proj}_2, \text{proj}_1)_{\#} \gamma \in \Gamma_o(\nu, \mu)\). So,
\[
J(\mu) - J(\nu) \geq \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\nu)(y), x - y \rangle \ d\gamma(x, y) + \frac{\alpha}{2} W_2(\mu, \nu)^2
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\nu)(y), x - y \rangle \ d\gamma(x, y) + \frac{\alpha}{2} W_2(\mu, \nu)^2
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle -\nabla \mu J(\nu)(y), y - x \rangle \ d\gamma(x, y) + \frac{\alpha}{2} W_2(\mu, \nu)^2.
\]

Finally, the “sum” of (10) and (67) establishes (11). \(\square\)

**Proof of Proposition 2.9.** Let \( \nu \in \mathcal{P}_2(\mathbb{R}^d) \) and \( \gamma \in \Gamma_o(\mu, \nu) \). Then,
\[
g(J(\nu)) - g(J(\mu)) = g'(J(\mu))(J(\nu) - J(\mu)) + o(|J(\nu) - J(\mu)|)
= g'(J(\mu)) \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla \mu J(\mu)(x), y - x \rangle \ d\gamma(x, y) + o(W_2(\nu, \mu)) \right)
+ o(|J(\nu) - J(\mu)|)
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle g'(J(\mu)) \nabla \mu J(\mu)(x), y - x \rangle \ d\gamma(x, y)
+ g'(J(\mu)) o(W_2(\nu, \mu)) + o(|J(\nu) - J(\mu)|).
\]

By differentiability (and thus continuity, by Proposition 2.7) of \( J \) we have
\[
\lim_{W_2(\nu, \mu) \to 0} \frac{o(|J(\nu) - J(\mu)|)}{W_2(\nu, \mu)} = \lim_{W_2(\nu, \mu) \to 0} \frac{o(|J(\nu) - J(\mu)|)}{|J(\nu) - J(\mu)|} \frac{|J(\nu) - J(\mu)|}{W_2(\nu, \mu)} = 0.
\]

This concludes the proof. \(\square\)

**Proof of Proposition 2.10.** First, by continuity and non-negativity of \( c \), \( J \) is well defined (e.g., see [29, Chapter 4]). We prove the statements separately.

(i) Non-negativity follows directly from non-negativity of \( c \). Moreover, since \((\text{Id}, \text{Id})_{\#} \mu \in \Gamma(\mu, \mu)\), \( J(\mu) \leq \int_{\mathbb{R}^d} c(y) d\mu(y) \leq C \). Thus, \( J \) is proper.

(ii) Since weak convergence in \( \mathcal{P}_2(\mathbb{R}^d) \) implies narrow convergence, the statement follows from (ii).

(iii) The statement is given in [29, Remark 6.12] and in [28, Proposition 7.4].
(iv) Let \( \mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d) \), \( \gamma \in \Gamma(\mu_0, \mu_1) \), and consider the interpolation
\[
\mu_t = ((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma.
\]
The proof simply leverages the \( \alpha \)-convexity of \( c(\cdot, y) \); i.e.,
\[
-c((1 - t)x_0 + tx_1, y) \leq -(1 - t)c(x_0, y) - tc(x_1, y) - \frac{\alpha}{2} t(1 - t) \| x_0 - x_1 \|^2.
\]
Moreover, from [69, Lemma 3.3], for Polish spaces \( X, Y, Z \), probability measures \( \nu_0 \in \mathcal{P}(X) \), \( \nu_1 \in \mathcal{P}(Y) \), and a Borel map \( f : X \to Z \)
\[
(f \times \text{Id}_Y) _\# \Gamma(\nu_0, \nu_1) = \Gamma(f _\# \nu_0, \nu_1) \subset \mathcal{P}(Z \times Y),
\]
where \( \text{Id}_Y \) is the identity map on \( Y \). Then,
\[
-J(\mu_t) = - \min_{\tilde{\gamma} \in \Gamma((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}(x, y)
\]
\[
= - \min_{\tilde{\gamma} \in \Gamma((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}(x, y)
\]
\[
= - \min_{\tilde{\gamma} \in \Gamma((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}(x, y)
\]
\[
= - \min_{\tilde{\gamma} \in \Gamma((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c((1 - t)x_0 + x_1, y) d\tilde{\gamma}(x_0, x_1, y)
\]
\[
= \max_{\tilde{\gamma} \in \Gamma((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma} (1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}(x, y) - \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_0 - x_1 \|^2 d\tilde{\gamma}(x_0, x_1, y)
\]
\[
\leq (1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}(x_0, x_1, y)
\]
\[
- \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_0 - x_1 \|^2 d\tilde{\gamma}(x_0, x_1, y)
\]
\[
\leq (1 - t) \min_{\tilde{\gamma} \in \Gamma((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}(x, y)
\]
\[
- \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_0 - x_1 \|^2 d\tilde{\gamma}(x_0, x_1, y)
\]
\[
\leq (1 - t) \min_{\tilde{\gamma} \in \Gamma((1 - t) \text{proj}_1 + t \text{proj}_2) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}_0(x, y)
\]
\[
- \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_0 - x_1 \|^2 d\tilde{\gamma}_0(x_0, x_1, y)
\]
\[
\leq (1 - t) \min_{\tilde{\gamma}_0 \in \Gamma(\text{proj}_1 \times \text{Id}) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}_0(x_0, x_1, y)
\]
\[
- \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_0 - x_1 \|^2 d\tilde{\gamma}_0(x_0, x_1, y)
\]
\[
\leq (1 - t) \min_{\tilde{\gamma}_1 \in \Gamma(\text{proj}_2 \times \text{Id}) _\# \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}_1(x_0, x_1, y)
\]
\[
- \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_0 - x_1 \|^2 d\tilde{\gamma}_1(x_0, x_1, y)
\]
\[
\leq \frac{1}{\alpha} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) d\tilde{\gamma}_1(x_0, x_1, y)
\]
\[
- \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \| x_0 - x_1 \|^2 d\tilde{\gamma}_1(x_0, x_1, y)
\]
This proves \( \alpha \)-convexity of \(-J\) along any interpolating curve.

(v) First, observe that

\[
((1 - t) \text{proj}_2 + t \text{proj}_3, \text{proj}_1)\# \gamma \in \Gamma(\mu, \bar{\mu}).
\]

Thus,

\[
J(\mu) \leq \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x,y) \text{d}((1 - t) \text{proj}_2 + t \text{proj}_3, \text{proj}_1)\# \gamma(x,y)
\]

\[
= \int_{\mathbb{R}^d \times \mathbb{R}^d} c((1 - t)x_0 + tx_1), x) \text{d} \gamma(x, x_0, x_1)
\]

\[
\leq (1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x_0, x) \text{d} \gamma(x, x_0, x_1) + t \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x_1, x) \text{d} \gamma(x, x_0, x_1)
\]

\[
- \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_0 - x_1\|^2 \text{d} \gamma(x, x_0, x_1)
\]

\[
= (1 - t)J(\mu) + tJ(\nu) - \frac{\alpha}{2} t(1 - t) \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_0 - x_1\|^2 \text{d} \gamma(x, x_0, x_1)
\]

\[
\leq (1 - t)J(\mu) + tJ(\nu) - \frac{\alpha}{2} t(1 - t) W_2(\mu, \nu)^2.
\]

(vi) To show that the Wasserstein gradient is well defined observe that

\[
\int_{\mathbb{R}^d} \|\nabla_x c(x, T^\mu_\bar{\nu}(x))\|^2 \text{d} \mu(x) \leq \int_{\mathbb{R}^d} M \left(1 + \|x\|^2 + \|T^\mu_\bar{\nu}(x)\|^2\right) \text{d} \mu(x)
\]

\[
= M \left(1 + \int_{\mathbb{R}^d} \|x\|^2 \text{d} \bar{\mu}(x) + \int_{\mathbb{R}^d} \|T^\mu_\bar{\nu}(x)\|^2 \text{d} \bar{\mu}(x)\right)
\]

\[
< +\infty,
\]

since \(\mu, \bar{\mu} \in \mathcal{P}_2(\mathbb{R}^d)\). Then, we prove subdifferentiability and superdifferentiability separately.

- **Superdifferentiability:** Let \((\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d)\) so that \(\mu_n \rightharpoonup \mu\) and let \(\gamma_n \in \Gamma_c(\mu, \mu_n)\). Via a Taylor’s expansion (recall (63) and (64) in the proof of Proposition 2.6), we have that

\[
c(x_1, y) - c(x_0, y) \leq \langle \nabla_x c(x_0, y), x_1 - x_0 \rangle + \frac{M}{2} \|x_1 - x_0\|^2,
\]

where we used that the norm of Hessian \(\nabla_x^2 c(x_0, y)\) is uniformly bounded. Then,

\[
-J(\nu) + J(\mu) \geq - \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x_1, T^\mu_\bar{\nu}(x_0)) \text{d} \gamma(x_0, x_1) + \int_{\mathbb{R}^d} c(x_0, T^\mu_\bar{\nu}(x_0)) \text{d} \mu(x_0)
\]

\[
= - \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x_1, T^\mu_\bar{\nu}(x_0)) - c(x_0, T^\mu_\bar{\nu}(x_0)) \text{d} \gamma(x_0, x_1)
\]

\[
\geq - \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_x c(x_0, T^\mu_\bar{\nu}(x_0)), x_1 - x_0 \rangle + \frac{M}{2} \|x_0 - x_1\|^2 \text{d} \gamma(x_0, x_1)
\]

\[
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle -\nabla_x c(x_0, T^\mu_\bar{\nu}(x_0)), x_1 - x_0 \rangle \text{d} \gamma(x_0, x_1) + \frac{M}{2} W_2(\mu, \nu)^2.
\]

This proves that \(-\nabla_x c(\cdot, T^\mu_\bar{\nu}(\cdot)) \in \partial^-(J)\), and thus superdifferentiability.
• Subdifferentiability: Let \((\mu_n)_{n \in \mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d)\) so that \(\mu_n \rightharpoonup \mu\). Define \(\gamma_n \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)\) so that
\[
(\text{proj}_{13})\# \gamma_n \in \Gamma_o(\mu, \mu_n) \quad (\text{proj}_{12})\# \gamma_n = (\text{Id}, T^n_\mu)\# \mu,
\]
which exists by Gluing Lemma (Proposition A.4 in Appendix A). Informally, \(\gamma_n\) is optimal from \(\mu\) to \(\mu_n\), and optimal from \(\mu\) to \(\bar{\mu}\). Moreover, again by Gluing Lemma (Proposition A.4 in Appendix A), define \(\beta_n \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)\) so that
\[
(\text{proj}_{13})\# \beta_n = (\text{proj}_{13})\# \gamma_n, \quad (\text{proj}_{23})\# \beta_n \in \Gamma_o(\bar{\mu}, \mu_n).
\]
Informally, \(\beta_n\) is optimal from \(\mu\) to \(\mu_n\) (analogously to \(\gamma_n\)), and optimal from \(\bar{\mu}\) to \(\mu_n\), and thus does not coincide with \(\gamma_n\). Accordingly, \(\beta_n\) is generally not optimal from \(\mu\) to \(\bar{\mu}\); i.e.,
\[
J(\mu) = \int_{\mathbb{R}^d} c(x, T^n_\mu(x))d\mu(x) \leq \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} c(x_1, x_2) d\beta_n(x_1, x_2, x_3).
\]
Define \(\varepsilon_n := W_2(\mu_n, \mu) \to 0\), and define the “rescaled plans”
\[
\hat{\gamma}_n := \left(\text{proj}_1, \text{proj}_2, \frac{\text{proj}_3 - \text{proj}_1}{\varepsilon_n}\right)\# \gamma_n, \\
\hat{\beta}_n := \left(\text{proj}_1, \text{proj}_2, \frac{\text{proj}_3 - \text{proj}_1}{\varepsilon_n}\right)\# \beta_n.
\]
Then,
\[
J(\mu_n) - J(\mu) \geq \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} c(x_3, x_2) - c(x_1, x_2) d\beta_n(x_1, x_2, x_3) \\
= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} c(x_1 + \varepsilon_n x_3, x_2) - c(x_1, x_2) d\hat{\beta}_n(x_1, x_2, x_3) \\
\geq \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_x c(x_1, x_2), \varepsilon_n x_3 \rangle - \frac{M}{2} \varepsilon_n^2 \|x_3\|^2 d\hat{\beta}_n(x_1, x_2, x_3) \\
= \varepsilon_n \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_x c(x_1, x_2), x_3 \rangle d\hat{\beta}_n(x_1, x_2, x_3) \\
- \frac{M}{2} \varepsilon_n^2 \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_3\|^2 d\hat{\beta}_n(x_1, x_2, x_3),
\]
and for any \(\hat{\gamma}_n \in \Gamma_o(\mu, \mu_n)\)
\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_x c(x_1, T^n_{\bar{\mu}}(x_1), x_3 - x_1) \rangle d\hat{\gamma}_n(x_1, x_3) \\
= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_x c(x_1, x_2), x_3 - x_1 \rangle d\gamma_n(x_1, x_2, x_3) \\
= \varepsilon_n \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_x c(x_1, x_2), x_3 \rangle d\hat{\gamma}_n(x_1, x_2, x_3).
\]
We now claim that \(\bar{\mu}_n\) and \(\bar{\beta}_n\) converge narrowly (up to subsequences) to some \(\bar{\mu}\) and \(\bar{\beta}\) with finite second moment:

– Narrow convergence: We equivalently show that the sets \(\{\hat{\gamma}_n\}_{n \in \mathbb{N}}\) and \(\{\hat{\beta}_n\}_{n \in \mathbb{N}}\) are tight, which automatically establishes convergence to some \(\hat{\gamma}\) and \(\hat{\beta}\) by Prokhorov’s theorem (Theorem A.2 in Appendix A). To show tightness it suffices to prove that
\[
\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_1\|^2 + \|x_2\|^2 + \|x_3\|^2 d\hat{\gamma}_n(x_1, x_2, x_3) < +\infty,
\]
by Lemma A.1 in Appendix A. In particular,

\[
\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x_1\|^2 + \|x_2\|^2 + \|x_3\|^2 d\tilde{\gamma}_n(x_1, x_2, x_3)
\]

\[
= \sup_n \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + \int_{\mathbb{R}^d} \|x\|^2 d\bar{\mu}(x) \int_{\mathbb{R}^d \times \mathbb{R}^d} \left\| \frac{x_3 - x_1}{\varepsilon_n} \right\|^2 d\gamma_n(x_1, x_2, x_3)
\]

\[
= \sup_n \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + \int_{\mathbb{R}^d} \|x\|^2 d\bar{\mu}(x) + 1
\]

\[
< +\infty,
\]

where we used that the first marginal of \(\gamma_n\) is \(\mu\), the second marginal is \(\bar{\mu}\), and both \(\mu\) and \(\bar{\mu}\) have finite second moment. Analogously,

\[
\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_1\|^2 + \|x_2\|^2 + \|x_3\|^2 d\tilde{\beta}_n(x_1, x_2, x_3)
\]

\[
\leq \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + \int_{\mathbb{R}^d} \|x\|^2 d\bar{\mu}(x) + 1
\]

\[
< +\infty,
\]

and the set \(\{\beta_n\}_{n \in \mathbb{N}}\) is tight. Thus, \(\gamma_n\) and \(\beta_n\) converge narrowly (up to subsequences) to \(\bar{\mu}\) and \(\bar{\beta}\).

- Finite second moment: Since \((x_1, x_2, x_3) \mapsto \|x_1\|^2 + \|x_2\|^2 + \|x_3\|^2\) is non-negative and lower semi-continuous, \(\gamma \mapsto \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_1\|^2 + \|x_2\|^2 + \|x_3\|^2 d\gamma(x_1, x_2, x_3)\) is lower semi-continuous w.r.t. narrow convergence (see Proposition 2.12 below or [27, Lemma 5.1.7]). Thus,

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_1\|^2 + \|x_2\|^2 + \|x_3\|^2 d\hat{\gamma}(x_1, x_2, x_3)
\]

\[
\leq \liminf_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_1\|^2 + \|x_2\|^2 + \|x_3\|^2 d\tilde{\gamma}_n(x_1, x_2, x_3)
\]

\[
\leq \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) + \int_{\mathbb{R}^d} \|x\|^2 d\bar{\mu}(x) + 1,
\]

which implies \(\hat{\gamma}\) has finite second moment. Analogously, \(\hat{\beta}\) has finite second moment.

Moreover, by construction of \(\tilde{\beta}_n\),

\[
(\text{proj}_{13})\# \hat{\gamma} = (\text{proj}_{13})\# \hat{\beta}.
\]

Indeed, for any \(\phi \in C_b(\mathbb{R}^d \times \mathbb{R}^d)\), which by approximation suffices to prove (75), we have

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} \phi(x_1, x_3) d(\text{proj}_{13})\# \hat{\gamma}(x_1, x_3) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \phi(x_1, x_3) d\hat{\gamma}(x_1, x_2 x_3)
\]

\[
= \lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \phi(x_1, x_3) d\tilde{\gamma}_n(x_1, x_2, x_3)
\]

\[
= \lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \phi(x_1, x_3) d\tilde{\beta}_n(x_1, x_2, x_3)
\]

\[
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \phi(x_1, x_3) d((\text{proj}_{13})\# \hat{\beta})(x_1, x_3).
\]
Since \((\text{proj}_{12})_\# \hat{\gamma}\) is induced by a transport, by [27, Lemma 10.2.8], we have

\[
\hat{\beta} = (\text{Id}, T^\mu) \# \mu.
\]

By Gluing Lemma (Proposition A.4 in Appendix A), given that \((\text{proj}_{12})_\# \hat{\gamma} = (\text{proj}_{12})_\# \hat{\beta}\) is induced by a transport, we conclude \(\hat{\gamma} = \hat{\beta}\). Next, we seek to prove that

\[
\lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\gamma}_n(x_1, x_2, x_3) = \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\gamma}(x_1, x_2, x_3). \tag{76}
\]

Note that the inner product is continuous, but not bounded, so the result does not follow directly from the definition of narrow convergence. Nonetheless, by Proposition A.3, we have

\[
\lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\gamma}_n(x_1, x_2, x_3) = \lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle y, x_3 \rangle \, d(\nabla_x c(\cdot, \cdot) \times \text{Id})_\# \hat{\gamma}_n(y, x_3)
\]

\[
= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle y, x_3 \rangle \, d(\nabla_x c(\cdot, \cdot) \times \text{Id})_\# \hat{\gamma}(y, x_3)
\]

\[
= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\gamma}(x_1, x_2, x_3),
\]

where we used that

- if \(\hat{\gamma}_n\) converges narrowly to \(\hat{\gamma}\), then \((\nabla_x c(\cdot, \cdot) \times \text{Id})_\# \hat{\gamma}_n\) converges narrowly to \((\nabla_x c(\cdot, \cdot) \times \text{Id})_\# \hat{\gamma}\) (by continuity of \(\nabla_x c\));

- the fact that

\[
\sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x\|^2 + \|y\|^2 \, d((\nabla_x c(\cdot, \cdot) \times \text{Id})_\# \hat{\gamma}_n)(y, x)
\]

\[
\leq \sup_n \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_3\|^2 + \|\nabla_x c(x_1, x_2)\|^2 \, d\hat{\gamma}_n(x_1, x_2, x_3)
\]

\[
= \sup_n \int_{\mathbb{R}^d} \|x_3\|^2 + M \left(1 + \|x_1\|^2 + \|x_2\|^2\right) \, d\hat{\gamma}_n(x_1, x_2, x_3)
\]

\[
< +\infty;
\]

- the fact that \((\text{proj}_{12})_\# (\nabla_x c(\cdot, \cdot) \times \text{Id})_\# \hat{\gamma}_n = \mu_n\) has uniformly integrable 2-moments since \(\mu_n \to \mu\) in \(\mathcal{P}_2(\mathbb{R}^d)\) (see [27, Proposition 7.1.5]).

A similar argument gives

\[
\lim_{n \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\beta}_n(x_1, x_2, x_3) = \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\beta}(x_1, x_2, x_3). \tag{77}
\]

Thus,

\[
\lim_{n \to \infty} \inf \frac{J(\mu_n) - J(\mu) - \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \langle \nabla_x c(x_1, T^\mu_\epsilon(x_1)), x_2 - x_1 \rangle \, d\hat{\gamma}(x_1, x_2)}{\epsilon_n} \geq \lim_{n \to \infty} \inf \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\beta}_n(x_1, x_2, x_3)
\]

\[
- \frac{M}{2} \epsilon_n \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|x_3\|^2 \, d\hat{\beta}_n(x_1, x_2, x_3)
\]

\[
- \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} (\nabla_x c(x_1, x_2), x_3) \, d\hat{\gamma}_n(x_1, x_2, x_3)
\]
Proof of Corollary 2.11. We prove the statements separately:

(i) Since $W_2(\cdot, \cdot)$ is distance on $\mathcal{P}_2(\mathbb{R}^d)$, it is non-negative and it does not evaluate to $+\infty$. Thus, $D(J) = \mathcal{P}_2(\mathbb{R}^d)$, $J$ is proper, and $J(\mu) \geq 0$ for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$.

(ii) Continuity w.r.t. weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$ follows directly from triangle inequality and continuity of $x^2/2$.

(iii) Lower semi-continuity w.r.t. narrow convergence follows from Proposition 2.10 and monotonicity of $x^2/2$.

(iv) It suffices to observe that $-\|x - y\|^2$ is $-2$-convex for all $y \in \mathbb{R}^d$, and deploy Proposition 2.10.

(v) It suffices to observe that $\|x - y\|^2$ is $2$-convex for all $y \in \mathbb{R}^d$, and deploy Proposition 2.10.

(vi) It suffices to observe that $\nabla_x \|x - y\|^2 = 2(x - y)$, and deploy Theorem 2.1 and Proposition 2.10.

\[ \text{Proof of Proposition 2.12.} \text{ We prove the statements separately:} \]

(i) It suffices to prove that $V$ has at most quadratic growth, i.e., that there exists $C > 0$ so that

\[ |V(x)| \leq C(1 + \|x\|^2). \]

Then, the statement follows from Jensen’s inequality:

\[ |\mathbb{E}^\mu [V(x)]| \leq \int_{\mathbb{R}^d} |V(x)| d\mu(x) \leq \int_{\mathbb{R}^d} C(1 + \|x\|^2) d\mu(x) < +\infty, \]

which also directly establishes properness. To see that $V$ has at most quadratic growth, observe that by Taylor’s expansion there exists $z \in \mathbb{R}^d$ so that

\[ V(x) = V(0) + \langle \nabla_x V(0), x \rangle + \frac{1}{2} \langle x, \nabla^2_x V(z)x \rangle \]

\[ \leq V(0) + \|\nabla_x V(0)\| \|x\| + \frac{M}{2} \|x\|^2 \]

\[ \leq V(0) + \frac{M}{2} \left( \frac{\|\nabla_x V(0)\|}{M} + \|x\| \right)^2 \]

\[ \leq V(0) + \frac{\|\nabla_x V(0)\|^2}{M} + M \|x\|^2 \]

\[ \leq C(1 + \|x\|^2) \]
(iii) [70, Theorem 3] proves an analogous statement for upper semi-continuity; the proof of lower semi-continuity follows *muta mutandis*.

(iv) See [27, Proposition 9.3.2].

(v) A more sophisticated proof involving subdifferentials can be found in [27, Proposition 10.4.2]; we provide a simplified proof for the differentiable case. Let \( \nu \in \mathcal{P}_2(\mathbb{R}) \) and \( \gamma \in \Gamma_o(\mu, \nu) \). Then,

\[
J(\nu) - J(\mu) = \int_{\mathbb{R}^d} V(x) d\nu(x) - \int_{\mathbb{R}^d} V(x) d\mu(x) = \int_{\mathbb{R}^d \times \mathbb{R}^d} V(y) d\gamma(x, y) - \int_{\mathbb{R}^d \times \mathbb{R}^d} V(x) d\gamma(x, y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} (\nabla_x V(x), y - x) d\gamma(x, y) + \int_{\mathbb{R}^d \times \mathbb{R}^d} R_x(y - x) d\gamma(x, y),
\]

where \( R_x(\cdot) \) is the remainder term of the Taylor’s series expansion at \( x \) of \( V \). Since the Hessian of \( V \) is uniformly bounded, by Taylor’s (multivariate) remainder formula we have that there exists \( z \in \mathbb{R}^d \) so that \( R_x(x - y) = \frac{1}{2} \left( x - y, \nabla^2 V(z)(x - y) \right) \), and so

\[
|R_x(y - x)| \leq \frac{M}{2} \| y - x \|^2.
\]

Thus,

\[
\left| \int_{\mathbb{R}^d \times \mathbb{R}^d} R_x(y - x) d\gamma(x, y) \right| \leq \int_{\mathbb{R}^d \times \mathbb{R}^d} |R_x(y - x)| d\gamma(x, y) \leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{M}{2} \| y - x \|^2 d\gamma(x, y) = \frac{M}{2} W_2(\mu, \nu)^2,
\]

which clearly approaches 0 as \( W_2(\mu, \nu) \to 0 \). Hence,

\[
J(\nu) - J(\mu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} (\nabla_x V(x), y - x) d\gamma(x, y) + o(W_2(\mu, \nu)).
\]  

By Definition 2.3, (78) directly gives subdifferential and superdifferential. These coincide and thus \( \nabla_x J(\mu) = \nabla_x V \). Finally, since \( V \) has bounded Hessian, \( \nabla_x V \) is Lipschitz continuous (with Lipschitz constant, say, \( L \geq 0 \)), and

\[
\int_{\mathbb{R}^d} \| \nabla_x V(x) \|^2 d\mu(x) \leq \int_{\mathbb{R}^d} \left( \| \nabla_x V(x) - \nabla_x V(0) \| + \| \nabla_x V(0) \| \right)^2 d\mu(x) \leq 2 \| \nabla_x V(0) \|^2 + 2 \int_{\mathbb{R}^d} \| \nabla_x V(x) - \nabla_x V(0) \|^2 d\mu(x) \leq 2 \| \nabla_x V(0) \|^2 + 2L^2 \int_{\mathbb{R}^d} \| x \|^2 d\mu(x) < +\infty.
\]

Hence, \( \nabla_x V \in L^2(\mathbb{R}^d, \mathbb{R}^d, \mu) \). \( \Box \)
Proof of Proposition 2.13. Since $U$ has bounded Hessian, we have $U(z) \leq C(1 + \|z\|^2)$ for some $C > 0$ (see (i) in the proof of Proposition 2.12). Thus,

$$
\int_{\mathbb{R}^d} \left( \int_{\mathbb{R}^d} |U(x - y)|\,d\mu(y) \right) \,d\mu(x) \leq \int_{\mathbb{R}^d} \left( \int_{\mathbb{R}^d} C(1 + \|x - y\|^2)\,d\mu(y) \right) \,d\mu(x)
$$

$$
= C + 2C \int_{\mathbb{R}^d} \left( \int_{\mathbb{R}^d} \|x\|^2 + \|y\|^2\,d\mu(y) \right) \,d\mu(x)
$$

$$
= C + 2C \left( \int_{\mathbb{R}^d} \|x\|^2\,d\mu(x) \right)^2 < +\infty.
$$

Thus, by Fubini’s Theorem [51, Theorem 8.8], the order of integration does not matter, and $J$ is well defined. Also, without loss of generality, we can assume that $U$ is even. If not, $U$ can be written as the sum of an even function $U_e$ and an odd function $U_o$. On one hand, since $U_o$ is odd,

$$
\int_{\mathbb{R}^d \times \mathbb{R}^d} U_o(x - y)\,d(\mu \times \mu)(x, y) = -\int_{\mathbb{R}^d \times \mathbb{R}^d} U_o(y - x)\,d(\mu \times \mu)(x, y),
$$

but on the other hand, by “relabeling” $x$ with $y$ and Fubini’s Theorem [51, Theorem 8.8],

$$
\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} U_o(x - y)\,d\mu(x)\,d\mu(y) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} U_o(y - x)\,d\mu(y)\,d\mu(x) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} U_o(y - x)\,d\mu(x)\,d\mu(y)
$$

which implies $\int_{\mathbb{R}^d \times \mathbb{R}^d} U_o(x - y)\,d(\mu \times \mu)(x, y) = 0$. Thus,

$$
\int_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y)\,d(\mu \times \mu)(x, y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} U_e(x - y)\,d(\mu \times \mu)(x, y) + \int_{\mathbb{R}^d \times \mathbb{R}^d} U_o(x - y)\,d(\mu \times \mu)(x, y)
$$

which equals

$$
\int_{\mathbb{R}^d \times \mathbb{R}^d} U_e(x - y)\,d(\mu \times \mu)(x, y).
$$

Then, we prove the statements separately:

(i) Since $|J(\mu)| \leq \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} |U(x - y)|\,d(\mu \times \mu)(x, y)$, the statement follows directly from (79). Properness follows from $D(J) \neq \emptyset$.

(ii) Since $\mu_n \rightharpoonup \mu_n$ implies $\mu_n \times \mu_n \rightharpoonup \mu \times \mu$ [27, Eq. 9.3.7], continuity follows from Proposition 2.12.

(iii) Since narrow convergence of $\mu_n$ to $\mu$ implies narrow convergence of $\mu_n \times \mu_n$ to $\mu \times \mu$ [28, Lemma 7.3], lower semi-continuity follows from Proposition 2.12.

(iv) A proof can be found in [27, Proposition 9.3.5]; we provide a more direct proof for completeness. Let $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, and $\gamma \in \Gamma(\mu_0, \mu_1)$. Let $\mu_t := ((1 - t)\,\text{proj}_1 + t\,\text{proj}_2)\#\gamma$. Then,

$$
J(\mu_t) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y)\,d(\mu \times \mu_t)(x, y)
$$

$$
= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} U((1 - t)x + tx' - ((1 - t)y + y'))\,d\gamma(x, x')\,d\gamma(y, y')
$$

$$
\leq \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} (1 - t)U(x - y) + tU(x' - y')\,d\gamma(x, x')\,d\gamma(y, y')
$$

$$
= \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} U(x - y)\,d\mu_0(x)\,d\mu_1(y) + \frac{t}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} U(x' - y')\,d\mu_0(x')\,d\mu_1(y')
$$

$$
= (1 - t)J(\mu_0) + tJ(\mu_1).
$$

(v) See [27, Theorem 10.4.11].
(vi) A more sophisticated proof involving subdifferentials can be found in [27, Proposition 10.4.11];
we provide a simplified proof here for the smooth case. Let $\nu \in P_2(\mathbb{R})$ and $\gamma \in \Gamma_o(\mu, \nu)$. Then,

$$J(\nu) - J(\mu) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} U(x' - y')d(\nu \times \nu)(x', y') - \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y)d(\mu \times \mu)(x, y)$$

$$= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} U(x' - y')d\gamma(x, x')d\gamma(y, y')$$

$$- \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} U(x - y)d\gamma(x, x')d\gamma(y, y')$$

$$= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \nabla U(x - y), (x' - y') - (x - y) \rangle d\gamma(x, x')d\gamma(y, y')$$

$$+ \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} R_{x-y}((x' - y') - (x - y)) d\gamma(x, x')d\gamma(y, y'),$$

where $R_{x-y}(\cdot)$ is the remainder term of the Taylor’s series expansion of $U$ at $x - y \in \mathbb{R}^d$. Since the Hessian of $U$ is uniformly bounded, by Taylor’s (multivariate) remainder formula we have that there exists $z \in \mathbb{R}^d$ so that

$$R_{x-y}((x' - y') - (x - y)) = \frac{1}{2} \langle (x' - y') - (x - y), \nabla^2 U(z)((x' - y') - (x - y)) \rangle,$$

and so

$$|R((x' - y') - (x - y))| \leq \frac{M}{2} \|(x' - y') - (x - y)\|^2 \leq M \left(\|x - x'\|^2 + \|y - y'\|^2\right).$$

Thus,

$$\left| \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} R((x' - y') - (x - y)) d\gamma(x, x')d\gamma(y, y') \right|$$

$$\leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} |R((x' - y') - (x - y))| d\gamma(x, x')d\gamma(y, y')$$

$$\leq M \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - x'\|^2 + \|y - y'\|^2 d\gamma(x, x')d\gamma(y, y')$$

$$\leq M \left( \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - x'\|^2 d\gamma(x, x') + \int_{\mathbb{R}^d \times \mathbb{R}^d} \|y - y'\|^2 d\gamma(y, y') \right)$$

$$= 2M \cdot W_2(\mu, \nu)^2,$$
which clearly approaches 0 as \( W_2(\mu, \nu) \to 0 \). Hence,

\[
J(\nu) - J(\mu) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( \nabla U(x - y), (x' - y') - (x - y) \right) d\gamma(x, x') d\gamma(y, y') + o(W_2(\mu, \nu))
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( \int_{\mathbb{R}^d} \nabla U(x - y) d\mu(y), x' - x \right) d\gamma(x, x')
\]

\[
\quad + \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( \int_{\mathbb{R}^d} -\nabla U(x - y) d\mu(x), y' - y \right) d\gamma(y, y') + o(W_2(\mu, \nu))
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( \int_{\mathbb{R}^d} \nabla U(x - y) d\mu(y), x' - x \right) d\gamma(x, x')
\]

\[
\quad + \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( \int_{\mathbb{R}^d} -\nabla U(y - x) d\mu(x), y' - y \right) d\gamma(y, y') + o(W_2(\mu, \nu))
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( (\nabla U \ast \mu)(x), x' - x \right) d\gamma(x, x')
\]

\[
\quad + \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( (\nabla U \ast \mu)(y), y' - y \right) d\gamma(y, y') + o(W_2(\mu, \nu))
\]

\[
= \int_{\mathbb{R}^d \times \mathbb{R}^d} \left( (\nabla U \ast \mu)(x), x' - x \right) d\gamma(x, x') + o(W_2(\mu, \nu)),
\]

where we used that the gradient of an even function is odd (i.e., \( -\nabla U(x - y) = \nabla U(y - x) \)). By Definition 2.3, this directly gives subdifferential and superdifferential. These coincide and thus \( \nabla \mu J(\mu) = \nabla x V \). \( \square \)

**Proof of Corollary 2.14.** First, observe that for a real random variable \( X \) the variance can be rewritten as follows:

\[
\text{Var}^\mu [X] = \int_{\mathbb{R}^d} xx^\top d\mu(x) - \mathbb{E}^\mu [X] \mathbb{E}^\mu [X]^\top
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^d} xx^\top d\mu(x) + \frac{1}{2} \int_{\mathbb{R}^d} yy^\top d\mu(y) - \int_{\mathbb{R}^d} xd\mu(x) \int_{\mathbb{R}^d} x^\top d\mu(x)
\]

\[
= \frac{1}{2} \left( \int_{\mathbb{R}^d} xx^\top d\mu(x) + \int_{\mathbb{R}^d} yy^\top d\mu(y)
\]

\[
\quad - \int_{\mathbb{R}^d} xd\mu(x) \int_{\mathbb{R}^d} y^\top d\mu(y) - \int_{\mathbb{R}^d} yd\mu(y) \int_{\mathbb{R}^d} x^\top d\mu(x) \right)
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} xx^\top + yy^\top - xy^\top - yx^\top d(\mu \times \mu)(x, y)
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} (x - y)(x - y)^\top d(\mu \times \mu)(x, y).
\]

In our case,

\[
J(\mu) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} (a, x - y)^2 d(\mu \times \mu)(x, y).
\]
Clearly, $U(z) = \langle a, z \rangle^2$ is differentiable, convex, and has bounded Hessian. So, Proposition 2.13 directly gives continuity w.r.t. weak convergence and convexity. To compute the gradient, we first show that $U(x + y) \leq 2(U(x) + U(y))$. Indeed,

$$U(x + y) = \langle a, x + y \rangle^2 \leq (\langle a, x \rangle + \langle a, y \rangle)^2 \leq 2(\langle a, x \rangle^2 + \langle a, y \rangle^2) = 2(U(x) + U(y)).$$

Hence, by Proposition 2.13,

$$\nabla J(\mu)(x) = \left( \nabla U^{*}\mu \right)(x) = 2a \left( \int_{\mathbb{R}^d} x - y d\mu(x) \right) = 2a \left( a, x - \mathbb{E}\mu [x] \right),$$

where we used $\nabla U(z) = 2a \langle a, z \rangle$.

Proof of Proposition 2.15. All proofs are in [27]. In particular:

(i) The statement is an obvious consequence of the definition of $J$. To show that $J$ is proper, consider the uniform probability measure over the $d$-dimensional ball in $\mathbb{R}$, for which $J$ is finite.

(ii) It follows from (i).

(iii) See [27, Lemma 9.4.3].

(iv) See [27, Proposition 9.3.9], by noting that $F^-$ is trivially integrable.

(v) See [27, Theorem 10.4.6].

Proof of Proposition 2.16. All proofs are in [27]. In particular:

(i) The statement is an obvious consequence of the definition of $J$. To show that $J$ is proper, consider $J(\tilde{\mu}) = \int_{\mathbb{R}^d} F(1) d\tilde{\mu}(x) = F(1) < +\infty$.

(ii) It follows from (i).

(iii) See [27, Lemma 9.4.3].

(iv) See [27, Theorem 9.4.12].

(v) See [27, Theorem 10.4.9].

Proof of Proposition 4.2. We prove the two statements for completeness; alternative (but slightly more sophisticated) proofs are in [27, 70].

(i) Closedness follows from triangle inequality. To see that $\bar{B}_\varepsilon(\mu)$ is generally not compact, let $d = 1$, $\mu = \delta_0$, and $\varepsilon = 1$. Define $(\mu_n)_{n \in \mathbb{N}} \subset \bar{B}_1(\delta_0)$ by $\mu_n := (1 - \frac{1}{n^2})\delta_0 + \frac{1}{n} \delta_n$. Assume that there exists a subsequence $\mu_{k_n} \rightharpoonup \mu \in \bar{B}_1(\delta_0)$. Since $\mu_n$ converges narrowly to $\delta_0$, it necessarily holds $\mu = \delta_0$; else, since weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$ implies narrow convergence, $\mu_{k_n}$ would converge narrowly to two limits, which is absurd (since narrow convergence is induced by a distance [27, Remark 5.1.1] and in metric spaces limits are unique). However, by definition of weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$,

$$W_2(\mu_{k_n}, \delta_0) = \int_{\mathbb{R}} x^2 d\mu_{k_n}(x) = \frac{1}{k_n^2} k_n^2 = 1 \rightarrow \int_{\mathbb{R}} x^2 d\mu(x) = W_2(\mu, \delta_0).$$

That is, $W_2(\mu, \delta_0) = 1$. Since the Wasserstein distance metrizes weak convergence in $\mathcal{P}_2(\mathbb{R}^d)$, this contradicts $\mu_{k_n} \rightharpoonup \delta_0$. So, $(\mu_n)_{n \in \mathbb{N}}$ does not admit a convergent subsequence, and $\bar{B}_1(\delta_0)$ is not compact.
(ii) By Corollary 2.11, \( \mu \mapsto W_2(\mu, \hat{\mu}) \) is lower semi-continuous w.r.t. narrow convergence, thus its level sets \( \overline{B}_\varepsilon(\hat{\mu}) \) are closed: Let \((\mu_n)_{n \in \mathbb{N}} \subset \overline{B}_\varepsilon(\hat{\mu})\) narrowly converge to \( \mu \in \mathcal{P}_2(\mathbb{R}^d) \), then

\[
W_2(\mu, \hat{\mu}) \leq \liminf_{n \to \infty} W_2(\mu_n, \hat{\mu}) \leq \varepsilon,
\]

and so \( \mu \in \overline{B}_\varepsilon(\hat{\mu}) \). Thus, it suffices to prove that Wasserstein balls are relatively compact (i.e., the closure w.r.t. narrow convergence is compact). By Prokhorov’s theorem (Theorem A.2 in Appendix A), relative compactness is equivalent to \( \overline{B}_\varepsilon(\hat{\mu}) \) being tight. Since

\[
\sup_{\mu \in \overline{B}_\varepsilon(\hat{\mu})} \int_{\mathbb{R}^d} \|x\|^2 d\mu(x) = \sup_{\mu \in \overline{B}_\varepsilon(\hat{\mu})} W_2(\mu, \delta_0)^2 \leq (\varepsilon + W_2(\hat{\mu}, \delta_0))^2 < +\infty.
\]
tightness follows from Lemma A.1. \( \square \)