Bounds on Wasserstein distances between continuous distributions using independent samples

Tamás Papp\textsuperscript{1}\textsuperscript{*}
Chris Sherlock\textsuperscript{2}
\textsuperscript{1}STOR-i CDT, Lancaster University, UK
\textsuperscript{2}Department of Mathematics and Statistics, Lancaster University, UK

Abstract

The plug-in estimator of the Wasserstein distance is known to be conservative, however its usefulness is severely limited when the distributions are similar as its bias does not decay to zero with the true Wasserstein distance. We propose a linear combination of plug-in estimators for the squared 2-Wasserstein distance with a reduced bias that decays to zero with the true distance. The new estimator is provably conservative provided one distribution is appropriately overdispersed with respect the other, and is unbiased when the distributions are equal. We apply it to approximately bound from above the 2-Wasserstein distance between the target and current distribution in Markov chain Monte Carlo, running multiple identically distributed chains which start, and remain, overdispersed with respect to the target. Our bound consistently outperforms the current state-of-the-art bound, which uses coupling, improving mixing time bounds by up to an order of magnitude.

Keywords: jackknife estimator of variance, Markov chain Monte Carlo, optimal transport, stochastic ordering, Wasserstein distance.

1 Introduction

Wasserstein distances (Villani, 2009) are a class of metrics between probability measures, which have found extensive use in probability (Villani, 2003, 2009), statistics (Panaretos and Zemel, 2019; Ramdas et al., 2017), and machine learning (Arjovsky et al., 2017; Peyré and Cuturi, 2019). Wasserstein distances metrize weak convergence, and have been used in Markov chain Monte Carlo to theoretically assess the convergence of sampling algorithms to their stationary distribution and the asymptotic bias of approximate sampling algorithms (Durmus and Moulines, 2019; Durmus and Eberle, 2021).

Wasserstein distances are analytically intractable for all but a few special cases. In practice, one can estimate them from a plug-in estimator constructed using independent samples from the distributions of interest. While relatively well-behaved in the discrete case (Sommerfeld and Munk, 2018; Tameling et al., 2019), the plug-in estimator suffers from the curse of dimensionality in the continuous case, with its rate of decay with the sample size worsening exponentially as the dimension of the problem increases (Fournier

\textsuperscript{*}t.papp@lancaster.ac.uk
and Guillin, 2015; Weed and Bach, 2019; Chizat et al., 2020). This translates into a significant upward bias for all but extremely large sample sizes. Worse, the plug-in estimator essentially attains a minimax optimal rate of convergence without additional assumptions beyond continuity (Niles-Weed and Rigollet, 2022).

Thus, a search for a general estimator which decays more quickly as the number of samples increases would be futile. Instead, we aim to obtain consistent estimators which are additionally meaningful bounds on the distance, especially as the distance shrinks. We achieve this by linearly combining plug-in estimators, in essence subtracting off a large portion of the bias of the plug-in estimator. We characterize when it is possible to do so and still obtain an upper bound in expectation, and we show that is straightforward to obtain an estimator of a lower bound in expectation. Our bounds converge no slower than the plug-in estimators they partially debias, and we show that the probability that the point estimators of our bounds are not themselves bounds decays exponentially with the sample size. We also propose an algorithm to compute the jackknife variance estimator of our bounds, which enables uncertainty quantification at no increase in computational complexity with the sample size, relative to solving for the bounds exactly.

An attractive feature of our upper and lower bound estimators is that, in contrast with the plug-in estimator, whatever the sample size, their biases decrease in proportion to the Wasserstein distance itself. We therefore apply our bounds to Markov chain Monte Carlo, quantifying the convergence of Markov chains in Wasserstein distance through direct empirical estimates. The idea is to run several independent and identically distributed Markov chains until convergence, and to graph the plug-in estimator of the squared 2-Wasserstein distance between the marginal distributions and stationary distribution. If the chains are started overdispersed with respect to the target and stay so until convergence, one can subtract off the asymptote in the graph and obtain an upper bound on the squared distance whose expectation decays to zero when the chains converge. The analogous procedure on the scale of the Wasserstein distance, instead of its square, achieves a lower bound on the distance. In effect, one backtracks and declares convergence when the asymptote occurs, similarly to the popular potential scale reduction factor \( \hat{\mathcal{R}} \) (Gelman and Rubin, 1992; Brooks and Gelman, 1998; Vehtari et al., 2021). We believe that our bounds will prove useful to compare the convergence of different Markov chains targeting the same stationary distribution, and to complement theoretical studies on Markov chain convergence with numerical results.

More closely related to our proposed bounds is the \( L \)-lag coupling upper bound proposed in Biswas et al. (2019), which can also be used to quantify the convergence of Markov chains. The bound applies to a certain class of integral probability metrics (Sriperumbudur et al., 2012) including the total variation distance and the 1-Wasserstein distance. The methodology can however be extended straightforwardly to 2-Wasserstein distances, and so can be directly compared to our bounds. Similarities between our bounds and the coupling bound include the use of many identically distributed Markov chains, and the eventual decay of the bounds towards zero as the chains converge. As opposed to our bounds, the coupling bound does not require overdispersion, and applies to discretely supported measures as well. At the same time, the coupling bound is not a consistent estimator, and need not decay in proportion to the true distance it bounds. As we show in the simulations of Section 4.4, even state-of-the-art couplings can be sub-optimal to a large extent, making the coupling bound very loose in comparison to our empirical bounds.
1.1 Wasserstein distances

Let \((\mathbb{R}^d, \|\cdot\|)\) be the \(d\)-dimensional real space endowed with the usual Euclidean norm. For two Borel probability measures \(\mu, \nu\) on \(\mathbb{R}^d\), the Wasserstein distance of order 2, or \(2\)-Wasserstein distance is

\[
W_2(\mu, \nu) = \left( \inf_{(X,Y) \in \Gamma(\mu, \nu)} \mathbb{E} \|X - Y\|^2 \right)^{1/2},
\]

where \(\Gamma(\mu, \nu)\) is the set of all couplings, that is probability measures in \(\mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)\) with marginals \(\mu, \nu\). The Wasserstein distance defines a metric on the space of probability measures with finite second moment. Convergence in the Wasserstein distribution is equivalent to convergence in distribution alongside convergence in the second moment (Villani, 2009).

There exists a unique optimal coupling \(\pi\) of \(\mu, \nu\) (Villani, 2009, Theorem 4.1). Under suitable regularity conditions on the distributions \(\mu, \nu\), for instance if both are continuous (Brenier, 1991; McCann, 1995), there exists an optimal transport map \(T\) which pushes forward \(\mu\) to \(\nu\), such that

\[
W_2(\mu, \nu) = \left( \mathbb{E}_\mu \|X - T(X)\|^2 \right)^{1/2}.
\]

If \(\mu\) and \(\nu\) are continuous, then \(T = \nabla \varphi\) uniquely \((d\nu\)-almost everywhere) for a convex function \(\varphi : \mathbb{R}^d \to \mathbb{R}\) called the Brenier potential from \(\mu\) to \(\nu\). Conversely, there exists a convex \(\tilde{\varphi} : \mathbb{R}^d \to \mathbb{R}\) such that the optimal transport map from \(\nu\) to \(\mu\) is \(T^{-1} = \nabla \tilde{\varphi}\) uniquely \((d\mu\)-almost everywhere), and \(\tilde{\varphi}\) is the associated Brenier potential from \(\nu\) to \(\mu\). See Appendix A for a precise statement and additional background on optimal transport and convexity.

For ease of exposition, we avoid presenting \(p\)-Wasserstein distances with exponents \(p \neq 2\) and general transportation costs in the main body of this work. We however introduce these concepts in the supplementary material. This is both to explain how certain results, such as the lower bound (2), generalize, as well as to aid in the proofs.

1.1.1 Empirical Wasserstein distance

Let \(\hat{\mu}_n, \hat{\nu}_n\) be independent empirical measures, each comprising of \(n\) equally weighted independent samples with weight \(1/n\). Based on \(\hat{\mu}_n\) and \(\hat{\nu}_n\), the empirical Wasserstein distance between \(\mu\) and \(\nu\) is \(W_2(\hat{\mu}_n, \hat{\nu}_n)\). We briefly summarize theoretical and computational properties of this plug-in estimator; see the review Panaretos and Zemel (2019) for an overview of statistical aspects, and the monograph Peyré and Cuturi (2019) for computational aspects.

The empirical Wasserstein distance is known to be consistent, converging almost surely to \(W_2(\mu, \nu)\) as \(n \to \infty\) (Villani, 2009, Corollary 6.11). When \(\mu, \nu\) are both discrete, the estimator is well-behaved (see Sommerfeld and Munk, 2018; Tameling et al., 2019, for limit theorems). The one-dimensional continuous case is also well-behaved, see the review of Bobkov and Ledoux (2019) for rates of mean-convergence, and del Barrio et al. (2005, 2019) for limit theorems. Whether \(\mu, \nu\) are continuous or discrete, the computation of \(W_2(\hat{\mu}_n, \hat{\nu}_n)\) is straightforward in the one-dimensional case, with the optimal coupling being a pairing of order statistics, for \(O(n \log n)\) cost.

Our focus is on the moderate-to-high dimensional continuous setting, when the plug-in estimator is known to suffer from the curse of dimensionality (Fournier and Guillin,
2015; Weed and Bach, 2019; Chizat et al., 2020). The estimator however concentrates well around its mean (Weed and Bach, 2019; Chizat et al., 2020), obeying a central limit theorem (del Barrio and Loubes, 2019; del Barrio et al., 2019, 2021) under minor regularity assumptions.

In general, one can compute the empirical Wasserstein distance by solving a linear program, for which exact \( \tilde{O}(n^3) \) algorithms exist, where the notation \( \tilde{O} \) obscures logarithmic factors. Interpreting the problem as one of optimal assignment, one could use the classical Hungarian algorithm (Kuhn (1955); see the discussions in Jonker and Volgenant (1986), Jonker and Volgenant (1987), Crouse (2016) for optimizations). However, algorithms which are tailored to the more general optimization problem of finding the minimum cost flow in a network are often more efficient in practice (see Kovács, 2015, for a comprehensive discussion). Our experiments are in the moderate sample size regime (up to \( n = 1000 \)), where exact computations are feasible, and so we employ exact solvers throughout. The cubic complexity of exact algorithms may however be prohibitive for large instances \( n \). In such scenarios, one might consider targeting an entropically regularized version of the transportation cost instead. This offers both computational and statistical advantages (Cuturi, 2013; Mena and Niles-Weed, 2019), although the entropic estimator is no longer consistent for the transportation cost.

1.2 Overview of results

1.2.1 Bounds

We informally describe out main results. For continuous measures \( \mu \) and \( \nu \) with \( \nu \) overdispersed (see below) with respect to \( \mu \), let \( \hat{\nu}_n, \hat{\mu}_n \) and \( \hat{\mu}'_n \) be independent samples of size \( n \) from \( \nu, \mu \) and \( \mu \) respectively. Theorem 1 essentially states that

\[
\mathbb{E}[W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\mu}'_n, \hat{\mu}_n)] \geq W_2^2(\mu, \nu).
\]  

(1)

Our sufficient condition, informally termed “overdispersed”, asks for the optimal transport map from \( \nu \) to \( \mu \) to be 1-Lipschitz. We refer to this as contractive optimal transport. If \( \nu \) and \( \mu \) differ only by a shift in mean, equality is attained in (1). As \( \nu \) approaches \( \mu \), the left-hand side of equation (1) decays in proportion to \( W_2(\mu, \nu) \). As a converse to the upper bound, if \( \nu \) is underdispersed with respect to \( \mu \), the reverse inequality holds. Further, assuming only that the samples are independent, it holds that

\[
|\mathbb{E}[W_2(\hat{\nu}_n, \hat{\mu}_n) - W_2(\hat{\mu}'_n, \hat{\mu}_n)]| \leq W_2(\mu, \nu).
\]  

(2)

We apply our bounds to estimate, from samples, the convergence in Wasserstein distance of a Markov chain targeting a continuous distribution. Multiple independent and identically distributed copies of the chain are started from a distribution \( \pi_0 \) which is overdispersed with respect to the stationary distribution \( \pi_\infty \), and run until they each approximately draw at least two independent samples from the stationary distribution \( \pi_\infty \). Let \( \pi_t \) denote the marginal distribution of the chain at time \( t \). Plotting the squared Wasserstein distance between the samples at iterations \( t \geq 0 \) and a collection of samples which are approximately from the stationary distribution will reveal an asymptote. Subtracting off the asymptote yields an estimate of the upper bound (1) on \( W_2^2(\pi_t, \pi_\infty) \) for \( t \geq 0 \), which goes to zero as the chain approaches stationarity. The analogous procedure, now on the scale of the Wasserstein distance, rather than its square, estimates the lower bound (2) on \( W_2(\pi_t, \pi_\infty) \).
1.2.2 Variance estimation and confidence intervals

We propose the Flapjack algorithm to efficiently compute the jackknife variance estimate of any statistic which can be computed via a linear assignment problem. Variance estimates can thus be obtained for any (balanced) empirical transportation cost, as well as for the estimators

\[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\nu}'_n, \hat{\mu}_n), \quad W_2(\hat{\nu}_n, \hat{\mu}_n) - W_2(\hat{\mu}'_n, \hat{\mu}_n) \]

of the left-hand sides of inequalities (1) and (2). The jackknife variance estimate is conservative (Efron and Stein, 1981), and we use it to construct asymptotic confidence intervals for the bounds (1) and (2). A central limit theorem (Section 3.1, derived from del Barrio and Loubes, 2019; del Barrio et al., 2021) motivates Gaussian confidence intervals for the upper bound (1). The lack of a satisfactory central limit for the term \( W_2(\hat{\mu}'_n, \hat{\mu}_n) \), however, hinders the construction of asymptotic confidence intervals for the lower bound (2). We therefore suggest using Chebyshev’s inequality to construct conservative confidence intervals for the lower bound.

1.3 Organization of the paper

In Section 2 we formally state our main results, characterize our main assumption on the contractivity of the optimal transportation map, and establish that point estimators for the bounds (1) and (2) are themselves bounds on the quantity of interest with high probability. Numerically, we compare our bounds with the plug-in estimator of the Wasserstein distance in synthetic examples, and we investigate the necessity of the contractive assumption on the optimal transport map.

Section 3 is concerned with uncertainty quantification for the bounds (1) and (2). We state a Gaussian central limit theorem for the point estimator of the upper bound (1). We introduce the Flapjack algorithm for the efficient computation of leave-one-out estimates of empirical transportation costs, which is also applicable to point estimators of the bounds (1) and (2). We then numerically verify the coverage of jackknife confidence intervals.

In Section 4 we apply our bounds to quantify convergence in multiple-chain Markov chain Monte Carlo. We investigate when the chains remain overdispersed with respect to the target when started overdispersed, both analytically and numerically. Further numerical experiments compare our bounds with the \( W_2 \)-analogue of the coupling bound proposed in Biswas et al. (2019). In Section 5, we conclude with a discussion of our findings and directions for future research. All proofs are deferred to Appendix B.

1.4 Notation

Let \( d \in \mathbb{N} \). For a function \( f : \mathbb{R}^d \to \mathbb{R} \), we write \( \nabla f \) for its gradient and \( \nabla^\otimes 2 f \) for its Hessian, which we allow to be undefined on a set of Lebesgue measure zero where appropriate. For \( x \in \mathbb{R}^d \), \( \| x \| = (\sum_{i=1}^d x_i^2)^{1/2} \) denotes its Euclidean norm. We write \( I_d \) for the \( d \)-dimensional identity matrix, and for \( x \in \mathbb{R}^d \) we use \( \text{diag}(x) \) to denote the diagonal matrix with diagonal \( x \) and all other entries null. The Loewner ordering of positive semidefinite matrices is indicated by \( \succeq \). For sequences \((a_n)_{n \geq 0}, (b_n)_{n \geq 0}\) of real numbers, we write \( a_n \lesssim b_n \) if there exists a \( C > 0 \) which does not depend on \( n \) such that \( a_n \leq Cb_n \) for all large enough \( n \geq 1 \). We let \( \mathcal{P}(\mathbb{R}^d) \) be the set of Borel probability measures on \( \mathbb{R}^d \). We
write $\mathcal{N}_d$ for a $d$-dimensional normal distribution, writing $\mathcal{N}$ instead of $\mathcal{N}_1$. Subscripts on expectations, such as $\mathbb{E}_\mu$, denote expectations with respect to random variables drawn from the distribution $\mu$.

## 2 Empirical bounds on the Wasserstein distance

As alluded to in Section 1, the problem of estimating the Wasserstein distance between two distributions from independent samples is particularly challenging when the distributions are continuous. The plug-in estimator $W_2^2(\hat{\mu}_n, \hat{\nu}_n)$ of the squared distance suffers from an average rate of convergence of $n^{-2/d}$ with the sample size $n$ in a space of dimension $d \geq 5$, a rate which is minimax under no additional restrictions (Chizat et al., 2020; Niles-Weed and Rigollet, 2022). Imposing smoothness assumptions on the distributions $\mu$ and $\nu$, plug-in estimators with better rates can be obtained by smoothing the empirical measures (Deb et al., 2021), at an increased computational cost. By considering slices or by smoothing, one can obtain a metric closely related to the Wasserstein distance, whose plug-in estimators converge at a rate in the sample size $n$ that is independent of the dimension (Nadjahi et al., 2020; Nietert et al., 2021).

We relax the objective of estimating the Wasserstein distance itself, and instead seek to estimate meaningful bounds on the distance from independent samples. The plug-in estimator $W_2^2(\hat{\mu}_n, \hat{\nu}_n)$ of the squared distance is known to be an upper bound on average (we also show its positive bias in Appendix B.1). However, the bias of this estimator does not decay in proportion to the distance $W_2(\mu, \nu)$ at any finite sample size $n$. This becomes abundantly clear when $\mu = \nu$ and at the sample size $n = 1$, in which case the bias of $W_2^2(\hat{\mu}_n, \hat{\nu}_n)$ is twice the squared centered moment of $\mu$, while the distance to be estimated is zero. In this section, we shall characterize when one can subtract off a significant portion of the bias of the plug-in estimator of the Wasserstein distance, such that on average one obtains a bound which decays in proportion to the distance.

### 2.1 Assumptions and main results

We make the structural assumption that independent samples are available from two distributions with finite second moments. The moment condition guarantees that all (expected) Wasserstein distances are well-defined.

**Assumption 1** (Second moment and independence). $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ have finite second moments, that is $\mathbb{E}_\mu \|X\|^2 \leq \infty$ and $\mathbb{E}_\nu \|Y\|^2 \leq \infty$. Furthermore, samples $X_1, \ldots, X_n, Z_1, \ldots, Z_n \sim \mu$ and $Y_1, \ldots, Y_n \sim \nu$ are all independent, and

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}, \quad \hat{\nu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{Y_i}, \quad \hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{Z_i}.$$

**Remark 1** (On the independence of empirical measure). All our results generalize straightforwardly, albeit with potentially worse constants, to independent samples of pairs of $(X_i, Y_i)$ with marginals $\mu$ and $\nu$ but an arbitrary joint distribution. More generally, the left-hand sides of equations (1), (2) are invariant to the dependence between between $\hat{\mu}_n$ and $\hat{\nu}_n$, as long as $\hat{\mu}_n$ is independent of both these measures.

If the measures $\mu$ and $\nu$ are continuous, then, by Brenier’s theorem (e.g. Villani (2003), Theorem 2.12) there exists a unique optimal transport map from $\mu$ to $\nu$. We shall
make the assumption that such an optimal transport map is 1-Lipschitz, in other words contractive.

**Definition 1** (Contraction). Let $f : \mathcal{X} \subseteq \mathbb{R}^d \to \mathbb{R}^d$. We say that $f$ is a contraction if, for all $x, y \in \mathcal{X}$,

$$\|f(x) - f(y)\| \leq \|x - y\|.$$  

Equivalently, $f$ is 1-Lipschitz continuous.

**Definition 2** (Contractive optimal transport). Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ be continuous measures. We write $\nu \overset{\text{cot}}{\rightsquigarrow} \mu$ or $\mu \overset{\text{cot}}{\rightsquigarrow} \nu$, and say that $\nu$ is contractively optimally transported to $\mu$, if the optimal transport map from $\nu$ to $\mu$ is a contraction and the Brenier potential $\hat{\phi}$ is differentiable.

As we shall argue, $\nu \overset{\text{cot}}{\rightsquigarrow} \mu$ asserts that $\nu$ is overdispersed relative to $\mu$ in a specific way. We characterize contractive optimal transport in Section 2.2, also relating it to the literature of stochastic orders (Shaked and Shanthikumar, 2007).

Theorem 1 below provides our key result. As with all our results, its proof is provided in Appendix B.

**Theorem 1** (Bounds for $W_2^2$). Let Assumption 1 hold, let $\mu, \nu$ be continuous, and consider $\overset{\text{cot}}{\rightsquigarrow}$ as defined in Definition 2. If $\nu \overset{\text{cot}}{\rightsquigarrow} \mu$, then inequality (1) holds:

$$E \left[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\mu}_n', \hat{\mu}_n) \right] \geq W_2^2(\mu, \nu).$$

Conversely, if $\mu \overset{\text{cot}}{\rightsquigarrow} \nu$, then

$$E \left[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\mu}_n', \hat{\mu}_n) \right] \leq W_2^2(\mu, \nu).$$

**Remark 2** (On the strength of the contractive assumption $\nu \overset{\text{cot}}{\rightsquigarrow} \mu$). This assumption is a strong one, and we expect it to be typically unverifiable in practice. In Section 2.4, we offer empirical evidence that the assumption is not strictly required in general.

**Remark 3** (On the necessity of overdispersion). Theorem 1, our experiments in Section 2.4, and the simple example below show that $\nu$ must be overdispersed with respect to $\mu$, at least in some weak sense, to guarantee that an upper bound of the type (1) holds. Letting $\hat{\nu}_n'$ be an independent copy of $\hat{\nu}_n$, then it is possible to have both

$$E \left[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\mu}_n', \hat{\mu}_n) \right] \leq W_2^2(\mu, \nu)$$

$$E \left[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\nu}_n', \hat{\nu}_n) \right] \leq W_2^2(\mu, \nu)$$

hold at once. Consider the following example, in $d = 2$ with sample size $n = 1$. Let $\mu = N_2(0, I_2)$ and $\nu = N_2(0, \text{diag}(2, 1/4))$. Then, $W_2^2(\mu, \nu) = 1/4 + (\sqrt{2} - 1)^2$, but

$$E \left[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\mu}_n', \hat{\mu}_n) \right] = 1/4 \quad \text{and} \quad E \left[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\nu}_n', \hat{\nu}_n) \right] = -1/4.$$

**Remark 4** (On the continuity assumption). In principle, provided one restates the overdispersion condition in terms of couplings of random variables, one need not enforce the continuity of the distributions $\mu, \nu$ for our main result to hold. However, continuity allows access to Brenier’s theorem, which asserts the existence of an optimal transport map, and allows for the simplified presentation above.

Compared to the naive estimator, the upper bound has the advantage of decaying in proportion to the Wasserstein distance $W_2(\mu, \nu)$ whatever the sample size.
Proposition 1. Let Assumption 1 hold. Then,

\[ \mathbb{E} \left[ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\nu}'_n, \hat{\mu}'_n) \right] \leq K(\mu, \nu) W_2(\mu, \nu), \]

where \( K(\mu, \nu) = 3 (\mathbb{E}\|X\|^2)^{1/2} + (\mathbb{E}\|Y\|^2)^{1/2} \) and \( X \sim \mu, Y \sim \nu. \)

Remark 5 (Unbiased in the shift case). Suppose \( \mu \) and \( \nu \) differ only by a shift in mean. Then, the optimal transport map is a translation, so both \( \nu^{\text{cov}} \sim \mu \) and \( \mu^{\text{cov}} \sim \nu \), and equality is attained: \( \mathbb{E}\left\{ W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\nu}'_n, \hat{\mu}'_n) \right\} = W_2^2(\mu, \nu). \)

Remark 6 (Infinite relative size if \( \mu \) and \( \nu \) are close). The bound of Proposition 1 suggests, but does not prove, that the relative size of the upper bound (1) grows to infinity as \( \nu \) approaches \( \mu \) in the Wasserstein distance (but does not reach \( \mu \)). Our empirical findings further support this behaviour for fixed sample sizes \( n \).

We also have the following lower bound for \( W_2 \), which is tight when \( \mu = \nu \).

Theorem 2 (Lower bound for \( W_2 \)). Under Assumption 1, inequality (2) holds:

\[ |\mathbb{E} [ W_2(\hat{\nu}_n, \hat{\mu}_n) - W_2(\hat{\nu}'_n, \hat{\mu}'_n)]| \leq W_2(\mu, \nu). \]

2.1.1 Estimation in practice

We suggest estimating the upper bound (1) with the estimator

\[ U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}'_n) = W_2^2(\hat{\nu}_n, \hat{\mu}_n) - W_2^2(\hat{\mu}'_n, \hat{\mu}_n), \]

and the lower bound (2) with

\[ L(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}'_n) = W_2(\hat{\nu}_n, \hat{\mu}_n) - W_2(\hat{\mu}'_n, \hat{\mu}_n). \]

The latter can be obtained for negligible computational cost once the upper bound has been estimated. We advise against modifying these estimators by taking absolute values, as this can mask pathological behaviour should the estimation noise be large enough to make either estimator negative with noticeable probability. Similarly, should the overdispersion assumption \( \nu^{\text{cov}} \sim \mu \) fail, and cause the upper bound estimate to become negative, this would also be masked by taking absolute values.

To use both bounds on the same scale, we suggest bringing the lower bound to the scale of \( W_2^2 \) by squaring and keeping the sign

\[ L_{sq}(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}'_n) = \text{sign}(W_2(\hat{\nu}_n, \hat{\mu}_n) - W_2(\hat{\mu}'_n, \hat{\mu}_n))[W_2(\hat{\nu}_n, \hat{\mu}_n) - W_2(\hat{\mu}'_n, \hat{\mu}_n)]^2. \]

While this estimator has the potential to overestimate \( W_2^2(\mu, \nu) \) in general, we have that

\[ \mathbb{P}(L_{sq} \leq W_2^2(\mu, \nu)) = \mathbb{P}(L \leq W_2(\mu, \nu)), \quad \mathbb{E}|L_{sq}| = (\mathbb{E}L)^2 + \text{Var}(L). \]

Firstly, on their respective scales, the point estimate \( L_{sq} \) is as good a lower bound as the point estimate \( L \) is. Secondly, if the absolute value of the bias of \( L \) decays much slower with \( n \) than the variance of \( L \) (as is known to occur in dimensions \( d \geq 5 \)) then the estimator \( L_{sq} \) will become a negatively biased estimator of \( W_2^2(\mu, \nu) \) for moderate sample sizes \( n \). All three estimators \( U, L \) and \( L_{sq} \) are consistent as \( n \to \infty. \)
2.2 Contractive optimal transport

Using Brenier’s theorem and facts from convex analysis (these and additional definitions are recalled in Appendix A), Theorem 3 provides conditions which are equivalent to contractive optimal transport.

**Theorem 3** (Equivalent notions of contractive optimal transport). Let \( \mu \) and \( \nu \) be continuous measures in \( \mathbb{R}^d \). Let \( \varphi \) be a Brenier potential from \( \mu \) to \( \nu \), \( T = \nabla \varphi \) be the optimal transport map from \( \mu \) to \( \nu \), and \( \tilde{\varphi} \) be a Brenier potential from \( \nu \) to \( \mu \). Then, the following are equivalent:

(i) \( \nu \sim cot \mu \).

(ii) \( \tilde{\varphi} \) is differentiable and \( T^{-1} = \nabla \tilde{\varphi} \) is 1-Lipschitz.

(iii) \( \varphi \) is 1-strongly convex.

If, additionally, \( \varphi \) and \( \tilde{\varphi} \) are twice continuously differentiable, then the above are also equivalent to:

(iv) \( \nabla^{\otimes 2} \tilde{\varphi} \preceq I_d \).

(v) \( \nabla^{\otimes 2} \varphi \succeq I_d \).

Shifting the mean of either distribution \( \mu \) or \( \nu \) only changes the optimal transport map by a translation. As such, if the map was contractive before the shift, it shall remain contractive afterwards. Contractive optimal transport \( \sim cot \) is therefore a shift-invariant (or location-free) relationship, and only relates the dispersion of the distributions. This motivates a comparison of \( \sim cot \) with stochastic orderings. In dimension \( d = 1 \), the univariate dispersive ordering \( \geq disp \) (Shaked, 1982) is equivalent to \( \sim cot \), as established in Shaked and Shanthikumar (2007, Equation 3.B.15). In order to establish the relationship \( \nu \sim cot \mu \) in the univariate case, one need only consider the relative separation of the quantiles of the two distributions \( \nu \) and \( \mu \) (Shaked and Shanthikumar, 2007, Equation 3.B.1). In general dimension, the strong dispersive ordering \( \geq SD \) (Giovagnoli and Wynn, 1995) is strictly weaker than \( \sim cot \) (Shaked and Shanthikumar, 2007, Equation 7.B.1).

The relationships \( \geq disp \) and \( \geq SD \) define partial orders on sets of distributions obeying mild regularity conditions. We have been unable to establish whether \( \sim cot \) defines a partial order under similar conditions; we however conjecture that it does not, and leave this problem as an open question. We note that a duality result exists for contractive optimal transport (Fathi et al., 2020, Theorem 2), which states that \( \nu \sim cot \mu \) if and only if \( \mu \) is the closest distribution to \( \nu \) in \( \mathcal{W}_2 \) among all distributions which dominate \( \nu \) in the convex ordering \( \geq c \) (Strassen, 1965).

The optimal transport map, as well as the squared Wasserstein distance, have known closed-form representations between Gaussians (Dowson and Landau, 1982; Peyré and Cuturi, 2019, Remark 2.31). In this case, contractive optimal transport reduces to the Loewner ordering of the covariances, as stated in Proposition 2 below. The result also extends straightforwardly to distributions belonging to the same family of elliptically-contoured distributions with finite second moments (see Peyré and Cuturi, 2019, Remark 2.32 and references therein).

**Proposition 2** (Contractive optimal transport in the Gaussian case). Let \( \mu \) and \( \nu \) be two Gaussian distributions on \( \mathbb{R}^d \) with covariances \( M \) and \( N \) respectively. Then, \( \nu \sim cot \mu \iff N \succeq M \).

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The optimal transport map between centered isotropic distributions $\mu$ and $\nu$ is completely determined by the optimal transport map between the radial components of these distributions. It follows that $\nu \overset{\text{cot}}{\rightsquigarrow} \mu$ if and only if $\nu \overset{\text{cot}}{\rightleftharpoons} \mu$ holds between the radial components of these distributions. For $d$-dimensional product distributions $\mu$ and $\nu$, the optimal transport map is $\nabla \varphi(x) = (\nabla \varphi_1(x), \ldots, \nabla \varphi_d(x))^T$, where $\nabla \varphi_i$ is the optimal map transporting $\mu_i$ to $\nu_i$ for all $i \in \{1, \ldots, d\}$. It follows that $\nu \overset{\text{cot}}{\rightleftharpoons} \mu$ if and only if $\nu_i \overset{\text{cot}}{\rightleftharpoons} \mu_i$ for all $i \in \{1, \ldots, d\}$.

Caffarelli’s Contraction Theorem (Caffarelli, 2000, Theorem 11), a seminal result in optimal transport, asserts that the optimal map transporting a Gaussian $\nu$ to a distribution $\mu$ which is “more log-concave” than $\nu$ is a contraction. We generalize this result in Theorem 4 below, allowing $\nu$ to be less log-concave than a Gaussian. The proof follows from a maximum principle argument (see Kolesnikov, 2010, for instance). Other generalizations of Caffarelli’s Contraction Theorem include the results of Valdimarsson (2007) ($\nu$ is a convolution of the Gaussian) and Kim and Milman (2012). See Chewi and Pooladian (2022, Theorem 5) for a generalization of Theorem 4 and for precise technical assumptions under which Theorem 4 holds.

**Theorem 4** (Caffarelli Contraction Theorem). Let $\mu$ and $\nu$ be continuous distributions on $\mathbb{R}^d$, with densities $d\mu(x) = e^{-U(x)}dx$ and $d\nu(x) = e^{-V(x)}dx$ where $U, V$ are twice continuously differentiable. If there exists a positive definite matrix $A$ such that $\nabla \otimes^2 U \succeq A \succeq \nabla \otimes^2 V$, then $\nu \overset{\text{cot}}{\rightleftharpoons} \mu$.

Thinking of $A$ as being a precision matrix, Theorem 4 provides some guidance in practice. When the distribution $\mu$ is a posterior distribution in a Bayesian inference problem, the Bernstein-von-Mises theorem asserts that it approaches Gaussianity as more data are collected. In this large-sample regime, if one is reasonably confident that the Hessian condition $\nabla \otimes^2 U \succeq \nabla \otimes^2 V$ holds, then the contractive condition $\nu \overset{\text{cot}}{\rightleftharpoons} \mu$ is approximately satisfied. As we show in the experiments of Section 2.4, the bound (1) is to some extent loose, so one might expect that in the approximate $\nu \overset{\text{cot}}{\rightleftharpoons} \mu$ regime the bound is valid.

The Loewner ordering induces a partial ordering on the set of positive semi-definite matrices, so Theorem 4 also induces a type of Gaussian-modulated dispersive ordering on the set of log-concave distributions. We note that Theorem 4 also generalizes Proposition 2 in one direction.

### 2.3 Concentration, convergence, and bounds with high probability

In this section, we show that, when $\mu \neq \nu$ and the dimension is large enough, the point estimates $U$ and $L$ are themselves upper, and respectively, lower bounds with high probability on the quantities of interest. Otherwise, when $\mu \equiv \nu$, both $U$ and $L$ have distributions which are symmetric about 0. We rely on bounds on the rate of convergence, as well as concentration bounds for empirical Wasserstein distance estimates, using results and techniques which we adapt from Fournier and Guillin (2015); Panaretos and Zemel (2019); Weed and Bach (2019); Chizat et al. (2020).

Such results require some additional assumptions. For a unified treatment, we shall assume that $\mu$ and $\nu$ are boundedly supported (without loss of generality, in the same subset of diameter 1). Progress can however be made even without assuming boundedness (Lei, 2020, Section 5).

**Assumption 2.** $\mu, \nu$ are supported in the same subset of diameter 1 of $\mathbb{R}^d$. 

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Theorem 5 states concentration bounds for the estimators $U$ and $L$ which are exponential in the sample size $n$. The estimator $U$ has sub-Gaussian concentration. For the estimator $L$ we obtain a concentration bound which is worse than sub-Gaussian, but which still shows that the tails of the estimator decay exponentially in the sample size $n$.

**Theorem 5 (Concentration bounds).** Consider Assumption 1, and let $\mu, \nu$ satisfy Assumption 2. Then, for all $t \geq 0$ it holds that
\[
\begin{align*}
    \mathbb{P}(|U - \mathbb{E}U| \geq t) &\leq 4 \exp\left(-nt^2/4\right), \\
    \mathbb{P}(|L - \mathbb{E}L| \geq t) &\leq 4 \exp\left(-nt^4/256\right).
\end{align*}
\]

Theorem 6 shows that the discrepancy between the empirical bounds $U, L$ and the truth decays polynomially with the number of samples, with the rate worsening exponentially as the dimension $d$ increases. This is typical behaviour for the plug-in estimator of the Wassestein distance, and indeed the rates below are minimax without additional assumptions on the smoothness of the measures (Niles-Weed and Rigollet, 2022).

**Theorem 6 (Rates of convergence).** Let $d \geq 5$ and $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$. Assume that $\mu \neq \nu$ satisfy Assumptions 1 and 2. Then,
\[
\begin{align*}
    \mathbb{E}|U - W_2^2(\mu, \nu)| &\lesssim n^{-2/d}, \\
    \mathbb{E}|W_2(\mu, \nu) - L| &\lesssim n^{-1/d}.
\end{align*}
\]

If $\mu, \nu$ are continuous and $\mu \neq \nu$, then
\[
W_2(\mu, \nu) - \mathbb{E}L \gtrsim n^{-1/d}.
\]

Theorems 5 and 6 suggest that the bias in the estimators $U$ and $L$ far outweighs the standard deviation if the dimension $d$ is high enough. This is formalized in the result below, essentially a corollary of the two theorems, which states that the probability that the bound point estimates $U$ and $L$ are not themselves bounds decays exponentially in the sample size $n$. This does not apply when $\mu \equiv \nu$, as then the point estimates $U$ and $L$ fluctuate around zero.

**Corollary 1 (Validity of point estimates).** Let $d \geq 5$, assume that $\mu \neq \nu$ are continuous and satisfy Assumptions 1 and 2. Then, there exists a constant $C_1 > 0$ such that
\[
\mathbb{P}(L_{sq} \leq W_2^2(\mu, \nu)) = \mathbb{P}(L \leq W_2(\mu, \nu)) \geq 1 - 2 \exp(-C_1 n^{1-4/d}).
\]

Furthermore, if $\mathbb{E}U - W_2^2(\mu, \nu) \gtrsim n^{-2/d}$, then there exists a constant $C_2 > 0$ such that
\[
\mathbb{P}(U \geq W_2^2(\mu, \nu)) \geq 1 - 2 \exp(-C_2 n^{1-4/d}).
\]

The constants $C_1, C_2$ in Corollary 1 depend on $\mu, \nu$ and the dimension $d$. In particular, $C_1$ and $C_2$ become smaller as $W_2(\mu, \nu)$ decreases. This is expected behaviour: on an absolute scale, the biases of the estimators $U$ and $L$ decay to 0 as the distance $W_2(\mu, \nu)$ decays to zero, while in the same regime the standard deviations of these estimators does not vanish as the distance $W_2(\mu, \nu)$ decays to zero.
2.4 Numerical illustrations

In this section, we compare our bounds \( U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu'}_n) \) and \( L_{sq}(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu'}_n) \) against the plug-in estimator \( \mathcal{W}^2_2(\hat{\mu}_n, \hat{\nu}_n) \) and the true squared distance \( \mathcal{W}^2_2(\mu, \nu) \) on a few synthetic examples. We first consider the case \( \mu = \mathcal{N}_d(0, I_d) \) and \( \nu = \mathcal{N}_d(0, \sigma^2 I_d) \), where the parameters are varied according to \((\sigma^2, d, n) \in \{1.1, 2, 10\} \times \{10, 100\} \times \{10, 100, 1000\}\). This ensures that \( \nu \approx \sqrt{\mu} \) throughout.

The results are presented in Figure 1. Relative to their biases, the noise in the estimators \( U \) and \( L_{sq} \) is under control at the higher sample sizes \( n \). Compared to the plug-in estimator \( \mathcal{W}^2_2(\hat{\mu}_n, \hat{\nu}_n) \), the upper bound estimator \( U \) has a greatly reduced absolute and relative error for the smaller values of \( \sigma^2 \). The relative error of the estimator \( U \) increases as \( \sigma^2 \) is decreased, as suggested by Proposition 1. As seen in Theorem 6, the rate of convergence of estimator \( U \) suffers from the curse of dimensionality similarly to the plug-in estimator \( \mathcal{W}^2_2(\hat{\mu}_n, \hat{\nu}_n) \).

The relative error of the estimator \( \mathbb{E}L_{sq} \) increases as \( \sigma^2 \) decreases, at sample size \( n = 1000 \) ranging between 0.14 and 0.69 in dimension \( d = 10 \), and ranging between 0.37 and 0.71 in dimension \( d = 100 \). As a bound for \( \mathcal{W}^2_2(\hat{\mu}_n, \hat{\nu}_n) \), \( \mathbb{E}L_{sq} \) appears to loosen slightly as \( n \) is increased. This is due to the differing rates of convergence of the two terms in the estimator \( L \) (recall that \( L_{sq} = \text{sign}(L)L^2 \)), where the first term \( \mathcal{W}^2_2(\hat{\mu}_n, \hat{\nu}_n) \) converges to \( \mathcal{W}^2_2(\mu, \nu) \) at rate \( n^{-2/d} \), while the second term \( \mathcal{W}^2_2(\hat{\mu}_n, \hat{\mu'}_n) \) converges to zero at a slower rate \( n^{-1/d} \). For large enough \( n \), the average \( \mathbb{E}L_{sq} \) does however converge from below to \( \mathcal{W}^2_2(\mu, \nu) \).

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Figure 1: Box plots for 100 of each estimator (left to right for each sample size) \( \mathcal{W}^2_2(\hat{\mu}_n, \hat{\nu}_n) \) \( (-) \), \( U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu'}_n) \) \( (\bullet) \) and \( L_{sq}(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu'}_n) \) \( (\star) \), compared with \( \mathcal{W}^2_2(\mu, \nu) \) \( (--) \). Distributions \( \mu = \mathcal{N}_d(0, I_d) \) and \( \nu = \mathcal{N}_d(0, \sigma^2 I_d) \) were compared. The sample size \( n \in \{10, 100, 1000\} \), the rows correspond to \( d \in \{10, 100\} \) and the columns correspond to \( \sigma^2 \in \{1.1, 2, 10\} \).

Secondly, we investigate how necessary the overdispersion condition \( \nu \sim \mu \) is for the upper bound of Theorem 1. For this, we plot the relative error of the estimator \( U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu'}_n) - \mathcal{W}^2_2(\mu, \nu) \), where \( \mu = \mathcal{N}_d(0, \text{diag}(1, 4, 1, 4, \ldots)) \), \( \nu = \mathcal{N}_d(0, \sigma^2 I_d) \), and the parameters vary
according to $(\sigma^2, d, n) \in \{1, 1.75, 2.5, 3.25, 4\} \times \{10, 100\} \times \{10, 100, 1000\}$. The range of \(\sigma^2\) is chosen so that \(\mu \sim \nu\) at \(\sigma^2 = 1\) (so that \(\mathbb{E}U\) is a lower bound according to Theorem 1), and \(\nu \sim \mu\) at \(\sigma^2 = 4\) (so that \(\mathbb{E}U\) is an upper bound according to Theorem 1). The results are shown in Figure 2, and suggest that overdispersion which is weaker than \(\nu \sim \mu\) may suffice for the upper bound of Theorem 1 to hold. The breaking point appears to be around \(\sigma^2 = 2.5\), at which point the traces of the covariances of \(\nu\) and \(\mu\) are identical, and above which the sum of the second moments of all components of \(\nu\) is larger than the corresponding quantity for \(\mu\).

![Figure 2: Box plots for the relative error of \(U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}'_n)\) (100 replicates) as an estimator of \(W_2^2(\mu, \nu)\), with dashed line at \(y = 0\). Distributions \(\mu = \mathcal{N}_d(0, \text{diag}(1, 4, 1, 4, \ldots))\) and \(\nu = \mathcal{N}_d(0, \sigma^2 I_d)\) were compared in dimension \(d = 10\) (left) and \(d = 100\) (right). Sample sizes were \(n = 10\) ( ), \(n = 100\) ( ), \(n = 1000\) ( ). Theorem 1 indicates a lower bound in expectation at the minimum of \(\sigma^2 = 1\), and an upper bound in expectation at the maximum of \(\sigma^2 = 4\).](image)

### 3 Uncertainty quantification

Having removed a large part of the bias in the empirical estimator of the Wasserstein distance, noise becomes a larger issue, and so now we quantify the uncertainty in the point estimators of the bounds (1), (2). We first derive a central limit theorem, following results in del Barrio and Loubes (2019); del Barrio et al. (2021). This motivates Gaussian confidence intervals for the upper bound (1). Lacking satisfactory distributional results, we suggest using Chebyshev’s theorem to obtain conservative confidence intervals for the lower bound (2).

Both types of confidence intervals rely on estimating the variance of the point estimators. We suggest doing so conservatively by the jackknife method (Efron and Stein, 1981), and we propose the Flapjack algorithm to compute the leave-one-out jackknife estimates efficiently.

#### 3.1 Central limit theorems and confidence intervals

We shall impose the following regularity conditions, borrowed from del Barrio et al. (2021).

**Assumption 3** (Regularity and bounded fourth moments). \(\mu, \nu \in \mathcal{P}(\mathbb{R}^d)\) are continuous, have connected supports with negligible boundary, and have finite moments of order \(4 + \delta\) for some \(\delta > 0\), that is \(\mathbb{E}_{\mu}\|X\|^{4+\delta} \leq \infty\) and \(\mathbb{E}_{\nu}\|Y\|^{4+\delta} \leq \infty\).
Under these conditions, a Gaussian central limit theorem holds for the estimator $U$. As noted by del Barrio and Loubes (2019); del Barrio et al. (2021), the limiting variance is null when $\mu = \nu$ (the Kantorovich potentials are constant). In this case, the theorem indicates that the variance of $U$ decreases strictly faster than the canonical rate $n^{-1}$. If a non-trivial limit of a similar type exists when $\mu = \nu$, its leading factor must grow strictly faster than $n^{1/2}$. The existence and form of such theorems are open questions for both $U$ and the plug-in estimator $W^2_2(\hat{\mu}_n, \hat{\nu}_n)$.

**Theorem 7** (Central limit theorem for the upper bound estimator). Under Assumptions 1 and 3, it holds that

$$n^{1/2}(U - E_U) \Rightarrow N(0, \sigma^2),$$

$$\lim_{n \to \infty} n \text{Var} U = \sigma^2.$$

$\sigma^2 = \text{Var}_\mu \varphi(X) + \text{Var}_\nu \psi(Y)$, and $(\varphi, \psi)$ are the Kantorovich potentials (see Appendix A) when transporting $\mu$ to $\nu$.

Theorem 7 motivates the usage of the usual Gaussian asymptotic confidence intervals for $E_U$ when $\mu \neq \nu$. Given an estimate $\hat{\sigma}^2$ of the variance of $U$, a $(1 - \alpha)$-level confidence interval is $[U - \hat{\sigma} z_{\alpha/2}, U + \hat{\sigma} z_{1-\alpha/2}]$. The coverage is asymptotically exact if the variance estimate $\hat{\sigma}^2$ is exact. When $\mu = \nu$, the asymptotic theory is lacking, and therefore such confidence intervals are currently out of reach (however note that the distribution of $U$ is symmetric about the origin). Chebyshev’s inequality could then be used to construct conservative confidence intervals for $U$, as we outline for the estimator $L$ below.

When $\mu \neq \nu$, following the proof of Theorem 4.9 in del Barrio et al. (2021) together with a simple observation, one can derive a non-trivial limit for $W_2(\hat{\nu}_n, \hat{\mu}_n)$ which is centered around its mean $E W_2(\hat{\nu}_n, \hat{\mu}_n)$ (see Appendix B.4). The method does not extend to obtain a centered limit for $W_2(\hat{\mu}_n', \hat{\mu}_n)$. As such, we have not been able to derive satisfactory central limits for the lower bound estimator $L$. In order to estimate conservative confidence intervals for $L$, we instead suggest using Chebyshev’s inequality. If $\hat{\tau}^2$ is an estimate of the variance of $L$, then a confidence interval with more than $(1 - \alpha)$ coverage is $[L - \hat{\tau} \alpha^{-1/2}, L + \hat{\tau} \alpha^{-1/2}]$. Compared to a Gaussian 95% confidence interval, a Chebyshev confidence interval is approximately 2.3 times wider.

### 3.2 Jackknife variance estimation

An estimate of the variance of a statistic $F(X_1, \ldots, X_n)$ can be obtained via the jackknife method (Efron and Stein, 1981). This proceeds by first computing the leave-one-out statistics $F_i = F(X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n)$ for $i = 1, \ldots, n$. Then, one combines these into the jackknife variance estimate

$$\frac{n-1}{n} \sum_{i=1}^{n} (F_i - \frac{1}{n} \sum_{i=1}^{n} F_i)^2.$$

The first term is a sample size correction, and the second term is a positively biased estimate of the sample size $n - 1$ variance, as per the Efron-Stein inequality (Efron and Stein, 1981).
3.2.1 The Flapjack algorithm

At sample size \( n \), an empirical transportation cost (including the squared empirical Wasserstein distance) is computed via a linear assignment problem of the following form,

\[
T = \min_x \sum_{i,j=1}^{n} c_{ij} x_{ij},
\]

\[
\text{s.t. } \sum_{k=1}^{n} x_{ik} = 1/n, \quad \sum_{k=1}^{n} x_{kj} = 1/n, \quad x_{ij} \geq 0, \quad \forall i,j = 1,\ldots,n.
\]

(3)

This is equivalent to the Kantorovich formulation of the optimal transportation problem. At the optimum, all \( x_{ij} \) are either 0 or \( 1/n \), such that there exists an optimal assignment (or matching) \( \sigma \in S_n \) with the property that \( i,j \in \{1,\ldots,n\}, x_{ij} = 1/n \) if and only if \( j = \sigma(i) \). This primal assignment problem admits the following dual formulation

\[
\max_{u,v} \frac{1}{n} \sum_{i=1}^{n} u_i + \frac{1}{n} \sum_{j=1}^{n} v_j,
\]

\[
\text{s.t. } u_i + v_j \leq c_{ij} \quad \forall i,j = 1,\ldots,n.
\]

To compute the jackknife variance estimate of the solution, one needs to first solve the \( n \) leave-one-out problems (3) at sample size \( n - 1 \). Since the exact computation of the sample size \( n \) problem takes \( O(n^3) \) time, naively computing the jackknife variance estimate would require a prohibitive \( O(n^4) \) time.

Starting from a joint solution of the sample size \( n \) primal and dual problems, it is however possible to compute the jackknife variance estimate of the cost in \( O(n^2) \) time, no worse than the complexity of solving the original optimization problem. As proven in Mills-Tettey et al. (2007), if only a single entry, row, or column of the cost matrix \( (c_{ij}) \) changes, then the Hungarian algorithm can be employed to solve the modified problem in \( O(n^2) \) time. This motivates the Flapjack algorithm (for Fast Linear Assignment Problem with JACKknife estimates), which repairs the sample size \( n \) optimal solution to solve the \( n \) sample size \( n - 1 \) sub-problems in \( O(n^2) \) time each. To compute the \( i \)-th leave-one-out estimate, we first change the cost \( c_{ii} \) to a small enough value, which forces \( x_{ii} = 1/n \) at the optimum, and then simply drop \( c_{ii} x_{ii} \) from the final objective value. The Flapjack algorithm is provided in Appendix E.1 as Algorithm 1.

3.3 Numerical illustration

In this section, we illustrate the behaviour of the jackknife variance estimator for \( U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}_{n}') \) when \( \mu = \mathcal{N}_d(0, I_d) \) and \( \nu = \mathcal{N}_d(0, \sigma^2 I_d) \) and the parameters vary according to \( (\sigma^2, d, n) \in \{1.1, 10\} \times \{10, 100\} \times \{10, 100, 1000\} \).

To simplify the presentation, and as the results are similar, we show no results for the plug-in estimator \( W^2_2(\hat{\mu}_n, \hat{\nu}_n) \) or the lower bound estimator \( L(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}_{n}') \). The jackknife variance estimates are compared with the variance of \( U \) in Figure 3. The jackknife variance estimates are conservative, and at worst are, in expectation, approximately a factor of 2 larger than the true variance. As \( \sigma^2 \) decreases, the jackknife estimates become progressively more conservative. We also find that 95%-level jackknife confidence intervals for the estimator \( U \), derived from the Gaussian limit of Theorem 7, have at least the nominal coverage for sample sizes \( n \geq 100 \).
Figure 3: Box plots of jackknife variance estimates for $U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}'_n)$ (■); empirical variance with bootstrap 95% confidence intervals (▪). Distributions $\mu = \mathcal{N}_d(0, I_d)$ and $\nu = \mathcal{N}_d(0, \sigma^2 I_d)$ were compared with, left to right, $\{(10, 1.1), (100, 1.1), (10, 10), (100, 10)\}$. For each sample size $n \in \{10, 100, 1000\}$, 500 replicates of the estimator and its jackknife variance estimator were computed. These 500 replicates were used to compute the empirical variance. Confidence intervals for the empirical variance were computed with 500 bootstrap samples.

4 Bounding the Wasserstein distance in MCMC

Let $(X_t)_{t \geq 0}$ represent an MCMC Markov chain where the time-$t$ marginals, $\pi_t$, and the stationary distribution, $\pi_\infty$, are all continuous and have finite second moments. Multiple independent copies of the chain are run generating empirical measures $\hat{\pi}_t$ for $t \geq 0$; with the same number of samples each, the two empirical measures $\hat{\pi}_\infty, \hat{\pi}'_\infty$ are drawn independently from the stationary distribution.

As long as the chain remains overdispersed with respect to its stationary distribution for all iterations $t \geq 0$, our empirical bounds can be applied to quantify the convergence of the Markov chain. In the following corollary, the first inequality restates Proposition 1, the second restates Theorem 1, and the third restates Theorem 2.

**Corollary 2** (Bounds for MCMC). Let $K$ be as in Proposition 1. If $\pi_t \overset{\text{cot}}{\leadsto} \pi_\infty$, then

$$K(\pi_t, \pi_\infty)W_2(\pi_t, \pi_\infty) \geq \mathbb{E} \left[ W_2^2(\hat{\pi}_t, \hat{\pi}_\infty) - W_2^2(\hat{\pi}'_\infty, \hat{\pi}_\infty) \right] \geq W_2^2(\pi_t, \pi_\infty).$$

In practice, independent samples from $\pi_\infty$ will not be available directly. However, we may estimate $\hat{\pi}_\infty \approx \hat{\pi}_T$ and $\hat{\pi}'_\infty \approx \hat{\pi}'_{T'}$ for some large for some large $T' < T$, chosen such that $X_T$ and $X_{T'}$ are approximately independent. In other words, we declare a priori that the chain has converged by time $T'$, and run it until a further iteration $T$ which produces samples approximately independently from iteration $T'$. The upper bound is useful to assess when before $T'$ the chain has reached the stationary distribution, and how it has done so.

4.1 Persistence of overdispersion in MCMC

In practice, one is unlikely to be able to verify the condition $\pi_t \overset{\text{cot}}{\leadsto} \pi_\infty$ for all $t \geq 0$, whether analytically or numerically. However, if one starts off a Markov chain from $\pi_0 \overset{\text{cot}}{\leadsto} \pi_\infty$, then one may hope that, throughout its lifetime, the Markov chain does remain overdispersed.
with respect to its target, or at least approximately so. This subsection is concerned
with checking whether this heuristic is reasonable, and when it might fail. We begin with
analytically tractable Gaussian scenarios, where the answer is affirmative, and follow up
with simulations in scenarios which are numerically tractable.

### 4.1.1 Analytically tractable scenarios

ULA and Gibbs chains which have Gaussian stationary and starting distributions also
have analytically tractable Gaussian marginals. As per Proposition 2, we can therefore
verify whether the overdispersion propagates throughout the marginals $\pi_t$, $t \geq 0$. We find
that this is indeed the case. However, caution is required: not starting the chains suitably
overdispersed also ensures that $\pi_0^{\cot} \not\sim \pi_\infty$.

**Theorem 8** (\(~\cot\) for chains with Gaussian marginals). Suppose that $\pi_t$ is the Gaussian
marginal distribution at time $t \geq 0$ of a Markov chain converging to a Gaussian stationary
distribution $\pi_\infty$. If the algorithm is (i) a deterministically updating Gibbs sampler, or (ii)
an unadjusted Langevin algorithm, then

$$
\pi_0^{\cot} \sim \pi_\infty \iff \pi_t^{\cot} \sim \pi_\infty \text{ for all } t \geq 0.
$$

The Gibbs sampler need not update its coordinates one-at-a-time, as the result remains
applicable for blocked Gibbs samplers as well.

### 4.1.2 Numerically tractable scenarios

Following Section 2.2, in dimension $d = 1$ one can check the condition $\pi_t^{\cot} \sim \pi$ by looking
at the relative separation of the quantiles of these distributions. Similarly, in general
dimension $d$, for samplers whose target $\pi$ and time-$t$ marginals $\pi_t$ are isotropic distribu-
tions, checking the condition $\pi_t^{\cot} \sim \pi$ simplifies to checking that the same relationship holds
between the radial components of these distributions. Samplers that are appropriately
isotropic include the random walk Metropolis (RWM) algorithm and the Metropolis-
Adjusted Langevin Algorithm (MALA) using proposals with isotropic Gaussian noise.

For the unimodal isotropic scenarios we investigated, $\pi_0^{\cot} \sim \pi_\infty$ caused $\pi_t^{\cot} \sim \pi_\infty$ for all $t \geq 0$. These examples correspond to diffusive MCMC samplers targeting unimodal
distributions, whose starting distributions are spread-out with respect to the target in
all directions. However, we found that multimodal targets can cause $\pi_t^{\cot} \sim \pi_\infty$ to not
hold for arbitrary $t > 0$, in spite of $\pi_0^{\cot} \sim \pi$ holding. For the RWM algorithm targeting
$\pi = 0.5\mathcal{N}_1(-5, 1) + 0.5\mathcal{N}_1(5, 1)$, a mixture distribution with well-separated modes, starting
from $\pi_0 = 0.5\mathcal{N}_1(-10, 4) + 0.5\mathcal{N}_1(10, 4)^{\cot}$ and using a step size $h = 2$ (an acceptance
rate of 50%), a single RWM chain seldom jumps between the modes, and $\pi_t^{\cot} \sim \pi_\infty$ holds
for all $t \geq 0$. Increasing the step size to $h = 6$ (an acceptance rate of 26%), a single RWM
chain jumps between the modes more frequently, causing $\pi_t^{\cot} \sim \pi_\infty$ to fail for iterations
$t \geq 1$. For the start $\pi_0 = 0.5\mathcal{N}_1(0, 1) + 0.5\mathcal{N}_1(10, 1)$, a shifted version of $\pi_\infty$, and $h = 2$,
the majority of the chains initially jump to one mode, causing $\pi_t^{\cot} \sim \pi_\infty$ to again fail for
$t \geq 1$. Figure 4, and Figure 9 in Appendix E.2 display the previously outlined results.

These examples highlight the potential challenges posed to our method by multimodal-
ity, while offering reassurance that $\pi_t^{\cot} \sim \pi_\infty$ for $t \geq 0$ can hold for diffusive MCMC samplers
started at $\pi_0^{\cot} \sim \pi_\infty$ and targeting unimodal distributions.
4.2 Confidence intervals in MCMC

Just as before in Section 3.1, we have a Gaussian central limit theorem for the upper bound estimator in MCMC. This follows from Proposition 3 (Appendix B).

**Theorem 9** (CLT for MCMC setting). Suppose that $\pi_t, \pi_T, \pi_T'$ satisfy Assumption 3. Then,

$$n^{1/2} \left( U(\hat{\pi}_t, \hat{\pi}_T, \hat{\pi}_{T'}) - \mathbb{E} U(\hat{\pi}_t, \hat{\pi}_T, \hat{\pi}_{T'}) \right) \Rightarrow \mathcal{N}(0, \sigma^2),$$

$$\lim_{n \to \infty} n \text{Var} U(\hat{\pi}_t, \hat{\pi}_T, \hat{\pi}_{T'}) = \sigma^2.$$

The limiting variance is $\sigma^2 = \text{Var}\{\phi_{t\to T}(X_t) + \phi_{T\to t}(X_T) + \phi_{T\to T'}(X_T) + \phi_{T'\to T}(X_T')\}$, where $\phi_{t\to T}$ is the Kantorovich potential (see Appendix A) associated to $\pi_t$ when transporting $\pi_t$ to $\pi_T$.

If $\pi_t, \pi_T, \pi_{T'}$ are all distinct, then both terms in $L(\hat{\pi}_t, \hat{\pi}_T, \hat{\pi}_{T'})$ have Gaussian weak limits. However, even if their linear combination were to have a Gaussian weak limit, our methodology relies on $\pi_{T'}$ and $\pi_T$ both being very close to $\pi$, and so we are perilously close to the boundary case where the distributional limit is unknown. We therefore opt for Chebyshev confidence intervals for $L$, obtained using jackknife variance estimates. To compute a confidence interval for $\mathbb{E} L_{sq}$, we scale up the confidence interval for $\mathbb{E} L$.

4.3 Proposed procedure

Provided one has confidence that the chain is close to stationarity by iteration $T$, and is at least close to overdispersed with respect to the stationary distribution at all time points $t$ of interest, we propose the following method in order to estimate upper and lower bounds on $W_2^2(\pi_t, \pi_\infty)$. We apply the subsequent procedure in all our numerical experiments.

Compute and plot $W_2^2(\hat{\pi}_t, \hat{\pi}_T)$ for $t \in \{0, 1, \ldots, T\}$. If the chain has reached stationarity some time before $T$, then the graph will have asymptoted parallel to the abscissa (for $t$ very close to $T$, the correlation of the samples in $\hat{\pi}_t$ and those in $\hat{\pi}_T$ means that
$W_2^2(\hat{\pi}_t, \hat{\pi}_T)$ leaves the asymptote and approaches zero). Samples $\hat{\pi}_t$ in the asymptote are essentially from the stationary distribution and are very weakly correlated with $\hat{\pi}_T$, so one would choose $T'$ to be somewhere in the asymptote. Therefore, as opposed to debiasing $W_2^2(\hat{\pi}_t, \hat{\pi}_T)$ by only a single term $W_2^2(\hat{\pi}_T', \hat{\pi}_T)$ in order to obtain the estimator $U$, instead “average in the asymptote” over all reasonable values of $T' \in A$ (for variance reduction purposes), and use the estimator

$$W_2^2(\hat{\pi}_t, \hat{\pi}_T) - \frac{1}{|A|} \sum_{T' \in A} W_2^2(\hat{\pi}_T', \hat{\pi}_T) \geq W_2^2(\pi_t, \pi_\infty)$$  \hspace{1cm} (4)

as the analogue of $U$. Similarly, on the scale of $W_2$ instead of its square, use

$$W_2(\hat{\pi}_t, \hat{\pi}_T) - \frac{1}{|A|} \sum_{T' \in A} W_2(\hat{\pi}_T', \hat{\pi}_T) \leq W_2(\pi_t, \pi_\infty).$$  \hspace{1cm} (5)

as the analogue of $L$. Analogously to the estimator $L_{sq}$, obtain an estimator of a lower bound on $W_2^2(\pi_t, \pi_\infty)$ by squaring and keeping the sign.

Uncertainty quantification for the time-averaged estimators can be achieved through jackknife variance estimates. Using the Flapjack algorithm (Algorithm 1), obtain the leave-one-out estimates for $W_2^2(\hat{\pi}_t, \hat{\pi}_T)$ for $t \in \{0, 1, \ldots, T\}$. By averaging these, and respectively square-rooting and then averaging, obtain the leave-one-out estimates for the estimators (4) and (5), from which jackknife variance estimates can be computed. Proposition 3 (Appendix B) generalizes Theorem 9, and motivates Gaussian confidence intervals for the estimator (4). Chebyshev-based confidence intervals for (5) are calculated as described in Section 4.2.

4.4 Numerical experiments

We illustrate the use of the estimators $U$ and $L_{sq}$ in MCMC on three examples. The first is an analytically tractable Gibbs sampler from Wilkinson (2020), where we are able to compute the exact squared Wasserstein distance. The second example, adapted from Biswas et al. (2019), concerns the dimensional scaling of the mixing times of the Unadjusted Langevin Algorithm (ULA) and its Metropolis-Adjusted variant (MALA). The final example is a stochastic volatility model adapted from from Liu (2001); Girolami and Calderhead (2011). Throughout, we compare our bounds to the 2-Wasserstein distance analogue of the coupling bound in Biswas et al. (2019) (see Appendix D). We use a sample of $n = 1000$ chains throughout the experiments. Appendix E contains further details on these numerical experiments.

4.4.1 Gaussian Gibbs sampler

A Gibbs sampler was run on a highly correlated Gaussian target $\pi$ in moderate dimension, starting from a version of the target which is spread-out by a factor of 2 (the densities are related by $\pi_0(x) \propto \pi(x/2)$, such that $\pi_0 \sim \pi$). In this setting, the squared Wasserstein distance $W_2^2(\pi_t, \pi)$ is available in closed form, and the empirical upper bound $U$ on $W_2^2(\pi_t, \pi)$ is known to be valid due to the overdispersed start (see Theorem 8).

The target is a multivariate Gaussian generated by an AR(1) process with a periodic boundary, in dimension $d = 50$ and with autocorrelation $\rho = 0.95$ (see Wilkinson, 2020, for a similar target). If $X = (X_1, \ldots, X_d)^T \sim \pi$, the random variable satisfies

$$X_{k+1} = \rho X_k + \varepsilon_k, \quad \varepsilon_k \sim \mathcal{N}(0, 1), \quad \text{for } k \in \{1, \ldots, d\},$$
\[ X_{d+1} = X_1. \]

The residuals \( \varepsilon_k \) are independent of each other, but are not independent of \( X_k \). The precision matrix of \( \pi \) is a sparse circulant matrix, having null entries apart from the tridiagonal and the top-right and bottom-left corners. The high correlation between the coordinates of the target causes the Gibbs sampler to mix slowly.

![Figure 5: Estimated bounds on \( W^2_2(\pi_t, \pi_\infty) \) for the Gibbs sampler (— U; — \( L_{sq} \); — coupling; — exact). Shaded areas represent 95% jackknife confidence intervals. The inset plot zooms in on the y-axis near 0.](image)

Figure 5 shows that the empirical upper bound \( U \) is close to the true squared distance for all but the first few iterations. This occurs even though the dimension \( (d = 50) \) is relatively large, because the target is approximately confined to a much lower-dimensional manifold, as is explained in more detail in Appendix E.3. The upper bound degenerates into pure noise at large enough iterations \( t \). The lower bound appears to be less noisy than the upper bound, but it is also looser than it. The coupling bound is also rather loose relative to the upper bound \( U \). For instance, considering the threshold \( W^2_2(\pi_t, \pi_\infty) \leq 10 \), the upper bound \( U \) reaches this after 500 iterations, while 2000 iterations are required for the coupling bound. The relatively poor performance of the coupling bound is due to the sub-optimal coupling employed. At the cost of additional tuning parameters, a multiscale coupling strategy which employs common random numbers when the chains are far apart, similarly to that in Bou-Rabee et al. (2020) for Hamiltonian Monte Carlo, may yield a tighter coupling bound in this example. However, we expect the empirical bound to still provide a noticeable improvement over this.

### 4.4.2 Dimensional scaling of ULA and MALA

The behaviour of the mixing time of the Metropolis-Adjusted Langevin Algorithm (MALA) and the Unadjusted Langevin Algorithm (ULA) has been extensively studied in the last few years, with particular attention being given to its dimensional dependence. See Durmus and Moulines (2019); Li et al. (2021); Chewi et al. (2021); Wu et al. (2021) for recent theoretical contributions to this area. In contrast to theoretical bounds, which may only be informative in the very high-dimensional regime, our empirical bounds are informative in the low-to-moderate dimensional setting as well.
Following Section 3.3 in Biswas et al. (2019), we bound the mixing time of ULA and MALA on the target \( \pi = \mathcal{N}_d(0, \Sigma) \), where \( \Sigma_{ij} = 0.5|\cdot - \cdot| \), and the dimension \( d \) is varied. As opposed to Biswas et al. (2019), we start from the initial distribution \( \pi_0 = \mathcal{N}_d(0, 3I_d) \) which satisfies \( \pi_0 \overset{\text{cot}}{\to} \pi \) (see Appendix E.4 for details). We scale MALA with \( h = d^{-1/6} \), for an acceptance rate of around 70%, following the optimal scaling result of Roberts and Rosenthal (1998) at stationarity. The step size of ULA is \( h = 0.2d^{-1/4} \), which maintains the stationary distribution of ULA close to \( \pi \) even as the dimension grows (see Durmus and Moulines, 2019, Corollary 9, and Durmus and Eberle, 2021).

![Figure 6: Estimated mixing time bounds at the \( \mathcal{W}_2^2(\pi_t, \pi_\infty) \leq 6 \) threshold (\( \blacktriangle \) U; \( \blacksquare \) \( L_{sq} \); \( \bullet \) coupling; \( \ast \) exact), for the MALA (solid lines) and ULA (dashed lines). The sequence of targets was Gaussian and satisfied a uniform condition number bound for dimensions \( d \in \{50, \ldots, 1000\} \). Both the y- and x-axes are on a log_{10}-scale.](image)

Results are displayed in Figure 6. While theoretical results which apply to our setting (Durmus and Moulines, 2019; Li et al., 2021) indicate a mixing time bound of \( O(d^{1/2} \log(d)) \) for ULA, we observe the mixing time to scale closer to \( \approx d^{4/5} \) in our experiment, improving slowly as the dimension is increased. While our largest dimension considered (\( d = 1000 \)) is relatively large in MCMC contexts, this appears to be relatively small for the asymptotic regime considered in Durmus and Moulines (2019); Li et al. (2021). Hence, while we expect the trend to approach \( d^{1/2} \log(d) \) as the dimension becomes large enough, our results suggest that, if only the dimension is considered, theoretical bounds on the mixing time can be misleading in scenarios of practical interest. Given the much larger step size of MALA, it is of no surprise that it converges much faster than ULA. At the same time, in spite of its step size scaling more favorably with the dimension, the mixing time of MALA seems to scale similarly to that of ULA.

The coupling bound suggests a similar scaling of the mixing time with the dimension for both samplers. However, our empirical upper bound improves on the coupling bound by a factor of 3 to 10 throughout. As the stationary distribution of ULA is overdispersed with respect to the target, our empirical upper and lower bounds can also be used to quantify the bias of ULA at stationarity (see Appendix E.4).
4.4.3 Stochastic volatility model

We investigate the stochastic volatility model in Liu (2001); Girolami and Calderhead (2011) for approximately a year’s worth of data (see Appendix E.5 for details). The hyperparameters are fixed at the true values, and the data are generated from the model. Inference is performed on the latent process conditional on the data, and all samplers are started from the prior distribution of the latent process as sampling from the prior is a frequently used technique to obtain a sample overdispersed with respect to the posterior. This start does not provably satisfy $\pi_0 \rightarrow \pi_\infty$, however a similar bound was obtained from a start which did satisfy the condition (see Appendix E.5), thereby lending credibility to the start-from-the-prior heuristic.

![Figure 7: Estimated bounds on $W^2_2(\pi_t, \pi_\infty)$ for optimally scaled MALA (left) and RWM (right) on the stochastic volatility model ($U$; $L_{sq}$; coupling). Shaded areas represent 95% jackknife confidence intervals. No coupling bound is computed for the RWM. The inset plots zoom in on the $y$-axis near $y = 0$.](image)

Scaling MALA and the RWM optimally for mixing (56% and 24% acceptance rates, respectively), we obtain the results in Figure 7. The empirical bounds suggest that MALA converges more than an order of magnitude quicker than the RWM. The coupling bound is relatively competitive for MALA, although it still suggests a factor of 2 to 3 worse mixing time than the empirical bound. For the RWM, however, the coupled chains coalesce extremely slowly, with 50 pilot chains all failing to meet within $10^8$ iterations, and so we are therefore unable to effectively use the coupling bound in this case.

![Figure 7: Estimated bounds on $W^2_2(\pi_t, \pi_\infty)$ for optimally scaled MALA (left) and RWM (right) on the stochastic volatility model ($U$; $L_{sq}$; coupling). Shaded areas represent 95% jackknife confidence intervals. No coupling bound is computed for the RWM. The inset plots zoom in on the $y$-axis near $y = 0$.](image)

Lowering the step size of the RWM by a factor of 2.5 (for an acceptance rate of 64%), the coupled chains now coalesce quicker, and we obtain the results in Figure 8. However, the coupling bound still suggests mixing times more than an order of magnitude larger than the empirical bound does. On the one hand, this shows the different objectives of optimal coalescence with a given coupling and optimal mixing may lead to conflicting tunings for MCMC algorithms. On the other hand, the simulation exposes the difficulty in designing effective practical couplings of Markov chains.

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Figure 8: Estimated bounds on $W^2_2(\pi_t, \pi_\infty)$ for the RWM with a small scaling, on the stochastic volatility model ($-U; -L_{sq}; -$ coupling). Shaded areas represent 95% jackknife confidence intervals. Left: zooming in on the empirical bounds, inset plot zooms in further near $y = 0$. Right: empirical and coupling bounds, $y$-axis transformed by $\log_{10}(1 + y)$, $x$-axis transformed by $\log_{10}x$.

5 Discussion

5.1 General remarks

Under a condition on the Lipschitz constant of the optimal transport map, which we interpret as an overdispersion condition, we show that an upper bound $U$ on the squared 2-Wasserstein distance can be obtained by a simple debiasing of the plug-in estimator. This is complemented by a lower bound $L$ on the Wasserstein distance, obtained at negligible additional cost. In comparison to the plug-in estimator, the debiased estimator $U$ has the advantage of decaying, on average, in proportion to the true Wasserstein distance. When the Wasserstein distance is relatively small, the debiased estimator attains a large improvement in average absolute error. At the same time, similar to the plug-in estimator, the average relative error of the debiased estimator becomes worse as the Wasserstein distance becomes smaller. As our estimator is a linear combination of plug-in estimators, we see no improvement in the rate of convergence to the true Wasserstein distance as the sample size increases. This stresses the fundamental difficulty in accurately estimating the Wasserstein distance from independent samples.

Under a compact support assumption, the point estimators $U$ and $L$ concentrate around their means with (nearly) sub-Gaussian tails. Coupled with results on the rate of convergence of these estimators under a continuity assumption, the point estimators themselves are seen to be reliable bounds with high probability. Namely, both the probability that $U$ is not an upper bound, and the probability that $L$ is not a lower bound, decay exponentially quickly in the sample size $n$.

Building on work in Mills-Tettey et al. (2007), we have suggested a procedure to efficiently compute the jackknife variance estimate to the solution of a linear assignment problem. This applies to empirical transportation costs, and all our suggested estimators. Central limit theorems enable the use of Gaussian jackknife confidence intervals for our estimator $U$ of the upper bound (1) on the squared Wasserstein distance. However, uncertainty quantification for our estimator $L$ of the lower bound (2) is hampered by a lack of satisfactory limit theorems for the unsquared Wasserstein distance. We leave such
limit theorems for future work, and suggest the use of Chebyshev confidence intervals instead.

5.2 MCMC

Our bounds can be used to understand the convergence properties of MCMC algorithms sampling continuous distributions, by running multiple chains which start and remain overdispersed with respect to their stationary distributions. As with the coupling upper bound of Biswas et al. (2019), our bounds can accurately quantify burn-in, and allow the comparison of various approximate or exact MCMC algorithms targeting the same distribution. Numerically, we find that mixing time upper bounds from our empirical upper bound uniformly improve on those from the coupling bound, even beyond an order of magnitude. The coupling bound requires no overdispersion assumption, and so applies more generally than our empirical upper bound. The usefulness of the coupling bound, however, crucially hinges on how effective the coupling is, and we found the empirical upper bound $U$ to be uniformly tighter than the coupling bound in our experiments in Section 4.4. Both the coupling and empirical techniques are embarrassingly parallel, and so are suitable for use in a massively parallel MCMC environment. We believe our bound will prove useful to researchers who wish to empirically compare the convergence of various samplers targeting the same distribution.

Due to the error incurred from discretizing the Langevin dynamics, in our experiment in Section 4.4.2 the stationary distribution of ULA was overdispersed with respect to the stationary distribution of MALA, in terms of our notion of contractive optimal transport. It would be of interest to see if this holds beyond the Gaussian case we have considered, and furthermore whether other approximate algorithms also converge to an overdispersed version of their intended target. If so, our upper bound \( U \) could be used to quantify the bias of approximate MCMC algorithms more generally.

The potential scale reduction factor $\hat{R}$ (Gelman and Rubin (1992); Brooks and Gelman (1998); see also the recent extension in Vehtari et al. (2021)) is a widely-used heuristic for assessing the convergence of Markov chains. Similarly to our work, the potential scale reduction factor assumes that multiple chains start and remain overdispersed with respect to the target, also considers information between chains, and the scalar statistic $\hat{R}$ converges (to a value of one) as the chains approach their limiting distributions. Our work is however better motivated theoretically, as our notion of overdispersion is explicitly defined, if in terms of an abstract condition. Moreover, our bounds are tied to a strong notion of convergence. While weak convergence of the chains is guaranteed by the convergence of the Wasserstein distance to zero, convergence of the potential scale reduction factor to one need not imply weak convergence, even if the Markov chains do not undergo pathological behaviour.

5.3 Additional related work

Very recent work has sought to exploit the smoothness and strong convexity of the Bre- nier potential in order to analyze the rate of convergence with the sample size $n$ of the plug-in Wassertein distance estimator (Ghosal and Sen, 2021; Hütter and Rigollet, 2021; Deb et al., 2021; Manole et al., 2021), propose estimators with improved rates of convergence under additional smoothness conditions on the potential (Hütter and Rigollet, 2021; Deb et al., 2021; Manole et al., 2021), and propose new estimation procedures for
the Wasserstein distance (Paty et al., 2020).

In particular, in independent parallel work (Manole et al., 2021, Proposition 12), a result similar to our Theorem 1 is obtained, under the condition that the Brenier potential is smooth and strongly convex. Termed a “stability bound”, such results have been used to analyze the convergence with the sample size \( n \) of estimators of Wasserstein distances and transportation costs (Ghosal and Sen, 2021; Hütter and Rigollet, 2021; Deb et al., 2021; Manole et al., 2021). Our contribution is inherently different, as we use our theoretical results to remove a large portion of the bias of the empirical Wasserstein distance, and also apply our work to accurately quantify the Wasserstein distance in MCMC. Nonetheless, the stability bound of (Manole et al., 2021, Proposition 12) can be used to prove the upper bound (1). Furthermore, it can be used to show that the rate of convergence of the upper bound estimator is no faster than \( n^{-2/d} \) when \( d \geq 5 \) (see Appendix C.1).

5.4 Further work

Our experiments in Section 2.4 suggest that the condition \( \nu^{\text{cot}} \rightharpoonup \mu \) is loose for the sufficiency of the upper bound (1). It may be possible to weaken this condition if one only wishes the upper bound (1) to hold for large finite values of \( n \).

Uncertainty quantification for the lower bound (2) is hindered by a lack of a central limit theorem for the term \( W_2(\hat{\nu}_n^\pi, \hat{\mu}_n) \). Even characterizing when the variance of this statistic decays at a rate faster than \( 1/n \) would immediately enable much tighter confidence intervals to be computed for the lower bound (2). Results on the validity of the bootstrap for optimal transportation costs in the continuous case are also of interest, since the procedure in Sommerfeld et al. (2019) could be used to efficiently compute both the empirical transportation cost and its bootstrap sample. Progress here has been made in the case where the distributions are known to be Gaussian (Rippl et al., 2016), although a different estimator of the Wasserstein distance is used.

Investigating whether it is possible to extend bounds of the type (1) to general transportation costs would be of interest. As Brenier’s theorem seems crucial to our characterization of a sufficient condition under which the bound (1) holds, the characterization of the optimal transport map for general costs (Gangbo and McCann, 1996) may prove to be key to the generalization. An extension of the bound (1) to entropic transportation costs would also be of interest. Such extensions would automatically imply stability bounds as in Manole et al. (2021).

In a multiple-chain MCMC context, the assignment computed with \( W_2^2(\hat{\pi}_t, \hat{\pi}_T) \) may contain additional information to complement the empirical bounds. For instance, if one tracks the assignments for iterations \( t \in \{0, 1, \ldots \} \) and observes clustering, that may indicate that the chains are trapped in local modes of the target.

Analytical derivations in the Gaussian case show that the stationary distribution of the ULA is overdispersed with respect to its target, in terms of a Loewner ordering of the covariance matrices. This enables the upper bound (1) to be used to quantify the stationary bias of the ULA. Formally establishing the overdispersion of the stationary distribution of ULA beyond the Gaussian case would increase the applicability of the upper bound (1) to quantify the stationary bias of the ULA. Similarly, it may also be possible to apply the bound (1) to quantify the bias of other types of approximate MCMC algorithms, such as stochastic gradient Markov chain Monte Carlo (e.g. Nemeth and Fearnhead, 2021).
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Supplementary material

The supplementary material contains additional background on optimal transport and convexity (Appendix A), all proofs (Appendix B), a discussion on immediate generalizations of results in the main body of the paper and of selected results related to the proofs (Appendix C), a discussion on extending the methodology in Biswas et al. (2019) to 2-Wasserstein distances (Appendix D), and finally additional details on the numerical experiments (Appendix E).

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A Additional background

A.1 Quadratic optimal transport

The squared Wasserstein distance \( W_2^2(\mu, \nu) \) admits a dual formulation (Villani, 2009, Theorem 5.10), which is often easier to manipulate than the primal formulation. Letting \( \Phi = \{ (\psi, \tilde{\psi}) \in L^1(\mu) \times L^1(\nu) : \psi(x) - \tilde{\psi}(y) \leq \|x - y\|^2 \} \), the (Kantorovich) dual formulation reads

\[
W_2^2(\mu, \nu) = \sup_{(\psi, \tilde{\psi}) \in \Phi} (\mathbb{E}_\mu \psi(X) - \mathbb{E}_\nu \tilde{\psi}(Y)).
\]  

(6)

When the measures \( \mu = \hat{\mu}_n = \sum_{i=1}^n \delta_{X_i}/n \) and \( \nu = \hat{\nu}_n = \sum_{i=1}^n \delta_{Y_i}/n \), the primal formulation of the squared Wasserstein distance \( W_2^2(\hat{\mu}_n, \hat{\nu}_n) \) can be rewritten in terms of a minimization problem over permutations, as follows:

\[
W_2^2(\hat{\mu}_n, \hat{\nu}_n) = \min_{\sigma \in S_n} \frac{1}{n} \sum_{i=1}^n \|X_i - Y_{\sigma(i)}\|^2.
\]  

(7)
The optimal coupling for the squared Wasserstein distance $W_2^2(\hat{\mu}_n, \hat{\nu}_n)$ is degenerate, in the sense that there exist one or more optimal permutations $\sigma \in \mathcal{S}_n$ mapping the points $(X_1, \ldots, X_n)$ to $(Y_1, \ldots, Y_n)$.

Another case in which an optimal transport map exists is when the measure $\mu$ is continuous (Brenier, 1991; McCann, 1995). Here, the result commonly known as Brenier’s Theorem states that there exists a unique map which transports $\mu$ to $\nu$ which is also the gradient of a convex function, and furthermore that this is the unique optimal transport map. The convex function associated to the map is known as a Brenier potential. If both $\mu$ and $\nu$ are continuous, then there similarly exists an optimal transport map from $\nu$ to $\mu$, uniquely determined as the gradient of a convex function. In this case, the Brenier potentials are Legendre-Fenchel conjugates of each other (see McCann, 1995, Remark 16). The Legendre-Fenchel conjugate $\tilde{\phi}$ of $\phi$ is defined as $\tilde{\phi}(x) = \sup_y \{x^T y - \phi(y)\}$. Theorem 10 below formally states the results described in this paragraph.

**Theorem 10** (Brenier’s Theorem). Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ have finite second moments.

(i) If $\mu$ is continuous, then there exists a convex function $\phi : \mathbb{R}^d \to \mathbb{R}$ such that its gradient $\nabla \phi$ pushes $\mu$ forward to $\nu$. The map $\nabla \phi$ is $d\mu$-almost everywhere uniquely determined among all gradients of convex functions which push $\mu$ forward to $\nu$. Furthermore, $\nabla \phi$ is the optimal transport map.

(ii) If furthermore $\nu$ is continuous, then the (convex) Legendre-Fenchel conjugate $\tilde{\phi} : \mathbb{R}^d \to \mathbb{R}$ of $\phi$ satisfies that its gradient $\nabla \tilde{\phi}$ is the $d\nu$-almost everywhere uniquely determined optimal transport map from $\nu$ to $\mu$. This map is the inverse of $\nabla \phi$ in the sense that $(\nabla \tilde{\phi} \circ \nabla \phi)(x) = x$ for $d\mu$-almost all $x$ and $(\nabla \phi \circ \nabla \tilde{\phi})(y) = y$ for $d\nu$-almost all $y$.

We emphasize that, as consequence of Theorem 10, once one finds a map which transports $\mu$ to $\nu$ which is of the form $\nabla \phi$ with $\phi$ convex, then one has also found the optimal transport map.

Let us also remark on some subtle technicalities regarding Theorem 10, which will however not pose additional challenges to our later proofs. In Theorem 10, the gradients $\nabla \phi$ and $\nabla \tilde{\phi}$ may not be defined everywhere on $\mathbb{R}^d$. As the functions $\phi, \tilde{\phi}$ are both convex, the gradients $\nabla \phi, \nabla \tilde{\phi}$ are however well-defined $d\mu$-almost everywhere and $d\nu$-almost everywhere, respectively, and so these gradients are also well-defined as push-forward maps. While the transport map $\nabla \phi$ is unique $d\mu$-almost everywhere, the associated Brenier potential $\phi$ need not be so in general, although it is unique up to the addition of a constant under mild regularity assumptions (see, for instance, del Barrio et al., 2021, Corollary 2.7).

### A.2 Duality between strong convexity and Lipschitz continuous gradient

We call $f : \mathbb{R}^d \to \mathbb{R}$ $m$-strongly convex ($m > 0$) if there exists a convex $g : \mathbb{R}^d \to \mathbb{R}$ such that for all $x \in \mathbb{R}^d$ it holds that $f(x) = m\|x\|^2/2 + g(x)$.

It is known that, for scalar fields, a duality result exists between strong convexity and Lipschitz continuous gradient (also known as “strong smoothness”). Specifically, a function $\phi : \mathbb{R}^d \to \mathbb{R}$ is $1/L$-strongly convex function if and only if its Legendre-Fenchel dual is $\tilde{\phi} : \mathbb{R}^d \to \mathbb{R}$ is differentiable and its gradient $\nabla \tilde{\phi}$ is $L$-Lipschitz. This is essentially proven in Kakade et al. (2012, Theorem 3), with the remark that their definition of
strong smoothness is equivalent to the potential $\tilde{\phi}$ being differentiable and its gradient being Lipschitz continuous.

**Lemma 1.** Let $L > 0$ and $\varphi$ and $\tilde{\varphi}$ be convex conjugates. Then, $\varphi$ is $(1/L)$-strongly convex if and only if $\tilde{\varphi}$ is differentiable and $\nabla \tilde{\varphi}$ is $L$-Lipschitz.

We additionally have the following lemma, which characterizes the form of differentiable convex functions with Lipschitz continuous gradient.

**Lemma 2.** Let $f : \mathbb{R}^d \to \mathbb{R}$ be a differentiable function. If $\nabla f$ is $1$-Lipschitz, then $g(x) = \|x\|^2/2 - f(x)$ is convex.

**Proof.** The map $g(x) = \|x\|^2/2 - f(x)$ is differentiable. It suffices to show that $g$ is convex. For all $x, y$ we have that

$$(x - y)^T(\nabla g(x) - \nabla g(y)) = (x - y)^T(x - y + \nabla f(x) - \nabla f(y))$$

$$= \|x - y\|^2 - (x - y)^T(\nabla f(x) - \nabla f(y))$$

$$\geq \|x - y\|^2 - \|x - y\|\|\nabla f(x) - \nabla f(y)\| \quad \text{(Cauchy-Schwarz)}$$

$$\geq \|x - y\|^2 - \|x - y\|^2 = 0. \quad \text{(}\nabla f\text{ is 1-Lipschitz)}$$

By the first-order definition of convexity, $g$ is convex, which completes the proof.

Theorem 10 asserts that Brenier potentials are convex conjugates of each other. As a corollary of Lemmas 1 and 2 therefore, the following result characterizes the form of the Brenier potentials when the overdispersion condition $\nu \sim \cot \mu$ holds. We shall use it in the proof of Theorem 1.

**Corollary 3.** Let $\varphi, \tilde{\varphi}$ be as in Brenier’s theorem. If $\tilde{\varphi}$ is differentiable and $\nabla \tilde{\varphi}$ is $1$-Lipschitz, then there exist convex functions $f, g : \mathbb{R}^d \to \mathbb{R}$ such that $\varphi(x) = \|x\|^2/2 + f(x)$ and $\tilde{\varphi}(x) = \|x\|^2/2 - g(x)$.

**Proof.** By Lemma 2, $\tilde{\varphi}(x) = \|x\|^2/2 - g(x)$ for some convex function $g$. Now, by Theorem 10, $\varphi$ and $\tilde{\varphi}$ are convex conjugates of each other. Since $\tilde{\varphi}$ is differentiable and $\nabla \tilde{\varphi}$ is 1-Lipschitz, by Lemma 1 it follows that $\varphi$ is 1-strongly convex. By the definition of strong convexity, it follows that $\varphi(x) = \|x\|^2/2 + f(x)$ for some convex $f$, which completes the proof.

**B Proofs**

A key ingredient to our proof of Theorem 1 is the non-negative bias of the empirical squared Wasserstein distance $W_2^2(\hat{\mu}_m, \hat{\nu}_n)$. This result also generalizes to arbitrary empirical transportation costs.

**Lemma 3.** Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ be two distributions with finite second moments. For $m, n \in \mathbb{N}$, draw $X_1, \ldots, X_m \sim \mu$ and $Y_1, \ldots, Y_n \sim \nu$ not necessarily independently, and define empirical measures $\hat{\mu}_m = \sum_{i=1}^m \delta_{X_i}/m$ and $\hat{\nu}_n = \sum_{i=1}^n \delta_{Y_i}/n$. Then,

$$\mathbb{E}W_2^2(\hat{\mu}_m, \hat{\nu}_n) \geq W_2^2(\mu, \nu).$$
Proof of Lemma 3. This is a straightforward consequence of Kantorovich duality. Let
\[ \hat{\Phi} = \{(\varphi, \psi) \in L^1(\hat{\mu}_m) \times L^1(\hat{\nu}_m) : \varphi(x) - \psi(y) \leq \|x - y\|^2 \}, \]
\[ \Phi = \{(\varphi, \psi) \in L^1(\mu) \times L^1(\nu) : \varphi(x) - \psi(y) \leq \|x - y\|^2 \}. \]
As \( L^1(\mu) \subseteq L^1(\hat{\mu}_m) \) and \( L^1(\nu) \subseteq L^1(\hat{\nu}_m) \), we have that \( \hat{\Phi} \subseteq \Phi \). Now, by Kantorovich duality (6),
\[ \mathbb{E}W_2^2(\hat{\mu}_m, \hat{\nu}_m) = \mathbb{E} \left[ \sup_{(\varphi, \psi) \in \hat{\Phi}} \left( \mathbb{E}_{\hat{\mu}_m, \varphi}(X) - \mathbb{E}_{\hat{\nu}_m, \psi}(Y) \right) \right] \]
\[ \geq \mathbb{E} \left[ \sup_{(\varphi, \psi) \in \Phi} \left( \mathbb{E}_{\mu_n, \varphi}(X) - \mathbb{E}_{\nu_n, \psi}(Y) \right) \right], \quad (\Phi \subseteq \hat{\Phi}) \]
which, by the convexity of the supremum and Jensen’s inequality, is
\[ \geq \sup_{(\varphi, \psi) \in \Phi} \mathbb{E} \left( \mathbb{E}_{\hat{\mu}_m, \varphi}(X) - \mathbb{E}_{\hat{\nu}_m, \psi}(Y) \right) \]
\[ = \sup_{(\varphi, \psi) \in \Phi} \left( \mathbb{E}_{\hat{\mu}_m, \varphi}(X) - \mathbb{E}_{\hat{\nu}_m, \psi}(Y) \right) \]
\[ = W_2^2(\hat{\mu}, \hat{\nu}). \quad \text{(Kantorovich duality)} \]
This completes the proof. \( \square \)

Another key ingredient to the proofs of Theorems 1, 2 and Proposition 1 is the following implication of Assumption 1. As long as \( \hat{\mu}_n \) is independent of both \( \hat{\nu}_n \) and \( \hat{\mu}_n \), notice that \( \mathbb{E}W_2^2(\hat{\nu}_n, \hat{\mu}_n) - \mathbb{E}W_2^2(\hat{\mu}_n', \hat{\mu}_n) \) remains the same whether the empirical measures \( \hat{\nu}_n \) and \( \hat{\mu}_n' \) are dependent or not. We shall induce a strong dependence between \( \hat{\nu}_n \) and \( \hat{\mu}_n' \) by sampling \((X_i, Y_i)\) from the optimal coupling of \( \mu, \nu \), independently for all \( i \in \{1, \ldots, n\} \).

### B.1 Main results

We prove our main result, Theorem 1, which states empirical bounds on \( W_2^2(\mu, \nu) \).

**Proof of Theorem 1.** Let \( X, Z \sim \mu \) and \( Y \sim \nu \). To simplify the notation, we drop the subscript \( n \) from the empirical measures \( \hat{\mu}_n, \hat{\mu}_n' \) and \( \hat{\nu}_n \), as well as from the set of permutations \( S_n \). Define \( A = W_2^2(\hat{\nu}, \hat{\mu}) - W_2^2(\hat{\mu}', \hat{\mu}) \). Let \( \pi \) be the optimal coupling of \( \mu \) and \( \nu \).

**The upper bound** By the definition of \( A \), and the primal formulation of \( W_2^2 \),
\[ A = \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^n \|Y_i - Z_{\sigma(i)}\|^2 - \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^n \|X_i - Z_{\sigma(i)}\|^2 \]
\[ \geq \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^n \left( \|Y_i - Z_{\sigma(i)}\|^2 - \|X_i - Z_{\sigma(i)}\|^2 \right), \quad \text{(min is concave)} \]
which, by expanding the squared norms, equals
\[ = \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^n \left( \|Z_{\sigma(i)}\|^2 - 2(Y_i - X_i)^T Z_{\sigma(i)} + \|Y_i\|^2 - \|X_i\|^2 - \|Z_{\sigma(i)}\|^2 \right). \]
Completing the square, then gathering all sums which are invariant to the permutation \( \sigma \), we obtain

\[
= \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} \| (Y_i - X_i) - Z_{\sigma(i)} \|^2 - \frac{1}{n} \sum_{i=1}^{n} (\| Y_i - X_i \|^2 - \| Y_i \|^2 + \| Z_i \|^2 + \| X_i \|^2).
\]

Taking expectations in the above (all expectations are finite by Assumption 1), we obtain

\[
\mathbb{E} A \geq \mathbb{E} \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} \| (Y_i - X_i) - Z_{\sigma(i)} \|^2 - \mathbb{E} \frac{1}{n} \sum_{i=1}^{n} \| Y_i - X_i \|^2 - \mathbb{E} \| Z \|^2 + \mathbb{E} \| Y \|^2 - \mathbb{E} \| X \|^2.
\]

We now handle the term (1). By Assumption 1, without changing \( \mathbb{E} A \), we choose to sample \((X_i, Y_i) \sim \pi \) independently for all \( i \in \{1, \ldots, n\} \). Since \( \nu \permute \mu \), by Corollary 3 there exists a convex \( f : \mathbb{R}^d \to \mathbb{R} \) such that \( Y_i - X_i = \nabla f(X_i) \) for all \( i \in \{1, \ldots, n\} \). We thus have that

\[
(1) = \mathbb{E} \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} \| \nabla f(X_i) - Z_{\sigma(i)} \|^2 - \mathbb{E} \frac{1}{n} \sum_{i=1}^{n} \| \nabla f(X_i) \|^2 - \mathbb{E} \| Z \|^2,
\]

and introducing the notation \( \psi = (\nabla f)_\#(\mu) \) and \( \hat{\psi} = (\nabla f)_\#(\hat{\mu}) \) we can rewrite this as

\[
= \mathbb{E} \mathcal{W}_2^2(\psi, \hat{\psi}) - \mathbb{E} \| \nabla f(X) \|^2 - \mathbb{E} \| X \|^2.
\]

Now, since \( f \) is convex and \( \psi = (\nabla f)_\#(\mu) \), Brenier’s Theorem 10(\( i \)) says that \( \nabla f \) is the optimal map which transports \( \mu \) to \( \psi \). It follows that \( \mathcal{W}_2^2(\psi, \mu) = \mathbb{E} \| \nabla f(X) \|^2 + \mathbb{E} \| X \|^2 - 2 \mathbb{E} \| \nabla f(X) \|^2 X \). Hence,

\[
(1) = \mathbb{E} \mathcal{W}_2^2(\psi, \hat{\psi}) - \mathcal{W}_2^2(\psi, \mu) - 2 \mathbb{E} \nabla f(X)^T X
\]

\[
\geq -2 \mathbb{E} \nabla f(X)^T X.
\]

(Lemma 3)

For the term (2), we have that

\[
(2) = (\mathbb{E} \| Y \|^2 + \mathbb{E} \| X \|^2) - 2 \mathbb{E} \| X \|^2
\]

\[
= \mathcal{W}_2^2(\mu, \nu) + 2 \sup_{(Y,X) \in \Gamma(\nu, \mu)} \mathbb{E} Y^T X - 2 \mathbb{E} \| X \|^2
\]

\[
= \mathcal{W}_2^2(\mu, \nu) + 2 \mathbb{E} (X + \nabla f(X))^T X - 2 \mathbb{E} \| X \|^2
\]

\[
= \mathcal{W}_2^2(\mu, \nu) + 2 \mathbb{E} \nabla f(X)^T X.
\]

(Corollary 3)

Overall, we have that

\[
\mathbb{E} A \geq (1) + (2) \geq \mathcal{W}_2^2(\mu, \nu),
\]

which concludes the proof of the upper bound.

**The lower bound** The proof of the lower bounds follows the same structure as that of the upper bound. We first begin by exploiting the symmetry in the expression for \( A \), namely

\[
A = \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} \| Y_i - Z_{\sigma(i)} \|^2 - \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} \| X_i - Z_{\sigma(i)} \|^2
\]

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\[
= -\left( \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} ||X_i - Z_{\sigma(i)}||^2 - \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} ||Y_i - Z_{\sigma(i)}||^2 \right),
\]

which, retracing the initial steps of the upper bound proof with \(X_i\) and \(Y_i\) swapped, is

\[
\leq \frac{1}{n} \sum_{i=1}^{n} (||X_i - Y_i||^2 - ||X_i||^2 + ||Z_i||^2 + ||Y_i||^2) - \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} ((X_i - Y_i) - Z_{\sigma(i)})^2.
\]

Take expectations to obtain

\[
\mathbb{E}A \leq \mathbb{E} \frac{1}{n} \sum_{i=1}^{n} ||X_i - Y_i||^2 + \mathbb{E} ||Z||^2 - \mathbb{E} \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} ((X_i - Y_i) - Z_{\sigma(i)})^2 + \mathbb{E} ||Y||^2 - \mathbb{E} ||X||^2.
\]

Again, to deal with the term (3), we sample \((X_i, Y_i) \sim \pi\) independently for all \(i \in \{1, \ldots, n\}\). This choice does not change \(\mathbb{E}A\). Since \(\mu \overset{cd}{=} \nu\), by Corollary 3 there exists a convex \(g : \mathbb{R}^d \to \mathbb{R}\) such that \(Y_i = X_i - \nabla g(X_i)\) for all \(i \in \{1, \ldots, n\}\). Hence, term (3) reduces to

\[
(3) = \mathbb{E} \frac{1}{n} \sum_{i=1}^{n} ||\nabla g(X_i)||^2 + \mathbb{E} ||Z||^2 - \mathbb{E} \min_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} ||\nabla g(X_i) - Z_{\sigma(i)}||^2.
\]

As with term (1) in the proof for the upper bound, we call \(\xi = \nabla g_{\#}(\mu)\) and \(\hat{\xi} = \nabla g_{\#}(\hat{\mu})\). By Brenier’s theorem \(\nabla g\) is the optimal transport map from \(\mu\) to \(\xi\), so

\[
(3) = 2\mathbb{E} \nabla g(X)^T X + W_2^2(\xi, \mu) - \mathbb{E} W_2^2(\hat{\xi}, \hat{\mu})
\leq 2\mathbb{E} \nabla g(X)^T X. \quad \text{(Lemma 3)}
\]

Term (2) has appeared in the upper bound proof, it equals

\[
(2) = W_2^2(\mu, \nu) + 2 \sup_{(Y, X) \in \Gamma(\nu, \mu)} \mathbb{E} Y^T X - 2\mathbb{E} ||X||^2
= W_2^2(\mu, \nu) + 2\mathbb{E}(X - \nabla g(X))^T X - 2\mathbb{E} ||X||^2 \quad \text{(Corollary 3)}
= W_2^2(\mu, \nu) - 2\mathbb{E} \nabla g(X)^T X.
\]

Altogether, we have that

\[
\mathbb{E}A \leq (3) + (2) \leq W_2^2(\mu, \nu),
\]

which concludes the proof of the lower bound.

Next, we prove Proposition 1, which asserts that the upper bound of Theorem 1 decays in proportion to the Wasserstein distance \(W_2(\mu, \nu)\).

**Proof of Proposition 1.** Let \(X, Z \sim \mu\) and \(Y \sim \nu\). To simplify the notation, we drop the subscript \(n\) from the empirical measures \(\hat{\mu}_n\), \(\hat{\mu}'_n\) and \(\hat{\nu}_n\), as well as from the set of permutations \(\mathcal{S}_n\). Define \(A = W_2^2(\hat{\nu}, \hat{\mu}) - W_2^2(\hat{\mu}', \hat{\mu})\). Let \(\pi\) be the optimal coupling of \(\mu\) and \(\nu\). Recall that \(\hat{\mu}' = \sum_{i=1}^{n} \delta_{X_i}/n\) and \(\hat{\nu} = \sum_{i=1}^{n} \delta_{Y_i}/n\). By Assumption 1, \(\mathbb{E}A\) is invariant to choosing \((X_i, Y_i) \sim \pi\) for all \(i \in \{1, \ldots, n\}\), where \(\pi\) is the optimal coupling of \(\mu\) and \(\nu\). In what follows, we make this choice.
\[
\mathbb{E}A = \mathbb{E}\|Y\|^2 - \mathbb{E}\|X\|^2 + 2\mathbb{E}\left(\max_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} X_i^T Z_{\sigma(i)} - \max_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} Y_i^T Z_{\sigma(i)}\right)
\]

\[
\leq \mathbb{E}\|Y\|^2 - \mathbb{E}\|X\|^2 + 2\mathbb{E}\max_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} (X_i - Y_i)^T Z_{\sigma(i)}. \quad \text{(convexity of max)}
\]

The term \(1\) is invariant to the coupling of \(X\) and \(Y\). Without loss of generality, assume \((X, Y) \sim \pi\). Then,

\[
1 = \mathbb{E}(Y - X)^T (Y + X)
\]

\[
\leq \mathbb{E}\|Y - X\||Y + X| \quad \text{(Cauchy-Schwarz)}
\]

\[
\leq (\mathbb{E}\|Y - X\|^2)^{1/2} (\mathbb{E}\|Y + X\|^2)^{1/2} \quad \text{(Cauchy-Schwarz)}
\]

\[
= \mathcal{W}_2(\mu, \nu) (\mathbb{E}\|Y + X\|^2)^{1/2}
\]

\[
= \mathcal{W}_2(\mu, \nu) (\mathbb{E}\|Y\|^2 + 2\mathbb{E}X^T Y + \mathbb{E}\|X\|^2)^{1/2}
\]

\[
\leq \mathcal{W}_2(\mu, \nu) (\mathbb{E}\|Y\|^2 + 2\mathbb{E}\|X\|\|Y\| + \mathbb{E}\|X\|^2)^{1/2} \quad \text{(Cauchy-Schwarz)}
\]

\[
\leq \mathcal{W}_2(\mu, \nu) [\mathbb{E}\|Y\|^2 + 2(\mathbb{E}\|X\|^2\mathbb{E}\|Y\|^2)^{1/2} + \mathbb{E}\|X\|^2]^{1/2} \quad \text{(Cauchy-Schwarz)}
\]

\[
= \mathcal{W}_2(\mu, \nu) [(\mathbb{E}\|X\|^2)^{1/2} + (\mathbb{E}\|Y\|^2)^{1/2}].
\]

For term \(2\),

\[
2 \leq 2\mathbb{E}\max_{\sigma \in S} \frac{1}{n} \sum_{i=1}^{n} \|X_i - Y_i\| \|Z_{\sigma(i)}\|
\]

\[
\leq 2\mathbb{E}\max_{\sigma \in S} \left(\frac{1}{n} \sum_{i=1}^{n} \|X_i - Y_i\|^2\right)^{1/2} \left(\frac{1}{n} \sum_{i=1}^{n} \|Z_{\sigma(i)}\|^2\right)^{1/2} \quad \text{(Cauchy-Schwarz)}
\]

\[
= 2\mathbb{E} \left(\frac{1}{n} \sum_{i=1}^{n} \|X_i - Y_i\|^2\right)^{1/2} \left(\frac{1}{n} \sum_{i=1}^{n} \|Z_i\|^2\right)^{1/2} \quad \text{(\(\sigma\) is a permutation)}
\]

\[
= 2\mathbb{E} \left(\frac{1}{n} \sum_{i=1}^{n} \|X_i - Y_i\|^2\right)^{1/2} \mathbb{E} \left(\frac{1}{n} \sum_{i=1}^{n} \|Z_i\|^2\right)^{1/2}, \quad \text{(independence)}
\]

and letting \((X, Y) \sim \pi\), this writes as

\[
= 2 (\mathbb{E}\|X - Y\|^2)^{1/2} (\mathbb{E}\|Z\|^2)^{1/2},
\]

which, since \((X, Y) \sim \pi\) and \(X, Z \sim \mu\), equals

\[
= 2\mathcal{W}_2(\mu, \nu) (\mathbb{E}\|X\|^2)^{1/2}.
\]

Altogether,

\[
\mathbb{E}A \leq 1 + 2 \leq \mathcal{W}_2(\mu, \nu) [3(\mathbb{E}\|X\|^2)^{1/2} + \mathbb{E}(\|Y\|^2)^{1/2}],
\]

which completes the proof.
We now turn to Theorem 2, which asserts an empirical lower bound on $W_2(\mu, \nu)$.

**Proof of Theorem 2.** Drop the subscripts from the empirical measures $\hat{\mu}_n$, $\hat{\nu}_n$, and the set of permutations $S_n$. Notice that the independence assumption on $\varphi$ makes $|E W_2(\hat{\nu}, \hat{\mu}) - E W_2(\hat{\mu}', \hat{\mu})|$ invariant to the dependence between $\hat{\nu}$ and $\hat{\mu}$. We shall induce a strong dependence between these measures by coupling samples optimally.

By the triangle inequality,

$$W_2(\hat{\nu}, \hat{\mu}) - W_2(\hat{\mu}', \hat{\mu}) \leq W_2(\hat{\mu}', \hat{\nu}).$$

Taking expectations, and noting that the expression also holds with $\hat{\mu}'$ and $\hat{\nu}$ swapped,

$$|E W_2(\hat{\nu}, \hat{\mu}) - E W_2(\hat{\mu}', \hat{\mu})| \leq E W_2(\hat{\mu}', \hat{\nu})$$

Let $\pi$ be the optimal coupling of $\mu, \nu$. As $|E W_2(\hat{\nu}, \hat{\mu}) - E W_2(\hat{\mu}', \hat{\mu})|$ is invariant to the dependence between $\hat{\nu}$ and $\hat{\mu}'$, without changing the left-hand-side of inequality (8), we choose to sample $(X_i, Y_i) \sim \pi$ independently for all $i \in \{1, \ldots, n\}$, where $\pi$ is the optimal coupling of $\mu$ and $\nu$. Then,

$$E W_2(\hat{\mu}', \hat{\nu}) = E \left( \min_{\sigma \in S_n} \frac{1}{n} \sum_{i=1}^{n} \|X_i - Y_{\sigma(i)}\|^2 \right)^{1/2}$$

$$\leq E \left( \frac{1}{n} \sum_{i=1}^{n} \|X_i - Y_i\|^2 \right)^{1/2}$$

$$\leq \left( E \frac{1}{n} \sum_{i=1}^{n} \|X_i - Y_i\|^2 \right)^{1/2}$$

(Jensen’s inequality)

$$= \left( E_{(X,Y) \sim \pi} \|X - Y\|^2 \right)^{1/2} = W_2(\mu, \nu).$$

(9)

Combining inequalities (8) and (9), we have that

$$|E W_2(\hat{\nu}, \hat{\mu}) - E W_2(\hat{\mu}', \hat{\mu})| \leq E W_2(\mu, \nu),$$

which completes the proof. 

**B.2 Contractive optimal transport**

**Proof of Theorem 3.** The equivalence $(i) \iff (ii)$ follows by definition. The equivalence $(ii) \iff (iii)$ is stated in Lemma 1. Let now $\varphi, \hat{\varphi}$ be twice continuously differentiable. The equivalence $(ii) \iff (iv)$ is shown in Nesterov (2004, Theorem 2.1.6). The equivalence $(iii) \iff (v)$ is shown in Nesterov (2004, Theorem 2.1.11). 

**Proof of Proposition 2.** Since $\cot \Rightarrow$ is shift-invariant, without loss of generality we may assume that $\mu$ and $\nu$ have mean 0. Following Peyré and Cuturi (2019, Remark 2.31), the optimal transport map from $\nu$ to $\mu$ is

$$T(x) = N^{-1/2} \left( N^{1/2} M N^{1/2} \right)^{1/2} N^{-1/2} x,$$

where $N^{1/2}$ denotes the symmetric positive definite matrix square root of symmetric positive definite matrix $N$. The transport map corresponds to the Brenier potential.
\( \dot{\varphi}(x) = x^T N^{-1/2} \left( N^{1/2} M N^{1/2} \right)^{1/2} N^{-1/2} x/2 \). The Brenier potential is twice continuously differentiable, so by Theorem 3\( (iii) \) we have that
\[
\nu \overset{\text{col}}{=} \mu \iff N^{-1/2} \left( N^{1/2} M N^{1/2} \right)^{1/2} N^{-1/2} \preceq I,
\]
now pre- and post-multiply by the positive definite \( N^{1/2} \) to equivalently get
\[
\iff \left( N^{1/2} M N^{1/2} \right)^{1/2} \preceq N,
\]
which, using the equivalence \( A \preceq B \iff A^{1/2} \preceq B^{1/2} \) for symmetric positive definite \( A \) and \( B \), is equivalently
\[
\iff N^{1/2} M N^{1/2} \preceq N^2,
\]
and finally pre- and post-multiply by the positive definite \( N^{-1/2} \) to equivalently get
\[
\iff M \preceq N,
\]
which concludes the proof. \( \square \)

We now turn to the proof of Theorem 4, which is a mild generalization of Caffarelli’s contraction theorem. We avoid technical details, and only offer a proof sketch which is based on the maximum principle argument (see, for instance, Kolesnikov, 2010).

**Proof of Theorem 4 (sketch).** We follow Kim and Milman (2012, Section 5.2) and Kolesnikov (2010, Proof of Theorem 2.5).

Assume that \( U, V \) and the Brenier potential \( \dot{\varphi} \) are sufficiently regular, in particular such that \( \dot{\varphi} \) is twice continuously differentiable and the Monge-Ampère (change of variables) equation holds
\[
\exp(-V(x)) = \exp\{-\nabla \dot{\varphi}(U(x))\} \det(\nabla^\otimes 2 U(x)).
\]
Kim and Milman (2012, Section 5.2) makes the regularity assumptions explicit, and argues how these can be removed by an approximation argument.

Let \( d \) be the dimension of the problem. As per Kim and Milman (2012, Section 5.2), if \( S^{d-1} \in \mathbb{R}^d \) is the set of \( d \)-dimensional unit vectors, then the function \( \sup_{e \in S^{d-1}} e^T \nabla^\otimes 2 \dot{\varphi}(x)e \) attains a maximum at some \( x_0 \in \mathbb{R}^d \). The Lipschitz constant of the transport map \( \nabla \dot{\varphi} \) equals \( e^T \nabla^\otimes 2 \dot{\varphi}(x_0)e \), where \( e \in S^{d-1} \) is the (normalized) eigenvector corresponding to the maximum eigenvalue of \( \nabla^\otimes 2 \dot{\varphi}(x_0) \). Since \( e \) is an eigenvector and it has unit length, its associated eigenvalue is \( e^T \nabla^\otimes 2 \dot{\varphi}(x_0)e \), and it holds that \( \nabla^\otimes 2 \dot{\varphi}(x_0)e = e^T \nabla^\otimes 2 \dot{\varphi}(x_0)e e \).

The Monge-Ampère equation yields Kim and Milman (2012, Equation (5.7)), and from there it holds that (see also Kolesnikov, 2010, Proof of Theorem 2.5)
\[
e^T \nabla^\otimes 2 U(x_0)e \geq e^T \nabla^\otimes 2 \dot{\varphi}(x_0) \nabla^\otimes 2 U(\nabla \dot{\varphi}(x_0)) \nabla^\otimes 2 \dot{\varphi}(x_0)e = e^T \{\nabla^\otimes 2 \dot{\varphi}(x_0)\}^2 e e^T \nabla^\otimes 2 U(\nabla \dot{\varphi}(x_0))e = e^T \nabla^\otimes 2 \dot{\varphi}(x_0)e e^T \nabla^\otimes 2 U(\nabla \dot{\varphi}(x_0))e, \tag{10}
\]
using the two lines that \( e \) is a unit eigenvector for \( \nabla^\otimes 2 \dot{\varphi}(x_0) \).

Since \( \nabla^\otimes 2 U \succeq A \succeq \nabla^\otimes 2 V \), there exist twice continuously differentiable convex functions \( P, Q : \mathbb{R}^d \rightarrow \mathbb{R} \) such that \( U(x) = x^T Ax/2 + P(x) \) and \( V(x) = x^T Ax/2 - Q(x) \) for all \( x \in \mathbb{R}^d \). Now, since \( P \) and \( Q \) are convex, it holds that \( e^T \nabla^\otimes 2 P(x_0)e \geq 0 \) and \( e^T \nabla^\otimes 2 Q(x_0)e \geq 0 \). From this and equation (10) it follows that
\[
e^T Ae \geq e^T A \{e^T \nabla^\otimes 2 \dot{\varphi}(x_0)e\}^2,
\]
and so \( 1 \geq \{e^T \nabla^\otimes 2 \dot{\varphi}(x_0)e\}^2 \). It follows that \( \dot{\varphi} \) is 1-Lipschitz, which concludes the proof. \( \square \)
B.3 Concentration and rates of convergence with the sample size

B.3.1 Proof of Theorem 5

We first focus on the the deviation bounds of Theorem 5. The first ingredient is Lemma 4 below, which states deviation bounds for the squared empirical estimator $W^2_2(\hat{\mu}_n, \hat{\nu}_n)$ under a bounded space assumption. For simplicity, we quote the proof of Chizat et al. (2020, Appendix C, Proposition 12), which follows that of Weed and Bach (2019, Proposition 20) and relies on the bounded difference inequalities of McDiarmid (1989). The concentration bound of Lemma 4 is stated as such in Chizat et al. (2020, Theorem 2). It is possible to generalize Lemma 4 to empirical transportation costs as long as the cost function has a bounded co-domain.

Lemma 4. Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ be supported in the same set of diameter at most 1. Then, for all $t \geq 0$,

\[
\mathbb{P}(W^2_2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}W^2_2(\hat{\mu}_n, \hat{\nu}_n) \leq -t) \leq \exp(-nt^2), \quad (11)
\]

\[
\mathbb{P}(W^2_2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}W^2_2(\hat{\mu}_n, \hat{\nu}_n) \geq t) \leq \exp(-nt^2). \quad (12)
\]

Hence, for all $t \geq 0$,

\[
\mathbb{P}(|W^2_2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}W^2_2(\hat{\mu}_n, \hat{\nu}_n)| \geq t) \leq 2\exp(-nt^2).
\]

Proof. Follow the proof of Chizat et al. (2020, Appendix C, Proposition 12) up to using McDiarmid’s bounded difference inequalities (McDiarmid, 1989). At this point, the deviation bounds (11) and (12) follow. The concentration bound follows by a union bound, thereby concluding the proof. \qed

The second ingredient to Theorem 5 is Lemma 5 below, which states deviation bounds for the empirical estimator $W_2(\hat{\mu}_n, \hat{\nu}_n)$ under a bounded space assumption. The proof has two separate parts: the lower deviation bound is a straightforward consequence of the bound (11), while the upper deviation bound has a significantly more technical proof, which we adapt from Boissard and Le Gouic (2014, Appendix A). For the latter part of the proof, it is first necessary to introduce the concepts of relative entropy (or Kullback-Leibler divergence) and generic transportation costs.

Definition 3 (Transportation cost). Let $\mathcal{X}$ be a Polish space, and let $\mu, \nu \in \mathcal{P}(\mathcal{X})$. Let $c : \mathcal{X} \times \mathcal{X} \to [0, \infty)$ be a lower semi-continuous cost function. The transportation cost from $\mu$ to $\nu$ is defined as

\[
\mathcal{T}_c(\mu, \nu) = \inf_{(X,Y) \sim \Gamma(\mu,\nu)} \mathbb{E}c(X,Y).
\]

Notice that $W^2_2(\mu, \nu) = \mathcal{T}_{\|\cdot\|^2}(\mu, \nu)$, where $\mathcal{T}_{\|\cdot\|^2}$ is the transportation cost with cost function $c(x, y) = \|x - y\|^2$.

Definition 4 (Relative entropy). Let $\mathcal{X}$ be a Polish space, and let $\mu, \nu \in \mathcal{P}(\mathcal{X})$. Let $\nu$ be absolutely continuous with respect to $\mu$, with Radon-Nikodym derivative $p$. The relative entropy of $\nu$ from $\mu$ is

\[
H(\nu \mid \mu) = \mathbb{E}_\nu(p(Y) \log p(Y)).
\]
Lemma 5. Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ be supported in the same set of diameter at most 1. Then, for all $t \geq 0$,

$$\mathbb{P}(\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) \leq -t) \leq \exp(-nt^4).$$

(13)

$$\mathbb{P}(\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) \geq t) \leq \exp(-nt^4/16).$$

(14)

Hence,

$$\mathbb{P}(|\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n)| \geq t) \leq 2\exp(-nt^4/16).$$

Proof. The concentration bound follows from the deviation bounds (13) and (14) and a union bound. It remains to prove the two deviation bounds.

Lower deviation By Lemma 4, for all $t \geq 0$,

$$\mathbb{P}(\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n) \leq -t) \leq \exp(-nt^2).$$

Manipulating the left-hand-side, for $t \geq 0$

$$\mathbb{P}(\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n) \leq -t) = \mathbb{P}(\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n) + t \leq \mathbb{E}\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n)),
$$

by Jensen’s inequality, $\mathbb{E}\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n) \geq (\mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n))^2$, so the above is

$$\geq \mathbb{P}(\mathcal{W}_2^2(\hat{\mu}_n, \hat{\nu}_n) + t \leq (\mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n))^2]
\geq \mathbb{P}((\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) + t^{1/2})^2 \leq (\mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n))^2]
= \mathbb{P}(\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) + t \leq \mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n))
= \mathbb{P}(\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) \leq -t^{1/2}).$$

The deviation bound (13) follows by a change of variables $t \leftarrow t^2$.

Upper deviation We follow the approach described in Boissard and Le Gouic (2014, Appendix A). Our main technical tools are transportation cost inequalities (see Gozlan and Léonard, 2007). Let us give an overview of the proof. We use the symbol $\otimes$ to denote products of measures, and for $n \in \mathbb{N}$ and $\mu \in \mathcal{P}(\mathbb{R}^d)$ we write $\mu^{\otimes n} = \bigotimes_{i=1}^n \mu$ for the product measure consisting of $n$ copies of $\mu$.

Step 1: By the compactness assumption on $\mathcal{X} = \text{Supp}(\mu) \cup \text{Supp}(\nu) \subset \mathbb{R}^d$, $\mu$ and $\nu$ satisfy a transportation cost inequality (Bolley and Villani, 2005, Particular case 2.5) with respect to the cost induced by the squared Euclidean norm.

Step 2: Tensorizing the squared Euclidean norm, we define a cost function on the $2n$-dimensional product space $\mathcal{X}^{2n}$, which is the square of some metric $d$. It follows (see Gozlan and Léonard, 2007, Section 4, Corollary 5) that the transportation cost inequality of Step 1 also tensorizes. Hence, the product measure $\mu^{\otimes n} \otimes \nu^{\otimes n}$ satisfies such an inequality as well with respect to the cost $d^2$.

Step 3: We apply Jensen’s inequality, obtaining that the product measure $\mu^{\otimes n} \otimes \nu^{\otimes n}$ satisfies a $T_1$ inequality (see Gozlan and Léonard, 2007, Section 1.2 for a definition) with metric $d$. Then, we show that the empirical 2-Wasserstein distance is $2^{1/2}n^{-1/2}$-Lipschitz when viewed as a functional of the product measure $\mu^{\otimes n} \otimes \nu^{\otimes n}$. We finally apply Gozlan and Léonard (2007, Section 6, Lemma 5), which brings us to an upper deviation inequality.

We now proceed with the proof.
Step 1: By Bolley and Villani (2005, Particular case 2.5), for all $Q \in \mathcal{P}(\mathcal{X})$ it holds that
\[
1/2 \mathcal{T}_{d_2}^2(\mu, Q) \leq H(Q | \mu), \quad 1/2 \mathcal{T}_{d_2}^2(\nu, Q) \leq H(Q | \nu).
\]

Step 2: Let $x_i, y_i, x'_i, y'_i \in \mathcal{X}$ for all $i \in \{1, \ldots, n\}$. Let $\mathbf{x} = (x_1, \ldots, x_n) \in \mathcal{X}^n$, and similarly $\mathbf{x}', \mathbf{y}$ and $\mathbf{y}'$. Define the function $d : \mathcal{X}^2 \times \mathcal{X}^2 \rightarrow [0, \infty)$ by
\[
d((\mathbf{x}, \mathbf{y}), (\mathbf{x}', \mathbf{y}')) = \left[ \sum_{i=1}^{n} (\|x_i - x'_i\|^2 + \|y_i - y'_i\|^2) \right]^{1/2}.
\]
Note that $d$ is a metric on $\mathcal{X}^2$ (one can show the triangle inequality by Minkowski’s inequality). We also have that
\[
d^2((\mathbf{x}, \mathbf{y}), (\mathbf{x}', \mathbf{y}')) = \sum_{i=1}^{n} (\|x_i - x'_i\|^2 + \|y_i - y'_i\|^2).
\]

Now, by equations (15) and (16), Gozlan and Léonard (2007, Section 4, Corollary 5) applies (with choice of map $\alpha : x \mapsto x^2/2$). For all $P \in \mathcal{P}(\mathcal{X}^2)$, it thus holds that
\[
1/4n \mathcal{T}_{d_2}^2(\mu \otimes^n \nu \otimes^n, P) \leq H(P | \mu \otimes^n \nu \otimes^n).
\]

Step 3: By Jensen’s inequality, we have that $\mathcal{T}_{d_2}^2(\mu \otimes^n \nu \otimes^n, P) \leq \mathcal{T}_{d_2}(\mu \otimes^n \nu \otimes^n, P)$. Combining this with equation (17) yields that, for all $P \in \mathcal{P}(\mathcal{X}^2)$,
\[
1/4n \mathcal{T}_{d_2}^2(\mu \otimes^n \nu \otimes^n, P) \leq H(P | \mu \otimes^n \nu \otimes^n).
\]

Let now $f : \mathcal{X}^2 \rightarrow [0, \infty)$ be $f(\mathbf{x}, \mathbf{y}) = \mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n)$. We will show that the function $f$ is $(2n)^{-1/2}$-Lipschitz with respect to metric $d : \mathcal{X}^2 \times \mathcal{X}^2 \rightarrow [0, \infty)$. We have that
\[
|f(\mathbf{x}, \mathbf{y}) - f(\mathbf{x}', \mathbf{y}')| \leq \left| f(\mathbf{x}, \mathbf{y}) - f(\mathbf{x}', \mathbf{y}) \right| + \left| f(\mathbf{x}', \mathbf{y}) - f(\mathbf{x}', \mathbf{y}') \right| \quad \text{(triangle inequality)}
\]
\[
\leq f(\mathbf{x}, \mathbf{x}') + f(\mathbf{y}, \mathbf{y}') \quad \text{(triangle inequality)}
\]
\[
\leq n^{-1/2} \left[ \left( \sum_{i=1}^{n} \|x_i - x'_i\|^2 \right)^{1/2} + \left( \sum_{i=1}^{n} \|y_i - y'_i\|^2 \right)^{1/2} \right],
\]
which, using elementary inequality $a^{1/2} + b^{1/2} \leq 2^{1/2}(a + b)^{1/2}$, is at most
\[
\leq 2^{1/2}n^{-1/2} \left[ \sum_{i=1}^{n} (\|x_i - x'_i\|^2 + \|y_i - y'_i\|^2) \right]^{1/2}
\]
\[
= 2^{1/2}n^{-1/2} d((\mathbf{x}, \mathbf{y}), (\mathbf{x}', \mathbf{y}')), \quad \text{so } f \text{ is } 2^{1/2}n^{-1/2}-\text{Lipschitz with respect to metric } d.
\]

By the 1-Lipschitz property of $(2n)^{1/2}f$, as well as equation (18), Gozlan and Léonard (2007, Section 6, Lemma 5) applies (with choice of map $\alpha : x \mapsto x^4/(4n)$). As a consequence, recalling that $f(\mathbf{x}, \mathbf{y}) = \mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n)$, we have that
\[
\mathbb{P} \left( 2^{1/2}n^{-1/2}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - 2^{1/2}n^{-1/2}\mathcal{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) \geq t \right) \leq \exp \left( -t^4/(4n) \right).
\]

Change variables to $t \leftarrow 2^{1/2}n^{-1/2}t$ to obtain the deviation bound (14), which concludes the proof.
The final auxiliary result required for the concentration bounds of Theorem 5 is the following union bound.

**Lemma 6.** For two real-valued random variables $A$ and $B$, and any $t \in \mathbb{R}$,
\[
\mathbb{P}(A - B \geq t) \leq \mathbb{P}(A \geq t/2) + \mathbb{P}(B < -t/2), \\
\mathbb{P}(A - B \leq -t) \leq \mathbb{P}(A < -t/2) + \mathbb{P}(B \geq t/2).
\]

Therefore, for all $t \geq 0$,
\[
\mathbb{P}(|A - B| \geq t) \leq \mathbb{P}(|A| \geq t/2) + \mathbb{P}(|B| \geq t/2).
\]

**Proof.** For the first inequality,
\[
\mathbb{P}(A - B \geq t) = \mathbb{P}(A \geq t + B) \\
= \mathbb{P}(A \geq t + B, t + B \geq t/2) + \mathbb{P}(A \geq t + B, t + B < t/2) \\
\leq \mathbb{P}(A \geq t/2) + \mathbb{P}(t + B < t/2) \\
= \mathbb{P}(A \geq t/2) + \mathbb{P}(B < -t/2).
\]

To obtain the second inequality, swap $A$ and $B$ in the first, then use $\mathbb{P}(B - A \geq t) = \mathbb{P}(A - B \leq -t)$. For the final inequality, add the first two. \(\square\)

We now proceed with the proof of Theorem 5.

**Proof of Theorem 5.** Estimator $U$: The deviation bound follows from Lemma 4 and a union bound. Let $A = \mathcal{W}_2^2(\hat{\nu}_n, \hat{\mu}_n) - \mathbb{E}\mathcal{W}_2^2(\hat{\nu}_n, \hat{\mu}_n)$ and $B = \mathcal{W}_2^2(\hat{\mu}_n', \hat{\mu}_n) - \mathbb{E}\mathcal{W}_2^2(\hat{\mu}_n', \hat{\mu}_n)$. Then,
\[
\mathbb{P}(|U - \mathbb{E}U| \geq t) = \mathbb{P}(|A - B| \geq t) \\
\leq \mathbb{P}(|A| \geq t/2) + \mathbb{P}(|B| \geq t/2) \qquad \text{(Lemma 6)} \\
\leq 4 \exp(-nt^2/4), \qquad \text{(Lemma 4)}
\]
which is the desired concentration bound.

Estimator $L$: Similarly to the above, let $C = \mathcal{W}_2^2(\hat{\nu}_n, \hat{\mu}_n) - \mathbb{E}\mathcal{W}_2^2(\hat{\nu}_n, \hat{\mu}_n)$ and $D = \mathcal{W}_2^2(\hat{\mu}_n', \hat{\mu}_n) - \mathbb{E}\mathcal{W}_2^2(\hat{\mu}_n', \hat{\mu}_n)$. Then, similarly to the proof for the estimator $U$,
\[
\mathbb{P}(|L - \mathbb{E}L| \geq t) = \mathbb{P}(|C - D| \geq t) \\
\leq \mathbb{P}(|C| \geq t/2) + \mathbb{P}(|D| \geq t/2) \qquad \text{(Lemma 6)} \\
\leq 4 \exp(-nt^4/256), \quad \text{(Lemma 5)}
\]
which concludes the proof. \(\square\)

**B.3.2 Proof of Theorem 6**

The proof of Theorem 6, in part, relies on sharp bounds on the rates of convergence of $\mathbb{E}\mathcal{W}_2^2(\hat{\mu}_n, \hat{\mu}_n')$ and $\mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\mu}_n')$ towards zero. We collect these in Lemma 7. These results are essentially well-known, however we were not able to find them stated as such in the literature, and so we also provide proofs. For the proof of Lemma 7, let us introduce the 1-Wasserstein distance,
\[
\mathcal{W}_1(\mu, \nu) = \inf_{(X,Y) \in \Gamma(\mu,\nu)} \mathbb{E}\|X - Y\|.
\]
By Jensen’s inequality, this satisfies \( \mathcal{W}_1(\mu, \nu) \leq \mathcal{W}_2(\mu, \nu) \). The 1-Wasserstein distance \( \mathcal{W}_1 \) also satisfies a Kantorovich duality similar to that for \( \mathcal{W}_2^2 \) (Villani, 2009, Theorem 5.10). If \( \Phi = \{ (\psi, \hat{\psi}) \in L^1(\mu) \times L^1(\nu) : \psi(x) - \hat{\psi}(y) \leq \|x - y\| \} \), the Kantorovich dual formulation reads

\[
\mathcal{W}_1(\mu, \nu) = \sup_{(\psi, \hat{\psi}) \in \Phi} (\mathbb{E}_\mu \psi(X) - \mathbb{E}_\nu \hat{\psi}(Y)).
\]

**Lemma 7.** Let \( d \geq 5 \) and let \( \mu \in \mathcal{P}(\mathbb{R}^d) \) be supported in a set of diameter 1. Define the empirical measures \( \tilde{\mu}_n = \sum_{i=1}^n \delta_{X_i/n} \) and \( \tilde{\nu}_n = \sum_{i=1}^n \delta_{X_i'/n} \), where \( X_1, \ldots, X_n, X_1', \ldots, X_n' \sim \mu \) are independent and identically distributed. Then,

\[
\mathbb{E}\mathcal{W}_2^2(\tilde{\mu}_n, \tilde{\nu}_n') \lesssim n^{-2/d}, \quad \mathbb{E}\mathcal{W}_2(\tilde{\mu}_n, \tilde{\nu}_n') \lesssim n^{-1/d}.
\]

If \( \mu, \nu \) are also continuous, then

\[
\mathbb{E}\mathcal{W}_2^2(\tilde{\mu}_n, \tilde{\nu}_n') \gtrsim n^{-2/d}, \quad \mathbb{E}\mathcal{W}_2(\tilde{\mu}_n, \tilde{\nu}_n') \gtrsim n^{-1/d}.
\]

**Proof.** The upper bounds: The bound \( \mathbb{E}\mathcal{W}_2^2(\tilde{\mu}_n, \tilde{\nu}_n') \lesssim n^{-2/d} \) follows by Chizat et al. (2020, Theorem 2). For the empirical Wasserstein distance now, use Jensen’s inequality to obtain

\[
\mathbb{E}\mathcal{W}_2(\tilde{\mu}_n, \tilde{\nu}_n') = \mathbb{E} \left[ (\mathcal{W}_2(\tilde{\mu}_n, \tilde{\nu}_n'))^{1/2} \right] \leq \left[ \mathbb{E}\mathcal{W}_2^2(\tilde{\mu}_n, \tilde{\nu}_n') \right]^{1/2} \lesssim n^{-1/d}.
\]

The lower bounds: Let us sketch the steps of the proof. We first follow Panaretos and Zemel (2019, Section 3.3) to show that \( \mathcal{W}_1(\tilde{\mu}_n, \mu) \gtrsim n^{-1/d} \) (note the lack of expectation on the left-hand-side). We then show that \( \mathbb{E}\mathcal{W}_1(\tilde{\mu}_n, \tilde{\nu}_n') \geq \mathbb{E}\mathcal{W}_1(\tilde{\mu}_n, \mu) \) along the same lines as the proof of Lemma 3. A few applications of Jensen’s inequality bring us the claimed lower bounds:

\[
\mathbb{E}\mathcal{W}_2^2(\tilde{\mu}_n, \tilde{\nu}_n') \geq \mathbb{E}\mathcal{W}_1^2(\tilde{\mu}_n, \tilde{\nu}_n') \geq \mathbb{E}\mathcal{W}_1(\tilde{\mu}_n, \tilde{\nu}_n')^2 \gtrsim n^{-2/d},
\]

\[
\mathbb{E}\mathcal{W}_2(\tilde{\mu}_n, \tilde{\nu}_n') \geq \mathbb{E}\mathcal{W}_1(\tilde{\mu}_n, \tilde{\nu}_n') \gtrsim n^{-1/d}.
\]

To show that \( \mathcal{W}_1(\tilde{\mu}_n, \mu) \gtrsim n^{-1/d} \), we shall use a metric entropy argument. For all \( i \in \{1, \ldots, n\} \), let \( B_i = B_\varepsilon(X_i, \|\cdot\|) \) represent the \( L_1 \)-ball of radius \( \varepsilon > 0 \) centered at \( X_i \). Let \( B = \bigcup_{i=1}^n B_i \), and hence \( \|x - y\| \geq \varepsilon \) for \( (x, y) \in \text{Supp}(\tilde{\mu}_n) \times (\text{Supp}(\mu) \setminus B) \).

By the definition of the 1-Wasserstein distance \( \mathcal{W}_1(\tilde{\mu}_n, \mu) \),

\[
\mathcal{W}_1(\tilde{\mu}_n, \mu) = \inf_{\pi \in \Gamma(\tilde{\mu}_n, \mu)} \int_{\text{Supp}(\tilde{\mu}_n) \times \text{Supp}(\mu)} \|x - y\|d\pi(x, y)
\geq \inf_{\pi \in \Gamma(\tilde{\mu}_n, \mu)} \int_{\text{Supp}(\tilde{\mu}_n) \times (\text{Supp}(\mu) \setminus B)} \|x - y\|d\pi(x, y)
\geq \inf_{\pi \in \Gamma(\tilde{\mu}_n, \mu)} \int_{\text{Supp}(\tilde{\mu}_n) \times (\text{Supp}(\mu) \setminus B)} \varepsilon d\pi(x, y)
= \varepsilon \mu(\text{Supp}(\mu) \setminus B).
\]

Letting \( \text{Vol} \) denote volume with respect to the Lebesgue measure, \( \text{Vol}B \leq n\varepsilon d n^{d/2} / \Gamma(d/2 + 1) \), where \( \Gamma(x) \) denotes the Gamma function when used with a single argument \( x \geq 0 \). Choose

\[
\varepsilon = n^{-1/d} \left[ \frac{\Gamma(d/2 + 1)}{2\pi^{d/2}} \text{Vol}(\text{Supp}(\mu)) \right]^{1/d},
\]

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which ensures that \( \text{Vol}B \leq \frac{1}{2} \text{Vol}(\text{Supp}(\mu)) \). By inequality (19), it follows that

\[
\mathcal{W}_1(\hat{\mu}_n, \mu) \geq n^{-1/d} \left[ \frac{\Gamma(d/2 + 1)}{2^{d/2}} \text{Vol}(\text{Supp}(\mu)) \right]^{1/d} \mu(\text{Supp}(\mu) \setminus B) \\
\geq n^{-1/d} \left[ \frac{\Gamma(d/2 + 1)}{2^{d/2}} \text{Vol}(\text{Supp}(\mu)) \right]^{1/d} \inf_{\text{Vol}(A) \geq \frac{1}{2} \text{Vol}(\text{Supp}(\mu))} \mu(A) \\
\geq n^{-1/d},
\]

since \( \mu \) is absolutely continuous with respect to the Lebesgue measure, which completes the proof of the first claim. (Notice that the penultimate bound only depends on \( \mu \), and holds with \( \hat{\mu}_n \) replaced by any probability measure supported on \( n \) points).

All that remains to be shown is the bound \( \mathbb{E} \mathcal{W}_1(\hat{\mu}_n, \hat{\mu}'_n) \geq \mathbb{E} \mathcal{W}_1(\hat{\mu}_n, \mu) \), which is a consequence of Kantorovich duality. Define sets

\[
\Phi' = \left\{ (\varphi, \psi) \in L^1(\hat{\mu}_n) \times L^1(\hat{\mu}'_n) : \varphi(x) - \psi(y) \leq \|x - y\| \right\}, \\
\Phi = \left\{ (\varphi, \psi) \in L^1(\hat{\mu}_n) \times L^1(\mu) : \varphi(x) - \psi(y) \leq \|x - y\| \right\}.
\]

As \( L^1(\mu) \subseteq L^1(\hat{\mu}'_n) \), we have that \( \Phi \subseteq \Phi' \). Recall that \( \hat{\mu}_n = \sum_{i=1}^n \delta_{X_i} / n \) and \( \hat{\mu}'_n = \sum_{i=1}^n \delta_{X'_i} / n \). Let \( \mathbb{E} \) denote the expectation jointly over all \( X_i \) and \( X'_i \), and let \( \mathbb{E}' \) be the expectation over \( X'_1, \ldots, X'_n \) only. Now, by Kantorovich duality,

\[
\mathbb{E} \mathcal{W}_1(\hat{\mu}_n, \hat{\mu}'_n) = \mathbb{E} \left[ \sup_{(\varphi, \psi) \in \Phi'} \left( \mathbb{E}_{\hat{\mu}_n} \varphi(X) - \mathbb{E}_{\hat{\mu}'_n} \psi(X') \right) \right] \\
\geq \mathbb{E} \left[ \sup_{(\varphi, \psi) \in \Phi} \left( \mathbb{E}_{\hat{\mu}_n} \varphi(X) - \mathbb{E}_{\hat{\mu}'_n} \psi(X') \right) \right] \\
= \mathbb{E} \mathbb{E}' \left[ \sup_{(\varphi, \psi) \in \Phi} \left( \mathbb{E}_{\hat{\mu}_n} \varphi(X) - \mathbb{E}_{\hat{\mu}'_n} \psi(X') \right) \right],
\]

which, by the convexity of the supremum and Jensen’s inequality, is

\[
\geq \mathbb{E} \sup_{(\varphi, \psi) \in \Phi} \mathbb{E}' \left( \mathbb{E}_{\hat{\mu}_n} \varphi(X) - \mathbb{E}_{\mu} \psi(X') \right) \\
= \mathbb{E} \sup_{(\varphi, \psi) \in \Phi} \left( \mathbb{E}_{\hat{\mu}_n} \varphi(X) - \mathbb{E}_{\mu} \psi(X') \right) \\
= \mathbb{E} \mathcal{W}_1(\hat{\mu}_n, \mu),
\]

(Kantorovich duality)

which is the desired bound. The proof is thus complete. \( \square \)

Theorem 6 follows from the rates of convergence established in Chizat et al. (2020, Theorem 2 and Corollary 1) and the rates of convergence in Lemma 7.

**Proof of Theorem 6. Estimator U:**

\[
\mathbb{E}|U - \mathcal{W}_2^2(\mu, \nu)| = \mathbb{E}|\mathcal{W}_2^2(\hat{\mu}_n, \hat{\mu}_n) - \mathcal{W}_2^2(\hat{\mu}'_n, \hat{\mu}_n) - \mathcal{W}_2^2(\hat{\mu}'_n, \mu, \nu)| \\
\leq \mathbb{E}|\mathcal{W}_2^2(\hat{\mu}_n, \hat{\mu}_n) - \mathcal{W}_2^2(\hat{\mu}'_n, \hat{\mu}_n)| + \mathbb{E} \mathcal{W}_2^2(\hat{\mu}'_n, \hat{\mu}_n). \quad \text{(triangle inequality)}
\]

Now, the first term is \( \lesssim n^{-2/d} \) by Chizat et al. (2020, Theorem 2) and the second is also \( \lesssim n^{-2/d} \) by Lemma 7. Overall, \( \mathbb{E}|U - \mathcal{W}_2^2(\mu, \nu)| \lesssim n^{-2/d} \).
**Estimator** $L$: For the upper bound in $n$,

\[
\mathbb{E}|\mathcal{W}_2(\mu, \nu) - L| = \mathbb{E}|\mathcal{W}_2(\mu, \nu) - \mathcal{W}_2(\hat{\nu}_n, \hat{\mu}_n) + \mathcal{W}_2(\hat{\mu}_n', \hat{\mu}_n)| \\
\leq \mathbb{E}|\mathcal{W}_2(\hat{\nu}_n, \hat{\mu}_n) - \mathcal{W}_2(\mu, \nu)| + \mathbb{E}\mathcal{W}_2(\hat{\mu}_n', \hat{\mu}_n). \quad \text{(triangle inequality)}
\]

The first term above is $\lesssim n^{-2/d}$ by Chizat et al. (2020, Corollary 1). The second term above is $\lesssim n^{-1/d}$ by Lemma 7. Overall $\mathbb{E}|\mathcal{W}_2(\mu, \nu) - L| \lesssim n^{-1/d}$, as claimed.

For the lower bound in $n$, first recall that $\mathcal{W}_2(\mu, \nu) - \mathbb{E}L \geq 0$ by Theorem 2. We have that

\[
\mathcal{W}_2(\mu, \nu) - \mathbb{E}L = \mathcal{W}_2(\mu, \nu) - \mathbb{E}\mathcal{W}_2(\hat{\nu}_n, \hat{\mu}_n) + \mathbb{E}\mathcal{W}_2(\hat{\mu}_n', \hat{\mu}_n) \\
= \mathbb{E}\mathcal{W}_2(\hat{\mu}_n', \hat{\mu}_n) - (\mathbb{E}\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathcal{W}_2(\mu, \nu)) \\
\geq \mathbb{E}\mathcal{W}_2(\hat{\mu}_n', \hat{\mu}_n) - |\mathbb{E}|\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathcal{W}_2(\mu, \nu)|. \quad \text{(20)}
\]

By Lemma 7, $\mathbb{E}\mathcal{W}_2(\hat{\mu}_n', \hat{\mu}_n) \gtrsim n^{-1/d}$. By Chizat et al. (2020, Corollary 1), $\mathbb{E}|\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathcal{W}_2(\mu, \nu)| \lesssim n^{-2/d}$. It follows that for large enough $n$ the right-hand-side of equation (20) is positive, and furthermore it holds that

\[
\mathbb{E}\mathcal{W}_2(\hat{\mu}_n', \hat{\mu}_n) - |\mathbb{E}|\mathcal{W}_2(\hat{\mu}_n, \hat{\nu}_n) - \mathcal{W}_2(\mu, \nu)| \gtrsim n^{-1/d}.
\]

Immediately, equation (20) implies that $\mathcal{W}_2(\mu, \nu) - \mathbb{E}L \gtrsim n^{-1/d}$, which completes the proof. \(\square\)

**B.3.3 Proof of Corollary 1**

We now turn to Corollary 1, which gives lower bounds on the point estimators $U$ and $L$ being themselves, respectively, upper and lower bounds. The result follows by the deviation bounds of Lemma 5 and the convergence rates of Theorem 6.

**Proof of Corollary 1. Estimator $L$:** It suffices to show the claimed bound for the estimator $L$ only, since $\mathbb{P}(L \leq \mathcal{W}_2(\mu, \nu)) = \mathbb{P}(\text{sign}(L)L^2 \leq \mathcal{W}_2^2(\mu, \nu)) = \mathbb{P}(L_{sq} \leq \mathcal{W}_2(\mu, \nu))$.

Similarly to the proof of Theorem 5, use Lemmas 5 and 6 and the continuity of $L$ to obtain, for all $t \geq 0$,

\[
\mathbb{P}(L - \mathbb{E}L \leq t) = 1 - \mathbb{P}(L - \mathbb{E}L \geq t) \geq 1 - 2\exp(-nt^4/256). \quad \text{(21)}
\]

Furthermore, by Theorem 6, there exists a constant $A_1 > 0$ such that $\mathcal{W}_2(\mu, \nu) - \mathbb{E}L \geq A_1 n^{-1/d}$ for all $n \in \mathbb{N}$. Hence,

\[
\mathbb{P}(L \leq \mathcal{W}_2(\mu, \nu)) = \mathbb{P}(L - \mathbb{E}L \leq \mathcal{W}_2(\mu, \nu) - \mathbb{E}L) \\
\geq 1 - 2\exp(-n(\mathcal{W}_2(\mu, \nu) - \mathbb{E}L)^4/256) \quad \text{(using equation (21))} \\
\geq 1 - 2\exp(-A_1^4 n^{1-4/d}/256) \\
= 1 - 2\exp(-C_1 n^{1-4/d}),
\]

for $C_1 = A_1^4/256 > 0$, which concludes the proof for the estimator $L$.

**Estimator $U$:** Similarly to the proof of Theorem 5, use Lemmas 4 and 6 and the continuity of $U$ to obtain, for all $t \geq 0$,

\[
\mathbb{P}(U - \mathbb{E}U \geq -t) = 1 - \mathbb{P}(U - \mathbb{E}U \leq -t) \geq 1 - 2\exp(-nt^2/4).
\]

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We have assumed that $\mathbb{E}U - W_2^2(\mu, \nu) \gtrsim n^{-2/d}$, so there exists a constant $A_2 > 0$ such that $\mathbb{E}U - W_2^2(\mu, \nu) \geq A_2 n^{-2/d}$. Hence,

$$
P(U \geq W_2^2(\mu, \nu)) = P(U - \mathbb{E}U \geq -(\mathbb{E}U - W_2^2(\mu, \nu))) \\
\geq 1 - 2 \exp(-n(\mathbb{E}U - W_2^2(\mu, \nu))^2/4) \quad \text{(equation (22))}
$$

for $C_2 = A_2^2/4 > 0$, which concludes the proof.

B.4 Distributional limits

To cover all distributional results in the paper, we now state and prove a central limit theorem for general linear combinations of squared empirical 2-Wasserstein distances. The result also covers the case of dependent empirical measures. The proof is essentially lifted from del Barrio and Loubes (2019) and the extension del Barrio et al. (2021), the main challenge being the more cumbersome notation.

We first state elementary upper and lower bounds on the variances of sums of random variables.

**Lemma 8.** Let $A_1, \ldots, A_k$ be real random variables with finite second moment. Then,

$$\text{Var} \sum_{i=1}^{k} A_i \leq \left( \sum_{i=1}^{k} (\text{Var} A_i)^{1/2} \right)^2.$$

In addition, $\text{Var}(A_1 + A_2) \geq [(\text{Var} A_1)^{1/2} - (\text{Var} A_2)^{1/2}]^2$.

**Proof.** The results are simple applications of Cauchy-Schwarz. For the upper bound, we have

$$\text{Var} \sum_{i=1}^{k} A_i = \sum_{i=1}^{k} \text{Var} A_i + 2 \sum_{1 \leq i < j \leq k} \text{Cov}(A_i, A_j) \\
\leq \sum_{i=1}^{k} \text{Var} A_i + 2 \sum_{1 \leq i < j \leq k} (\text{Var} A_i)^{1/2}(\text{Var} A_j)^{1/2} \quad \text{(Cauchy-Schwarz)}
$$

$$= \left[ \sum_{i=1}^{k} (\text{Var} A_i)^{1/2} \right]^2.$$

For the lower bound, we use the converse inequality $\text{Cov}(A_1, A_2) \geq -(\text{Var} A_1)^{1/2}(\text{Var} A_2)^{1/2}$.

With these bounds, we are ready to prove Proposition 3, the central limit theorem for linear combinations of squared Wasserstein distances.

**Proposition 3.** Let $\pi$ be a joint distribution of measures $(\mu^{(1)}, \ldots, \mu^{(k)}, \nu^{(1)}, \ldots, \nu^{(k)})$, where all $2k$ measures satisfy Assumption 3. Let $(X^{(i)}, \ldots, X^{(k)}, Y^{(1)}, \ldots, Y^{(k)}) \sim \pi$. Let $(\psi^{(i)}, \tilde{\psi}^{(i)})$ be the Kantorovich potentials from $X^{(i)} \sim \mu_i$ to $Y^{(i)} \sim \nu_i$. Sample $n$
times independently from \( \pi \), generating empirical measures \( \hat{\mu}_n^{(i)} = \sum_{j=1}^k \delta_{X_j^{(i)}} \) and \( \hat{\nu}_n^{(i)} = \sum_{j=1}^k \delta_{Y_j^{(i)}} \) for \( i \in \{1, \ldots, k\} \). Define

\[
A_n = \sum_{i=1}^k a_i W_2^2(\hat{\mu}_n^{(i)} , \hat{\nu}_n^{(i)}) , \quad \sigma^2 = \operatorname{Var}_\pi \sum_{i=1}^k a_i \left( \psi^{(i)}(X^{(i)}) + \tilde{\psi}^{(i)}(Y^{(i)}) \right). 
\]

Then,

\[
n^{1/2} \left( A_n - E A_n \right) \xrightarrow{\text{d}} \mathcal{N}(0, \sigma^2), \quad \lim_{n \to \infty} n \operatorname{Var} A_n = \sigma^2.
\]

Proof. We follow the same structure as in del Barrio and Loubes (2019). First, we show that \( (n \operatorname{Var} A_n)_{n \geq 0} \) is bounded. Then, letting \( (\psi_n^{(i)} , \tilde{\psi}_n^{(i)}) \) be the Kantorovich potentials from \( \hat{\mu}_n^{(i)} \) to \( \hat{\nu}_n^{(i)} \), we show that the residual

\[
R_n = A_n - \frac{1}{n} \sum_{j=1}^n \sum_{i=1}^k a_i \left( \psi^{(i)}(X_j^{(i)}) + \tilde{\psi}^{(i)}(Y_j^{(i)}) \right)
\]

\[
= \sum_{i=1}^k a_i \left[ W_2^2(\hat{\mu}_n^{(i)} , \hat{\nu}_n^{(i)}) - \frac{1}{n} \sum_{j=1}^n \left( \psi^{(i)}(X_j^{(i)}) - \tilde{\psi}^{(i)}(Y_j^{(i)}) \right) \right]
\]

satisfies \( \lim_{n \to \infty} n \operatorname{Var} R_n = 0 \). This is already sufficient to prove the convergence of the variance of \( A_n \). The limit theorem will follow by applying the Central Limit Theorem.

Let \( B_n^{(i)} = W_2^2(\hat{\mu}_n^{(i)} , \hat{\nu}_n^{(i)}) \) for all \( i \in \{1, \ldots, k\} \). By del Barrio and Loubes (2019, Theorem 3.3), the sequence \( (n \operatorname{Var} B_n^{(i)})_{n \geq 0} \) is bounded, and this holds for all \( i \in \{1, \ldots, k\} \).

By Lemma 8,

\[
n \operatorname{Var} A_n = n \operatorname{Var} \sum_{i=1}^k a_i B_n^{(i)} \leq \left[ \sum_{i=1}^k |a_i| (n \operatorname{Var} B_n^{(i)})^{1/2} \right]^2,
\]

so it follows that \( (n \operatorname{Var} A_n)_{n \geq 0} \) is bounded.

Now dealing with the residual, by Lemma 8,

\[
n \operatorname{Var} R_n \leq \left[ \sum_{i=1}^k |a_i| (n \operatorname{Var} C_n^{(i)})^{1/2} \right]^2, \tag{23}
\]

where \( C_n^{(i)} = W_2^2(\hat{\mu}_n^{(i)} , \hat{\nu}_n^{(i)}) - \sum_{j=1}^n \left( \psi^{(i)}(X_j^{(i)}) - \tilde{\psi}^{(i)}(Y_j^{(i)}) \right) / n \). Arguing similarly to del Barrio et al. (2021, proof of Theorem 4.10), but applying instead the Efron-Stein inequality to independent samples \( (X_j^{(i)} , Y_j^{(i)}) \) for all \( j \in \{1, \ldots, n\} \), we obtain that \( \lim_{n \to \infty} n \operatorname{Var} C_n^{(i)} = 0 \). It follows by equation (23) that \( \lim_{n \to \infty} n \operatorname{Var} R_n = 0 \).

To see that \( \lim_{n \to \infty} n \operatorname{Var} A_n = \sigma^2 \), using Lemma 8 and the definitions of \( R_n \) and \( \sigma^2 \), we have that

\[
[|\sigma| - (n \operatorname{Var} R_n)^{1/2}]^2 \leq n \operatorname{Var} A_n \leq [ |\sigma| + (n \operatorname{Var} R_n)^{1/2} ]^2.
\]

Since \( \lim_{n \to \infty} n \operatorname{Var} R_n = 0 \), the squeeze lemma implies that \( \lim_{n \to \infty} n \operatorname{Var} A_n = \sigma^2 \).
By definition, \( A \) for all \( \sum \) \( A \), which uses the mean-value theorem. Let \( \tau \) be a simplified version of the argument in del Barrio et al. (2021, Proof).

The first term \( n^{1/2} (A_n - \mathbb{E}A_n) \) converges to zero in probability, since \( \lim_{n \to \infty} n \text{Var} R_n = 0 \). By the Central Limit Theorem, the second term converges weakly as follows:

\[
\frac{1}{n} \sum_{j=1}^{n} f(Z_j) - \mathbb{E}_\pi f(Z) \to \mathcal{N}(0, \sigma^2),
\]

where \( \sigma^2 = \text{Var}_\pi f(Z) = \text{Var} \sum_{i=1}^{k} a_i (\psi(i)(X^i) + \tilde{\psi}(i)(Y^i)) \). Slutsky’s lemma implies that \( n^{1/2} (A_n - \mathbb{E}A_n) \to \mathcal{N}(0, \sigma^2) \), which completes the proof.

Theorems 7 and 9 follow by corollary from Proposition 3. One can see from Proposition 3 that Theorems 9 readily extends to estimators which average in the asymptote as well.

**Proof of Theorems 7 and 9.** Apply Proposition 3.

We also extend del Barrio et al. (2021, Theorems 4.9 and 4.10) to a central limit theorem for \( W_2^2(\mu_n, \nu_n) \) which is centered at \( \mathbb{E}W_2^2(\mu_n, \nu_n) \). This is only valid if \( \mu \neq \nu \), as otherwise the variance of the Gaussian limit is undefined.

**Proposition 4.** Let \( \pi \) be a joint distribution of measures \( \mu \neq \nu \), where \( \mu, \nu \) satisfy Assumption 3. Let \( (\psi, \tilde{\psi}) \) be the Kantorovich potentials from \( X \sim \mu \) to \( Y \sim \nu \). Sample \( n \) times independently from \( \pi \), generating empirical measures \( \hat{\mu}_n = \sum_{j=1}^{k} \delta_{X_j} \) and \( \hat{\nu}_n = \sum_{j=1}^{k} \delta_{Y_j} \). Then,

\[
n^{1/2} (W_2(\mu_n, \nu_n) - \mathbb{E}W_2(\mu_n, \nu_n)) \to \mathcal{N}(0, \tau^2),
\]

where \( \tau^2 = \text{Var}_\pi (\psi(X) + \tilde{\psi}(Y)) / (4W_2^2(\mu, \nu)) \).

**Proof.** We start with a simplified version of the argument in del Barrio et al. (2021, proof of Theorem 4.9), which uses the mean-value theorem. Let \( A_n = W_2(\mu_n, \nu_n) \), let \( A = W_2(\mu, \nu) \), and let \( \sigma^2 = \text{Var}_\pi (\psi(X) + \tilde{\psi}(Y)) \). Then,

\[
n^{1/2} (A_n - (\mathbb{E}A_n)^{1/2}) (A_n + (\mathbb{E}A_n)^{1/2}) = n^{1/2} (A_n^2 - \mathbb{E}A_n^2) \to \mathcal{N}(0, \sigma^2),
\]

using for the limit Proposition 3. Since \( A_n + (\mathbb{E}A_n)^{1/2} \to 2A > 0 \) almost surely as \( n \to \infty \), Slutsky’s lemma implies that

\[
n^{1/2} (A_n - (\mathbb{E}A_n)^{1/2}) \to \mathcal{N}(0, \sigma^2/(4A^2)) = \mathcal{N}(0, \tau^2). \quad (24)
\]
We will now show that the second moment of \( n^{1/2} \left( A_n - \left( E A_n^2 \right)^{1/2} \right) \) is uniformly bounded for all \( n \). We have

\[
\text{Var} \, A_n^2 = E (A_n^2 - E A_n^2)^2 \\
= E [A_n + (E A_n^2)^{1/2}]^2 [A_n - (E A_n^2)^{1/2}]^2 \\
\geq E A_n^2 E [A_n - (E A_n^2)^{1/2}]^2 \\
\geq A^2 E [A_n - (E A_n^2)^{1/2}]^2. \tag{Lemma 3}
\]

Hence, \( E \left[ n^{1/2} \left( A_n - \left( E A_n^2 \right)^{1/2} \right) \right]^2 \leq n \text{Var}(A_n^2)/A^2 \), which, by the proof of Proposition 3, is uniformly bounded for all \( n \).

By DasGupta (2008, Theorem 6.1), the sequence of random variables \( n^{1/2} \left( A_n - \left( E A_n^2 \right)^{1/2} \right) \) is therefore uniformly integrable, as its second moment is uniformly bounded for all \( n \). It follows by DasGupta (2008, Theorem 6.2) that convergence in the mean also holds in equation (24). Hence,

\[
\lim_{n \to \infty} n^{1/2} \left( E (A_n^2)^{1/2} - E A_n \right) = 0.
\]

Adding the above to equation (24) and using Slutsky’s lemma concludes the proof.

**B.5 Markov chains targeting Gaussian distributions**

In this appendix we characterize deterministic Gibbs samplers and the Unadjusted Langevin Algorithm (ULA) when all marginals are Gaussian. We write \( \pi = \mathcal{N}_d(\mu, \Sigma) \) for the \( d \)-dimensional target distribution and also use \( \pi \) to denote the target density.

Following Roberts and Sahu (1997, Section 2), we consider a blocked Gibbs sampler updating its coordinates in a deterministic order. By Roberts and Sahu (1997, Lemma 1), one full iteration of the Gibbs sampler is

\[
X_{t+1} \mid X_t \sim \mathcal{N}_d(BX_t + b, \Sigma - B\Sigma B^T), \tag{25}
\]

for a matrix \( B \) as defined in Roberts and Sahu (1997, equation (4)) and \( b = (I - B)\mu \). Suppose that we start from a Gaussian initial distribution \( \pi_0 = \mathcal{N}_d(\mu_0, \Sigma_0) \). Then, all marginals \( \pi_t \) at iterations \( t \geq 0 \) are Gaussian, and we write them as \( \pi_t = \mathcal{N}_d(\mu_t, \Sigma_t) \).

Taking expectations and variances, equation (25) reduces to the following updates for all \( t \geq 0 \):

\[
\mu_{t+1} - \mu = B(\mu_t - \mu), \quad \Sigma_{t+1} - \Sigma = B(\Sigma_t - \Sigma)B^T. \tag{26}
\]

ULA generates a Markov chain by the recurrence

\[
X_{t+1} = X_t + \frac{1}{2} h^2 \nabla \log \pi(X_t) + hZ_t, \quad Z_t \sim \mathcal{N}_d(0, I_d), \quad \text{for all } t \geq 0,
\]

which represents the Euler discretized dynamics of an overdamped Langevin diffusion with \( \pi \) as its stationary distribution. Provided the step size \( h > 0 \) is small enough to not produce diverging dynamics, the Markov chain \( (X_t)_{t \geq 0} \) converges to a stationary distribution \( \pi_\infty \). The stationary distribution is distinct from \( \pi \) due to the discretization error, however it converges to \( \pi \) as the step size \( h \to 0 \), under regularity conditions. For a Gaussian target \( \pi = \mathcal{N}_d(\mu, \Sigma) \), the recurrence becomes

\[
X_{t+1} - \mu = M(X_t - \mu) + hZ_t, \tag{27}
\]
where \( M = I_d - h^2 \Sigma^{-1}/2 \). Proposition 5 below (i) states the stationary distribution \( \pi_\infty \) of ULA, (ii) establishes that the stationary distribution of ULA is an overdispersed version of the target such that \( \pi_\infty \otimes \pi \), and (iii) that the stationary bias of ULA, as measured in squared Wasserstein distance \( W_2^2(\pi_\infty, \pi) \), is of sharp order \( h^4d^2 \) in high dimension \( d \).

In addition, when the algorithm is started from a Gaussian \( \pi_0 \), the proposition also (iv) characterizes the marginals \( \pi_t \) at iterations \( t \geq 0 \) in terms of a recurrence relation similar to the recurrence (26) for the Gibbs sampler. See also Wibisono (2018, Example 2) for a similar statement of parts (i) and (iii).

**Proposition 5** (ULA on a Gaussian target). Suppose that \( \pi = \mathcal{N}_d(\mu, \Sigma) \), \( h > 0 \) is small enough such that the spectral radius \( \rho(M) < 1 \), and \( \mathbb{E}\|X_0 - \mu\| < \infty \). It holds that:

(i) The stationary distribution of ULA targeting \( \pi \) is \( \pi_\infty = \mathcal{N}(\mu_\infty, \Sigma_\infty) \) where

\[
\mu_\infty = \mu, \quad \Sigma_\infty = h^2(I_d - M^2)^{-1} = (I_d - h^2\Sigma^{-1}/4)^{-1}\Sigma.
\]

(ii) \( \Sigma_\infty \succeq \Sigma \) and so \( \pi_\infty \otimes \pi \).

(iii) Let \( \Sigma \) vary with the dimension \( d \), such that there exist \( \alpha, \beta > 0 \) with \( \alpha I_d \succeq \Sigma \succeq \beta I_d \) for all \( d \). Then, \( W_2^2(\pi_\infty, \pi) = h^4 \text{tr}(\Sigma^{-1})/64 + O(h^6)d \).

(iv) If \( \pi_0 = \mathcal{N}_d(\mu_0, \Sigma_0) \), then \( \pi_t = \mathcal{N}_d(\mu_t, \Sigma_t) \) for all \( t \geq 0 \) satisfying the recurrence relations

\[
\mu_{t+1} - \mu_\infty = M(\mu_t - \mu_\infty), \quad \Sigma_{t+1} - \Sigma_\infty = M(\Sigma_t - \Sigma_\infty)M^T.
\]

**Proof.** For part (i), using the recurrence (27), we have that

\[
X_t - \mu = M^t(X_0 - \mu) + h \sum_{k=1}^t M^{t-k}Z_k,
\]

for all \( t \geq 0 \), with the convention that the sum is zero for \( t = 0 \). Dealing with term (1), since \( M^t \) is symmetric for all \( t \geq 0 \) it follows that \( \|M^t(X_0 - \mu)\| \leq \rho(M^t}\|X_0 - \mu\| = \rho(M)^t\|X_0 - \mu\|. \) Take expectations, then use that \( \mathbb{E}\|X_0 - \mu\| < \infty \) and \( \rho(M) < 1 \), to derive the limit \( \lim_{t \to \infty} \mathbb{E}\|M^t(X_0 - \mu)\| \leq \lim_{t \to \infty} \rho(M)^t\mathbb{E}\|X_0 - \mu\| = 0 \). It follows that (1) \( M^t(X_0 - \mu) \to 0 \) in probability as \( t \to \infty \). For term (2), since \( M \) is symmetric, we have that

\[
(2) = h \sum_{k=1}^t M^{t-k}Z_k \sim \mathcal{N}_d\left(0, h^2\sum_{j=0}^{t-1} (M^2)^j\right).
\]

Since \( \rho(M^2) = \rho(M)^2 < 1 \), by Higham (2008, Theorem 4.7) it follows that \( \lim_{t \to \infty} \sum_{j=0}^{t-1} (M^2)^j = (I_d - M^2)^{-1} \). Therefore, (2) \( \implies \mathcal{N}_d(0, h^2(I_d - M^2)^{-1}) \) as \( t \to \infty \). Overall, we have that

\[
X_t = \mu + (1) + (2) \implies \mathcal{N}_d(0, h^2(I_d - M^2)^{-1}) \quad \text{as} \quad t \to \infty,
\]

so \( \mu_\infty = \mu \). Finally, \( M^2 = I_d - h^2\Sigma^{-1} + h^4\Sigma^{-2}/4 \), so

\[
\Sigma_\infty = h^2(I_d - M^2)^{-1} = h^2\left\{h^2\Sigma^{-1} - h^4\Sigma^{-2}/4\right\}^{-1} = (I_d - h^2\Sigma^{-1}/4)^{-1}\Sigma,
\]

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which completes the proof of part (i).

For part (ii), by the definition of $M$ we have that $\Sigma = h^2\{2(I - M)\}^{-1}$. Since $\Sigma_\infty = h^2(I_d - M^2)^{-1}$, it follows that $\Sigma$ and $\Sigma_\infty$ commute. Hence,

$$\Sigma_\infty - \Sigma = \Sigma_\infty \Sigma (\Sigma_\infty - \Sigma_\infty^{-1}) = \Sigma_\infty \Sigma h^{-2}(I_d - 2M - I + M^2) = \Sigma_\infty \Sigma h^{-2}(I - M)^2 \geq 0.$$ 

Therefore $\Sigma_\infty \geq \Sigma$, and by Proposition 2 it follows that $\pi_\infty \sim \pi$, thus completing the proof of part (ii).

For part (iii), by Dowson and Landau (1982) we have $W^2_2(\pi_\infty, \pi) = \text{tr}(\Sigma) + \text{tr}(\Sigma_\infty) - 2 \text{tr}((\Sigma \Sigma_\infty)_{1/2})$. Let $\varepsilon = h^2/4$. Expanding the second term in the Wasserstein distance,

$$\text{tr}(\Sigma_\infty) = \text{tr}[(I_d - \varepsilon \Sigma^{-1})^{-1}\Sigma],$$

now using the Taylor series for $x \mapsto (1 - x)^{-1}$ and Higham (2008, Theorem 4.7),

$$= \text{tr} \left[ \sum_{i=0}^{\infty} (\varepsilon \Sigma^{-1})^i \right],$$

which, since $\text{tr}(\Sigma^{-i}) \in [\beta^{-i}d, \alpha^{-i}d]$ for all $i \geq 0$, is

$$= \text{tr}(\Sigma) + \varepsilon d + \varepsilon^2 \text{tr}(\Sigma^{-1}) + O(\varepsilon^3)d.$$

Expanding the third term in the Wasserstein distance,

$$\text{tr}[(\Sigma \Sigma_\infty)_{1/2}] = \text{tr} \left[ ((I_d - \varepsilon \Sigma^{-1})^{-1/2} \Sigma)^{1/2} \right]\quad (\text{since } (I_d - \varepsilon \Sigma^{-1})^{-1} \text{ and } \Sigma \text{ commute})$$

and now using Higham (2008, Theorem 4.7) with the Taylor series for $x \mapsto (1 - x)^{-1/2}$, and also that $\text{tr}(\Sigma^{-i}) \in [\beta^{-i}d, \alpha^{-i}d]$ for all $i \geq 0$, this is

$$= \text{tr}(\Sigma) + \varepsilon d/2 + 3\varepsilon^2 \text{tr}(\Sigma^{-1})/8 + O(\varepsilon^3)d.$$

Hence, $W^2_2(\pi_\infty, \pi) = \varepsilon^2 \text{tr}(\Sigma^{-1})/4 + O(\varepsilon^3)d = h^4 \text{tr}(\Sigma^{-1})/64 + O(h^6)d$, which completes the proof of part (iii).

For part (iv), equation (27) implies that all $\pi_t$ are Gaussian. Take expectations in equation (27) and use $\mu_\infty = \mu$ to obtain the recurrence $\mu_{t+1} = \mu_\infty + M(\mu_t - \mu_\infty)$. To see the recurrence for the variances, take variances in recurrence (27) to obtain

$$\Sigma_{t+1} = M\Sigma_t M^T + h^2 I_d.$$ \hfill (29)

But since $\Sigma_\infty$ is the covariance of the stationary distribution, it must also hold that

$$\Sigma_\infty = M\Sigma_\infty M^T + h^2 I_d.$$ \hfill (30)

Subtracting equation (30) from equation (29) gives $\Sigma_{t+1} - \Sigma_\infty = M(\Sigma_t - \Sigma_\infty)M^T$. This completes the proof of part (iv).

We now finally turn to the proof of Theorem 8.
Proof of Theorem 8. Let us start with the deterministic Gibbs sampler. The stationary distribution of the Gibbs sampler is \( \pi_\infty = \mathcal{N}_d(\mu_\infty, \Sigma_\infty) = \mathcal{N}_d(\mu, \Sigma) = \pi \). Apply the recurrence (26) to obtain \( \Sigma_t - \Sigma_\infty = B^t(\Sigma_0 - \Sigma_\infty)(B^t)^T \) for all \( t \geq 0 \). For all \( v \in \mathbb{R}^d \) and \( t \geq 0 \), it follows that

\[
v^T(\Sigma_t - \Sigma_\infty)v = \{(B^t)^Tv\}^T(\Sigma_0 - \Sigma_\infty)(B^t)^Tv,\]

and so \( \Sigma_0 \geq \Sigma_\infty \iff \Sigma_t \geq \Sigma_\infty \) for all \( t \geq 0 \). By Proposition 2 it follows that \( \pi_0 \sim \pi_\infty \iff \pi_t \sim \pi_\infty \) for all \( t \geq 0 \). This completes the proof for the Gibbs sampler; for ULA, notice the symmetry between the recurrences (26) and (28). The proof simply repeats the above steps, replacing the matrix \( B \) by the matrix \( M \).

One can see that if the matrices \( M \) and \( B \) are allowed to depend on the iteration \( t \geq 0 \), the proof of Theorem 8 carries through similarly. For ULA, this corresponds to the step size changing across iterations, while for the Gibbs sampler this corresponds to the order of the clock updates changing across iterations. This includes reversible Gibbs samplers, which alternate between updates in the increasing order of coordinate blocks with updates in the decreasing order of the blocks. The proof of Theorem 8 does not however extend to Gibbs samplers which scan through the coordinates at random. By Roberts and Sahu (1997), if the blocks are scanned in a random order \( z \), there exists a matrix \( B_z \) depending on \( z \) such that

\[
X_{t+1} \mid X_t, z \sim \mathcal{N}_d(B_zX_t + b, \Sigma - B_z\Sigma B_z^T).
\]

By integrating \( z \) out, the conditionals \( X_{t+1} \mid X_t \) are mixtures of Gaussian distributions. If the chain starts at a Gaussian \( \pi_0 \), then the marginals \( \pi_t \) are also mixtures of Gaussians. However, \( \pi_t \) need not be Gaussian for any finite \( t \geq 1 \), even though the target is Gaussian.

B.5.1 Computation of marginals by repeated squaring

Suppose that a marginal \( \pi_t = \mathcal{N}_d(\mu_t, \Sigma_t) \) for a relatively large value of \( t \geq 0 \) is of interest. An efficient strategy of computing this is as follows. Repeatedly applying the recurrence (28), we obtain for \( t \geq 0 \) that

\[
\mu_t - \mu_\infty = M^t(\mu_0 - \mu_\infty), \quad \Sigma_t - \Sigma_\infty = M^t(\Sigma_0 - \Sigma_\infty)M^t.
\]

The key to both of these computations is the matrix power \( M^t \). Consider the binary expansion \( t = \sum_{i=0}^{\lfloor \log_2 t \rfloor} b_i 2^i \). One can compute the matrices \( \{M, M^2, M^4, \ldots, M^{2^\lfloor \log_2 t \rfloor} \} \) by \( \lfloor \log_2 t \rfloor \) repeated squarings. Storing these matrices, one can reconstruct \( M^t \) by at most \( \lfloor \log_2 t \rfloor \) multiplications.

C Generalizations and extensions

Let \( p \geq 1 \), and \( \mu, \nu \) be measures with finite \( p \)-th moment in some Polish probability space \( \mathcal{X} \) equipped with metric \( d : \mathcal{X} \times \mathcal{X} \to [0, \infty) \). The Wasserstein distance of order \( p \) is

\[
\mathcal{W}_p(\mu, \nu) = \left( \inf_{(X,Y) \in \Gamma(\mu, \nu)} \mathbb{E}d(X,Y)^p \right)^{1/p},
\]

where \( \Gamma(\mu, \nu) \) is the set couplings of random variables \( X \sim \mu \) and \( Y \sim \nu \). By Villani (2009, Theorem 4.1) a coupling exists which is optimal for \( \mathcal{W}_p \).
Using essentially the same steps in the proof (the triangle inequality, sampling from an optimal coupling, and Jensen’s inequality), the lower bound of Theorem 2 theorem generalizes to Wasserstein distances of any order $p \geq 1$, on general metric spaces. Furthermore, one could also replace the reference measure $\mu_n$ by any probability measure $\varphi$ (which can be fixed or random) provided that $\varphi$ is independent of both $\mu'_n$ and $\nu_n$. The general version of Theorem 2 reads

$$
\|\mathbb{E}W_p(\hat{\mu}_n, \varphi) - \mathbb{E}W_p(\mu'_n, \varphi)\| \leq W_p(\mu, \nu).
$$

If $\varphi = \mu_n$ and $d(x, y) = \|x - y\|$, the rate of convergence for the lower bound estimator $L$ remains the sharp $n^{-1/d}$ for $d > 2p$, as stated in Theorem 6 for the case $p = 2$.

Under a compactness assumption, the concentration bounds of Theorem 5 generalize in the following ways. The sub-Gaussian bound for the estimator $U$, a linear combination of squared 2-Wasserstein distances, extends to linear combinations of empirical transportation costs, and maintains similar $\exp(-nt^2)$ tails. Similarly, the exponential bound for the estimator $L$, a linear combination of 2-Wasserstein distances, extends to linear combinations of $p$-Wasserstein distances, but the tails become of order $\exp(-nt^{2p})$. The probabilistic bound of Corollary 1 for the estimator $L$ generalizes to the $p \geq 1$ case when and $d(x, y) = \|x - y\|$, with the exponential becoming of order $\exp(-n^{1-2p/d})$ for $d > 2p$.

The limit in Proposition 4 extends to general distances $W_p(\hat{\mu}_n, \hat{\nu}_n)$ with centering constant $\mathbb{E}W_p(\hat{\mu}_n, \hat{\nu}_n)$. One can see that the proof does not extend to the case $\mu = \nu$ however, since division by zero would occur.

### C.1 Sharp rate of convergence for upper bound

Suppose that $\mu$ and $\nu$ are supported in the same compact set of diameter at most 1, the Brenier potential $\tilde{\varphi}$ from $\nu$ to $\mu$ is twice continuously differentiable, and $\nabla^{\otimes 2} \tilde{\varphi} \geq \lambda I_d$ for some $\lambda > 0$. Let $\sigma^*$ be the optimal permutation in equation (7), which solves for $W_2^2(\mu_n, \nu_n)$. Then, by Manole et al. (2021, Proposition 12), it follows that

$$
\mathbb{E}W_2^2(\hat{\mu}_n, \hat{\nu}_n) - W_2^2(\mu, \nu) \geq \lambda \mathbb{E} \frac{1}{n} \sum_{i=1}^{n} \|X_i - \nabla \tilde{\varphi}(Y_{\sigma^*(i)})\|^2
$$

$$
\geq \lambda \mathbb{E} \inf_{\sigma \in S_n} \frac{1}{n} \sum_{i=1}^{n} \|X_i - \nabla \tilde{\varphi}(Y_{\sigma(i)})\|^2
$$

$$
= \lambda \mathbb{E} W_2^2(\mu_n, \mu'_n),
$$

using in the last line that $\nabla \tilde{\varphi}(Y_i) \sim \mu$ independently for all $i$, and independently from all $X_i$. With $\lambda = 1$, the upper bound of Theorem 1 follows. If $\lambda = 1 + \varepsilon$ for some $\varepsilon > 0$, which essentially corresponds to $\nu \sim \mu$ and $\nu \neq \mu$, then it follows that

$$
\mathbb{E}U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}'_n) - W_2^2(\mu, \nu) = \mathbb{E}W_2^2(\hat{\mu}_n, \hat{\nu}_n) - \mathbb{E}W_2^2(\hat{\mu}_n, \hat{\mu}'_n) - W_2^2(\mu, \nu)
$$

$$
\geq \varepsilon \mathbb{E}W_2^2(\hat{\mu}_n, \hat{\mu}'_n).
$$

By Lemma 7, it thus follow that $\mathbb{E}U(\hat{\nu}_n, \hat{\mu}_n, \hat{\mu}'_n) - W_2^2(\mu, \nu) \gtrsim n^{-2/d}$ when $d > 5$. By Theorem 6, the upper bound $\mathbb{E}U$ to $W_2^2$ converges at a sharp rate $n^{-2/d}$ when $d > 5$.

### D Wasserstein coupling bound

In Biswas et al. (2019), the estimation of upper bounds on integral probability metrics (Gelbrich, 1990; Sriperumbudur et al., 2012) between $\pi_i$ and $\pi$ is proposed, via coupling.
We refer to this as the coupling bound. The bound applies to all integral probability metrics satisfying a Lipschitz-type condition, which includes all 1-Wasserstein distances. It is straightforward to extend the methodology in Biswas et al. (2019) to $p$-Wasserstein distances with $p > 1$. We now informally derive a coupling bound for the 2-Wasserstein distance $W_2(\pi_\infty, \pi_t)$, avoiding precise technical assumptions.

Suppose that $\lim_{t \to \infty} W_2(\pi_\infty, \pi_t) = 0$, and coupled chains $(X_t)_{t \geq 0}, (Y_t)_{t \geq 0} \sim (\pi_t)_{t \geq 0}$ are sampled via an $L$-lagged Markovian coupling, that is $(X_{t+L}, Y_t)$ is sampled conditionally on $(X_{t+L-1}, Y_{t-1})$ from a joint kernel $\tilde{K}$ for $t \geq 1$. The coupling kernel $\tilde{K}$ is designed to make the chains meet at an almost surely a finite time $\tau$, after which they take the same value. Then, for all $L \in \mathbb{N}$ it holds that

$$W_2(\pi_\infty, \pi_t) \leq \sum_{j=1}^{\infty} W_2(\pi_{t+jL}, \pi_{t+(j-1)L})$$

(triangle inequality)

$$\leq \sum_{j=1}^{\infty} \left( \mathbb{E}\|X_{t+jL} - Y_{t+(j-1)L}\|^2 \right)^{1/2},$$

(31)

using in the final line that $(X_{t+jL}, Y_{t+(j-1)L})$ is a coupling of $\pi_{t+jL}$ and $\pi_{t+(j-1)L}$.

Given $R$ replicates of the chains $(X, Y)$ denoted by $(X^{(r)}, Y^{(r)})$ for $r \in \{1, \ldots, R\}$ and meeting at finite times $\tau_1, \ldots, \tau_R$, we estimate the bound (31) by

$$\sum_{j=1}^{\infty} \left( \frac{1}{R} \sum_{r=1}^{R} \|X^{(r)}_{t+jL} - Y^{(r)}_{t+(j-1)L}\|^2 \right)^{1/2}.$$  

(32)

The chains are designed to meet at finite times $\tau_r$, so the infinite series truncates at $J = \max_{1 \leq r \leq R}\lfloor (\tau_r - L - t - 1)/L \rfloor$. The estimator (32) can computed efficiently in a parallel setting for all $t \geq 0$. For each pair of coupled chains $r$, only a vector of length $\tau_r - L$ needs to be stored, with entries $\|X^{(r)}_{t+jL} - Y^{(r)}_{t+(j-1)L}\|$ for $t \in \{0, \ldots, \tau_r - L - 1\}$.

Under suitable regularity conditions on the behaviour of the coupled chains, the bound (31) is finite and the estimator (32) converges to the bound (31) almost surely as the number of chains $R \to \infty$. While the estimator is known to be an upper bound in the large-sample regime, the estimator (32) is smaller in expectation than the 2-Wasserstein coupling bound for finite $R$. This is since

$$\mathbb{E}\left( \frac{1}{R} \sum_{i=1}^{R} \|X^{(i)}_{t+jL} - Y^{(i)}_{t+(j-1)L}\|^2 \right)^{1/2} \leq \left( \mathbb{E}\frac{1}{R} \sum_{i=1}^{R} \|X^{(i)}_{t+jL} - Y^{(i)}_{t+(j-1)L}\|^2 \right)^{1/2}$$

(Jensen)

$$= \left( \mathbb{E}\|X_{t+jL} - Y_{t+(j-1)L}\|^2 \right)^{1/2},$$

and so the expectation of the estimator (32) cannot be larger than the coupling bound (31). This behaviour contrasts with the coupling upper bound for integral probability metrics, which are unbiasedly estimated for any finite $R$. Our numerical investigations in Section 4.4 reveal that even state-of-the-art practically implementable couplings can be sub-optimal by a large margin. This suggests that, in the moderate sample size regime where the variability of the coupling bound estimator is under control, one can expect the estimate (32) to be conservative for $W_2(\pi_\infty, \pi_t)$.

Following Biswas et al. (2019), we note that choosing the lag $L$ to be large mitigates the inefficiency introduced by the triangle inequality into the coupling bound (31). In all our simulations apart from the RWM algorithm applied to the stochastic volatility model
(where, even with the smaller scaling, the meeting times are prohibitively large to do so),
the lag \( L \) is chosen to be large enough such that all \( R \) chains meet at times \( \tau_i \leq 2L \)
for \( i \in \{1, \ldots, R\} \). This ensures that the coupling bound is essentially completely
determined by the coupling kernel.

E  Numerics

The simulations were written in \( R \) (R Core Team, 2020), together with \( C++ \) code integrated
via the \( Rcpp \) package (Eddelbuettel and Balamuta, 2018), and were run on a Lenovo T490s
laptop equipped with 16GB of RAM and a four-core Intel i5-8265U processor. The code
to reproduce all experiments can be found in the repository http://www.github.com/tamaspapp/wassersteinbound.

E.1 The Flapjack algorithm

**Algorithm 1: Flapjack**

**Input:** Cost matrix \( C = (c_{ij}) \in \mathbb{R}^{n \times n} \).

**Output:** Assignment cost \( T \), leave-one-out assignment costs \( (T_1, T_2, \ldots, T_n) \).

**Initialize:** Solve the linear assignment problem (3), to obtain an optimal
assignment \( \sigma \in S_n \) and optimal dual variables \( u \in \mathbb{R}^n \) and \( v \in \mathbb{R}^n \). Store
\( T \leftarrow \sum_{i=1}^{n} c_{i\sigma(i)}/n \). Save the optima \( \sigma^* \leftarrow \sigma, u^* \leftarrow u \) and \( v^* \leftarrow v \), and also
\( c^* \leftarrow (c_{11}, c_{22}, \ldots, c_{nn}) \). Set \( \varepsilon \) to a small enough value to guarantee assignment,
say \( \varepsilon < 2 \min_{ij} c_{ij} - \max_{ij} c_{ij} \).

**Loop:** For \( j = 1, 2, \ldots, n \):
1. Remove the edge \((\sigma^{-1}(j), j)\) from the matching.
2. Set \( c_{jj} \leq \varepsilon \).
3. Set \( v_j \leftarrow \min_i (c_{ij} - u_i) \).
4. Starting from the feasible dual variables \((u, v)\), and the incomplete matching, solve
the assignment problem (3) with new cost matrix \( C \) to optimality using the
Hungarian algorithm, obtaining new optimal matching \( \sigma \).
5. Store \( T_j \leftarrow \sum_{i \neq j} c_{i\sigma(i)}/(n-1) \).
6. Restore \( \sigma \leftarrow \sigma^*, c_{jj} \leftarrow c_{jj}^*, u \leftarrow u^* \) and \( v \leftarrow v^* \).

We use the network simplex algorithm to solve for the size-\( n \) optimal assignment in
the first stage, as implemented in Bonneel et al. (2011). In the second stage, we compute
the \( n \) jackknife estimates using the Jonker-Volgenant successive shortest path algorithm
(Jonker and Volgenant, 1987), an efficient variant of the Hungarian algorithm (Jonker
and Volgenant, 1986; Crouse, 2016). We do not use its pre-solve heuristic, as we found
it to be unreliable for double precision cost matrices. Compared to only solving for the
size-\( n \) optimal assignment, additionally computing the jackknife estimates in Flapjack
makes the overall running time a factor of 2 to 5 larger. This is to be compared with
the factor of \( n \) larger that separately solving all of the \( n \) additional assignment problems
would entail. At sample size \( n = 1000 \), our implementation of Flapjack terminates in around 1 second.

### E.2 Contractive optimal transport in MCMC

The radial component of the \( d \)-dimensional multivariate logistic target has density \( h(r) \propto r^{d-1} \exp(-r)/(1 + \exp(-r))^2 \) (Gómez et al., 2003, Definition 1, Theorem 3). We sample this using adaptive rejection sampling (Gilks and Wild, 1992). Figure 9 displays additional findings discussed in Section 2.2.

![Figure 9: Quantiles of (left) the radial component of \( \pi_t \), and (right) \( \pi_t \), against iteration \( t \geq 0 \), from probability 0.005 (dark blue) to 0.995 (light blue). The RWM algorithm (left) targeted the logistic target \( \pi(x) \propto \exp(x)/(1 + \exp(x))^2 \) with starting density \( \pi_0(x) \propto \pi(x/2) \), and (left) targeted \( \pi = 0.5\mathcal{N}_1(-5, 1) + 0.5\mathcal{N}_1(5, 1) \) with \( \pi_0 = 0.5\mathcal{N}_1(0, 1) + 0.5\mathcal{N}_1(10, 1) \) and \( h = 2 \). The condition \( \pi_t \overset{\text{c.s.}}{\to} \pi_\infty \) holds for all \( t \geq 0 \) in the left plot, but fails for \( t > 0 \) in the right plot.

### E.3 Gibbs sampler

A thinning factor of 5 was used for both the empirical and the coupling bounds. For the empirical bound, \( T = 5000 \) was set, at which point the chain has been stationary for a substantial amount of iterations. The empirical bounds were debiased by averaging in the asymptote for \( T' \in \mathcal{A} = \{2000, 2005, \ldots, 4000\} \). The reflection-maximal coupling (Bou-Rabee et al., 2020; Jacob et al., 2020) was used, coordinate-wise, to compute the coupling bound at a lag of \( L = 5000 \). With this large value of \( L \), all meetings occurred before time \( L \) as measured at the \( Y \)-chain, and the coupling bound incurred virtually no loss due to the triangle inequality.

#### E.3.1 Explanation for the tightness of the bound \( U \)

The reason why the bound \( U \) closely follows the true squared Wasserstein distance is due to the essentially low-dimensional nature of the problem, as we now explain. The high
correlation in the AR(1) process causes the largest principal components of the target
to overshadow the rest (the sum of the five largest eigenvalues is over 90% of the trace),
and causes the sampler to explore more easily in the direction of the smallest principal
components than in the direction of the larger ones. For all but the earliest few iterations
\( t \), the marginals \( \pi_t \) of the Gibbs sampler approximately lie in the same low-dimensional
subspace, spanned by, say, the five largest principal components of the target \( \pi \). When
the distributions are approximately supported in a low-dimensional subset of \( \mathbb{R}^d \), the
empirical Wasserstein distance has been shown to converge faster than the canonical rate
\( n^{-1/d} \) for low-to-moderate sample sizes \( n \) (Weed and Bach, 2019, Section 5.3). A faster
rate therefore applies to our upper bound \( U \) as well. This rate, in conjunction with the
debiasing term present in \( U \), causes the estimator to have a very small bias at the sample
size we consider.

### E.4 Dimensional scaling of ULA and MALA

The target \( \pi = \mathcal{N}_d(0, \Sigma) \) with \( \Sigma_{ij} = 0.5^{|i-j|} \) corresponds to a \( d \)-dimensional AR(1) process
with correlation \( \rho = 0.5 \) and unit noise. Properties of such matrices \( \Sigma \) are listed in Trench
(1999, Section 1). The precision matrix \( \Sigma^{-1} \) is tridiagonal with a simple closed form,
leading to faster gradient computation. The eigenvalues of \( \Sigma \) fall between 1/3 and 3, the
covariance therefore satisfies \( I_d/3 \preceq \Sigma \preceq 3I_d \) and so is well-conditioned with a condition
number of 9. By Proposition 2, it follows that \( \mathcal{N}_d(0, 3I_d) = \pi_0 \overset{\text{cot}}{\rightsquigarrow} \pi = \mathcal{N}_d(0, \Sigma) \), and so
the start \( \pi_0 \) is appropriately overdispersed with respect to the target \( \pi \). The dimension
was set to \( d \in \{50, 100, 200, 300, 400, 500, 600, 800, 1000\} \).

For MALA, no thinning was used, and the empirical bounds were computed with
\( T = 2000 \) and debiased by averaging in the asymptote for \( T' \in \mathcal{A} = \{250, 251, \ldots, 500\} \).
For ULA, the empirical bounds used a thinning factor of 40, and the empirical bounds
were computed with \( T = 70000 \) and debiased by averaging in the asymptote for \( T' \in \mathcal{A} = \{8000, 8040, \ldots, 60000\} \). No thinning was used for the coupling bound, and both
algorithms used the reflection-maximal coupling (Bou-Rabee et al., 2020; Jacob et al.,
2020), with a lag of \( L = 2000 \) for MALA and a lag of \( L = 70000 \) for ULA. With these
large values of \( L \), all meetings occurred before time \( L \) as measured at the \( Y \)-chain. Relative
to MALA, the much larger choice of the lag \( L \) for ULA is due to the much slower mixing
of this algorithm. The gap between the debiasing interval \( \mathcal{A} \) and the endpoint \( T \) was
chosen significantly larger, in terms of relative size, for MALA than for ULA. This is
purely due to the convenience of selecting \( T = L \) in our simulations, and we emphasize
that the bound for MALA exhibits similar performance for smaller values of \( T \) as well.

Letting TV denote the total variation distance, for parity with the \( \text{TV}(\pi_t, \pi_\infty) \leq 0.25 \)
threshold used in Biswas et al. (2019) mixing times were computed at the threshold
\( W_2^2(\pi_t, \pi_\infty) \leq 6 \), because at these thresholds the coupling bounds for both the Wasserstein
and the total variation distances indicated similar mixing times.

We remark that for the larger values of \( d \) we consider, the stationary distribution of
ULA does not strictly satisfy \( \pi_0 \overset{\text{cot}}{\rightsquigarrow} \pi_\infty \), since we have seen numerically that \( 3I_d - \Sigma_\infty \)
has one negative eigenvalue. However, the absolute value of the negative eigenvalue is
invariably negligibly small compared to the others, and so \( \pi_0 \overset{\text{cot}}{\rightsquigarrow} \pi_\infty \) is approximately
satisfied. Our numerical results in Figure 6 confirm that our bounds are robust to this
slight discrepancy.
E.4.1 Stationary bias of ULA

By Proposition 5, ULA has a stationary distribution \( \pi_{\infty} = \mathcal{N}_d(0, \Sigma_{\infty}) \) with \( \Sigma_{\infty} \succeq \Sigma \). By Proposition 2 it follows that \( \pi_{\infty} \overset{\text{cot}}{\sim} \pi \), hence the stationary distribution of ULA is overdispersed with respect to its intended target. Theorem 1 thus enables us to directly quantify the bias of ULA due to its discretization error by an upper bound on \( W_2^2(\pi, \pi_{\infty}) \), which is complemented by the lower bound on \( W_2^2(\pi, \pi_{\infty}) \) from Theorem 2. Bringing these bounds to the same scale, Figure 10 displays the estimators \( U \) and \( L_{sq} \) for an ULA with step size \( h = d^{-1/6} \). The bounds are able to detect the stationary bias of ULA at this step size.

![Figure 10: Estimated bounds on \( W_2^2(\pi_{\infty}, \pi) \) for the ULA of Section 4.4.2 with a larger step size \( h = d^{-1/6} \). Box plots of 50 estimators \( U \) ( ■ ) and \( L_{sq} \) ( □ ) at sample size \( n = 1000 \), and exact squared distance ( × ). The y-axis is on a log\(_{10}\)-scale.](image)

E.4.2 Erratum for Biswas et al. (2019)

We note that our numerical results for the ULA vs MALA scaling are markedly different to those in Biswas et al. (2019, Section 3.3). While our choice of different step sizes and initial distribution are contributing factors, the discrepancy is largely due to an unfortunate error in the code associated to Biswas et al. (2019), as confirmed by the authors. As opposed to the intended scaling \( h \sim d^{-1/6} \), both ULA and MALA are instead scaled with a much larger \( h \sim d^{-1/12} \). This leads to vanishingly small acceptance probabilities for MALA as the dimension is increased. Compared to MALA, ULA does not have an acceptance step. Therefore, in large enough dimension, it converges to its stationary distribution faster than MALA, despite having a step size which was chosen to be a constant factor smaller. At the same time, the larger scaling causes ULA to converge to a stationary distribution which is substantially different from the intended target.
E.5 Stochastic volatility model

The stochastic volatility model we consider echoes (Liu, 2001, Section 9.6.2) and (Girolami and Calderhead, 2011, Section 8):

\[ Y_t = \beta \varepsilon_t \exp \left( \frac{X_t}{2} \right), \quad \varepsilon_t \sim \mathcal{N}(0, 1), \quad \text{for } t = 1, \ldots, T, \]
\[ X_{t+1} = \varphi X_t + \eta_{t+1}, \quad \eta_{t+1} \sim \mathcal{N}(0, \sigma^2), \quad \text{for } t = 1, \ldots, T - 1, \]
\[ X_1 \sim \mathcal{N} \left( 0, \frac{\sigma^2}{(1 - \varphi^2)} \right). \]

Here, \( X_{1:T} = (X_1, \ldots, X_T) \) is a latent AR(1) process, which drives the variance of the logarithm of the data \( Y_{1:T} = (Y_1, \ldots, Y_T) \). We assume that the parameters \( \beta, \varphi \) and \( \sigma \) are fixed. Having observed the data \( Y_{1:T} \), the log-posterior density \( f(X_{1:T} \mid Y_{1:T}) \) is, up to a constant offset,

\[ f(X_{1:T} \mid Y_{1:T}) = -\frac{1}{2} \left( \sum_{t=1}^{T} X_t + \frac{1}{\beta^2} \sum_{t=1}^{T} Y_t^2 \exp(-X_t) + \frac{1}{\sigma^2} \sum_{t=1}^{T-1} (\varphi X_t - X_{t+1})^2 + \frac{1 - \varphi^2}{\sigma^2} X_1^2 \right). \]

The gradient of the log-posterior \( f \) thus has components

\[ \frac{\partial f}{\partial X_1} = \frac{1}{2 \beta^2} Y_1^2 \exp(-X_1) - \frac{\varphi}{\sigma^2} (\varphi X_1 - X_2) - \frac{1 - \varphi^2}{\sigma^2} X_1, \]
\[ \frac{\partial f}{\partial X_t} = \frac{1}{2 \beta^2} Y_t^2 \exp(-X_t) - \frac{\varphi}{\sigma^2} (\varphi X_t - X_{t+1}) - \frac{1}{\sigma^2} (X_t - \varphi X_{t-1}), \quad \text{for } t = 2, \ldots, T - 1, \]
\[ \frac{\partial f}{\partial X_T} = \frac{1}{2 \beta^2} Y_T^2 \exp(-X_T) - \frac{1}{\sigma^2} (X_T - \varphi X_{T-1}). \]

When using a gradient-based Metropolis-Hastings algorithm, we evaluate the log-posterior and its gradient at proposal \( X_{1:T} \). We can reduce the total computation time of these steps, perhaps at the expense of additional memory usage. With all operations applied component-wise, we compute the vectors \( \exp(-X_{1:T}) \) and \( \varphi X_{1:T-1} - X_{2:T} \) exactly once, then re-use them for both the posterior and gradient calculation.

The dimension of the problem was \( T = 360 \), equivalent to approximately one year of daily data. Following Girolami and Calderhead (2011), the parameter values were fixed at \( \beta = 0.65, \varphi = 0.98 \) and \( \sigma = 0.15 \). The data \( Y_{1:T} \) were simulated from the model.

The MALA was run with a step-size of \( h = 0.13T^{-1/6} \), giving an acceptance rate of around 56%, which is known to be approximately optimal in certain high-dimensional settings (Roberts and Rosenthal, 1998). A thinning factor of 50 was used for both the empirical and coupling bounds. The empirical bounds used \( T = 60000 \), and employed debiasing by averaging in the asymptote for \( T' \in \mathcal{A} = \{20000, 20050, \ldots, 50000\} \). The coupling bound used the reflection-maximal coupling (Bou-Rabee et al., 2020; Jacob et al., 2020) with a lag of \( L = 60000 \). With this large value of \( L \), all meetings occurred before time \( L \) as measured at the \( Y \)-chain, and the coupling bound incurred virtually no loss due to the triangle inequality.

The RWM was first run with a step size of \( h = 0.25T^{-1/2} \), for an acceptance rate of around 24%, which is known to be approximately optimal in certain high-dimensional settings (Roberts et al., 1997). A thinning factor of 2000 was used for both the empirical and coupling bounds. The empirical bounds used \( T = 3000000 \) (two orders of magnitude larger than for the MALA), and employed debiasing by averaging in the asymptote for \( T' \in \mathcal{A} = \{1000000, 1002000, \ldots, 2000000\} \). No coupling was used, as all preliminary runs
with the reflection-maximal coupling failed to meet within iteration counts two orders of magnitude larger than those considered for the empirical bound. The RWM was then run with a smaller scaling of \( h = 0.1T^{-1/2} \), for an acceptance rate of around 64%. A thinning factor of 2000 was used for both the empirical and coupling bounds, and the empirical bound was computed similarly to the larger scaling. The coupling bound was computed with the reflection-maximal coupling and a lag of \( L = 2000000 \). As measured at the \( Y \)-chain, many meetings occur after iteration \( L \), causing the coupling bound to lose efficiency due to the triangle inequality. In this example, it was computationally infeasible to increase \( L \) to where the impact of the triangle inequality was negligible for the coupling bound.

### E.5.1 The start from the prior distribution is overdispersed

With the same parameters as outlined above, the MALA was also run started from a twice spread-out version of the target. Samples from the target were obtained from iteration \( T = 60000 \) of the previous MALA experiment, then were multiplied by a factor of 2, leading to a starting density \( \pi_0(x) \approx \pi(x/2) \) which satisfies \( \pi_0 \overset{\text{opt}}{\rightarrow} \pi \) (the optimal transport map is \( T(x) = x/2 \)). Figure 11 compares the empirical bounds obtained from this known overdispersed start to those obtained by starting from the prior. While the bounds indicate that the MALA converges slower when started from the prior, the overall shape of the bounds is similar for both starts, suggesting that the start from the prior is suitably overdispersed with respect to the target.

![Figure 11](image-url)

**Figure 11:** Empirical bounds on the squared Wasserstein distance \( W_2^2(\pi_t, \pi_\infty) \) (--- \( U \); --- \( L_{sq} \); shaded areas are 95% jackknife confidence intervals) for the MALA targeting the stochastic volatility model. The sampler is started from the prior (left) and a spread-out version of the target (right).

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