Asymptotic bias of inexact Markov Chain Monte Carlo methods in high dimension

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Abstract

Inexact Markov Chain Monte Carlo methods rely on Markov chains that do not exactly preserve the target distribution. Examples include the unadjusted Langevin algorithm (ULA) and unadjusted Hamiltonian Monte Carlo (uHMC). This paper establishes bounds on Wasserstein distances between the invariant probability measures of inexact MCMC methods and their target distributions with a focus on understanding the precise dependence of this asymptotic bias on both dimension and discretization step size. Assuming Wasserstein bounds on the convergence to equilibrium of either the exact or the approximate dynamics, we show that for both ULA and uHMC, the asymptotic bias depends on key quantities related to the target distribution or the stationary probability measure of the scheme. As a corollary, we conclude that for models with a limited amount of interactions such as mean-field models, finite range graphical models, and perturbations thereof, the asymptotic bias has a similar dependence on the step size and the dimension as for product measures.

1 Introduction

This paper deals with Markov Chain Monte Carlo (MCMC) methods based on Markov chains that do not exactly preserve a target distribution $\pi$ on $\mathbb{R}^d$. A simple example is the Unadjusted Langevin algorithm (ULA) where the Markov chain is an Euler-Maruyama (EM) discretization of an overdamped Langevin diffusion with invariant measure $\pi$. Alternatively, modifications of the EM scheme can be applied, such as Runge-Kutta and $\theta$ methods [33, 53, 60, 15, 1] or a taming strategy [9]. Further, in recent years, variants of the EM scheme have been developed in recent years specifically for certain forms of target distributions motivated by applications in computational statistics and machine

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Another important class of inexact MCMC methods is based on Hamiltonian dynamics which are approximated numerically by a symplectic integrator \[19, 44, 39\]. Unadjusted Hamiltonian Monte Carlo (uHMC) is one of the most popular schemes in this class. It consists of using the Störmer-Verlet (or leapfrog) integrator in combination with momentum randomizations. In general, the basic idea underlying inexact MCMC methods is to consider a continuous-time Markov process which is ergodic with respect to \( \pi \). Since an exact simulation of the continuous time dynamics is usually not possible, a discrete time approximation is adopted. Although in principle, it is possible in many cases to incorporate a Metropolis-Hastings accept/reject step to ensure that the target distribution \( \pi \) is invariant for the corresponding Markov chain, this is not always convenient since it may lead to high rejection probabilities and slow convergence of the method, see the discussion in Section 3.3. On the other hand, without adjustment, the discretization with time step size \( \gamma > 0 \) usually has an invariant measure \( \pi_\gamma \) that is only approximately equal to \( \pi \), and approaches \( \pi \) in the limit \( \gamma \to 0 \).

In recent years, a lot of work has been done on the analysis of the approximation error of inexact MCMC methods, focusing mainly on the unadjusted Langevin algorithm \[13, 22, 24, 9, 14, 40, 46, 41, 8, 6\]. In most of these works, the analysis of approximation bias is intertwined with the study of convergence to equilibrium. While this approach has yielded meaningful results, the intertwining of contraction properties and bias does not make it clear exactly which factors contribute to the dimension dependence of the resulting bounds and in which way. Therefore, to gain a better understanding, we propose to separate the two effects and to divide the error analysis into two parts: quantifying the mixing properties of the Markov chain, and quantifying the distance between its invariant measure \( \pi_\gamma \) and the target distribution \( \pi \). The focus of this work is on the second task. In particular, we provide a careful analysis of Wasserstein distances between \( \pi_\gamma \) and \( \pi \) and their dependence on both the dimension \( d \) and the discretization step size \( \gamma \). We will see that the results we obtain and their conclusion depend crucially on the type of Wasserstein distance that we consider.

There is already an extensive literature on the bias associated with numerical schemes for SDE, and in particular for Euler-Maruyama discretizations. The seminal works \[54, 55\] analyze the difference between the integrals \( \int_{\mathbb{R}^d} f \, d\pi \) and \( \int_{\mathbb{R}^d} f \, d\pi_\gamma \) for smooth functions \( f \). The regularity requirements for \( f \) have been relaxed considerably in later work \[2\]. In \[42\] the authors bound the distance between \( \pi \) and \( \pi_\gamma \) in metrics weaker than Wasserstein distances, and outline possible approaches to deriving Wasserstein bounds. Subsequently, convergence to equilibrium and Wasserstein and total variation bias for Euler-Maruyama discretizations have been studied in several papers including \[22, 24, 40, 46\]. These two distances are of interest for applications in Bayesian inference. The total variation distance, by definition, allows us to obtain guarantees for the estimates for highest posterior density regions produced by MCMC algorithms. As for the Wasserstein distance, it allows for guarantees when one wants to estimate the mean of the posterior distribution.

Our goal in the present work is to understand more precisely and more generally the
order in the step size \( \gamma \) and the dimension \( d \) of Wasserstein distances between \( \pi \) and \( \pi_{\gamma} \). To this end, we follow a simple approach outlined for example in [42, Remark 6.3], which is based on a triangle inequality trick, see Lemma 1 below. To implement this approach, we need two ingredients: a bound on the convergence to equilibrium in Wasserstein distance for either the exact dynamics or its numerical approximation, and a bound on the finite time accuracy of the approximation. Bounds of the first type have been derived systematically in recent years in various situations [27, 22, 24, 31, 40, 14, 28, 7, 8]. Our main contribution is therefore a careful study of the finite time Wasserstein accuracy in high dimension.

To explain our main results, we start with a simple but important example which can be easily analyzed. Suppose that \( \pi = \mu^d = \otimes_{i=1}^d \mu \) is a \( d \)-fold product of a probability measure \( \mu \) on \( \mathbb{R} \) which is absolutely continuous with respect to the Lebesgue measure, with density proportional to \( e^{-V} \) where \( V \) is a continuously differentiable function. Thus, \( \pi \) admits a density proportional to \( e^{-U} \) where for any \( x = (x_i)_{i=1}^d \in \mathbb{R}^d \),

\[
U(x) = \sum_{i=1}^d V(x_i) .
\]  

(1)

Under mild assumptions on \( V \), the measure \( \pi \) is invariant for the overdamped Langevin diffusion defined by the SDE

\[
dY_t = -\nabla U(Y_t) \, dt + \sqrt{2} \, dB_t ,
\]

where \((B_t)_{t \geq 0}\) is a Brownian motion in \( \mathbb{R}^d \). Now consider the Euler discretization

\[
X_{k+1} = X_k - \gamma \nabla U(X_k) + \sqrt{2} \gamma G_{k+1} ,
\]  

(2)

where \( \gamma > 0 \) is the step size, and \((G_k)_{k \geq 1}\) is a sequence of independent standard normal random variables in \( \mathbb{R}^d \). The recursion (2) defines a Markov chain with state space \( \mathbb{R}^d \) and transition kernel \( R_{\gamma} \). The unadjusted Langevin algorithm (ULA) consists in simulating the Markov chain \((X_k)_{k \geq 0}\) to get approximate samples from \( \pi \).

Recall that for a metric \( d : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_+ \), and probability measures \( \mu, \nu \in \mathcal{P}(\mathbb{R}^d) \), the \( L^p \) Wasserstein distance of order \( p \) associated with \( d \) is defined by

\[
W_{p,d}(\mu, \nu) = \inf \left\{ \int_{\mathbb{R}^d \times \mathbb{R}^d} d(x,y)^p \, d\zeta(x,y) : \zeta \in \Gamma(\mu, \nu) \right\}^{1/p} ,
\]

where \( \Gamma(\mu, \nu) \) is the set of all couplings of \( \mu \) and \( \nu \), i.e., all probability measures on \( \mathbb{R}^d \times \mathbb{R}^d \) with marginals \( \mu \) and \( \nu \). The \( L^p \) Wasserstein distance associated with the Euclidean distance is denoted by \( W_p \). Under mild assumptions, it can be shown that the Markov chain \((X_k)_{k \geq 0}\) defined by (2) has a unique invariant probability measure \( \pi_{\gamma} \), and the \( L^p \) Wasserstein distance \( W_p(\pi_{\gamma}, \pi) \) is of order \( O(\gamma) \) for every \( p \in [1, 2] \). This is well-known [24], and follows also from the results below. We are interested in the precise dependence of the corresponding bounds on both the dimension and the step size. In the particular case where \( U \) is of the form (1), the analysis is relatively simple. Indeed,
it is easy to verify that under mild assumptions on $V$, $\pi_\gamma$ is the $d$-fold product of the invariant measure $\mu_\gamma$ corresponding to ULA with one-dimensional target distribution $\mu$, and, therefore,

$$W_2(\pi_\gamma, \pi)^2 = W_2(\mu_\gamma^d, \mu^d)^2 = d W_2(\mu_\gamma, \mu)^2.$$ 

Thus for $p = 2$, $W_p(\pi_\gamma, \pi)$ is of order $O(d^{1/2}\gamma)$, and the same holds for any $p \leq 2$, since in this case, $W_p \leq W_2$. More generally, for any $q \geq 1$, we can endow $\mathbb{R}^d$ with either the $\ell^q$ distance

$$\ell^q(x, y) = \|x - y\|_{\ell^q} = \left(\sum_{i=1}^d |x_i - y_i|^q\right)^{1/q}, \quad x, y \in \mathbb{R}^d,$$  

or the normalized $\tilde{\ell}^q$ distance

$$\tilde{\ell}^q(x, y) = \|x - y\|_{\tilde{\ell}^q} = \left(d^{-1}\sum_{i=1}^d |x_i - y_i|^q\right)^{1/q}, \quad x, y \in \mathbb{R}^d,$$

and consider the corresponding Wasserstein distances $W_{p,\ell^q}$ and $W_{p,\tilde{\ell}^q}$ of order $p$ on the space of probability measures on $\mathbb{R}^d$. Note that for any $q \in [1, 2]$, we have $\|x\|_{\tilde{\ell}^q} = d^{1/q}\|x\|_{\ell^q}$ and $\|x\|_{\tilde{\ell}^q} \leq \|x\|_{\ell^2}$. Therefore, for any $p, q \in [1, 2]$,

$$W_{p,\tilde{\ell}^q}(\pi_\gamma, \pi) \leq W_{2,\tilde{\ell}^q}(\pi_\gamma, \pi) = d^{-1/2} W_2(\pi_\gamma, \pi) \in O(\gamma),$$

$$W_{p,\tilde{\ell}^q}(\pi_\gamma, \pi) = d^{1/q} W_{p,\ell^q}(\pi_\gamma, \pi) \in O(d^{1/q}\gamma).$$

On the other hand, an explicit computation in the case where $\mu$ and $\mu_\gamma$ are Gaussian measures shows that, at least for $q = 2$, this order is sharp, see Section 3.2 below. Thus in the product case, to obtain an accurate approximation of the invariant measure w.r.t. the $W_{p,\ell^q}$ distance, the step size $\gamma$ in the unadjusted Euler scheme should be chosen of order $O(d^{-1/q})$, whereas an accurate approximation in the $W_{p,\tilde{\ell}^q}$ distance can be achieved with a step size that is independent of the dimension. It follows that if one is only interested in approximating integrals $\int_{\mathbb{R}^d} f \, d\gamma$ for functions $f : \mathbb{R}^d \to \mathbb{R}$ that are Lipschitz continuous w.r.t. the $\ell^q$ metric with a Lipschitz constant that does not depend on the dimension $d$, then the step size can be chosen independently of $d$. This is often the case in molecular dynamics simulations when $f$ is an intensive quantity. Examples include averages $f(x) = \frac{1}{d} \sum_{i=1}^d \Phi(x,i)$, and more generally, U-statistics $f(x) = (d_k)^{-1} \sum_{1 \leq i_1 < i_2 < \ldots < i_d} \Phi(x_{i_1}, \ldots, x_{i_k})$, where $k \in \{1, \ldots, d\}$ is fixed, and $\Phi : \mathbb{R}^k \to \mathbb{R}$ is Lipschitz continuous. If, on the other hand, one is interested in the integrals of functions that are Lipschitz continuous w.r.t. the $\ell^q$ metric with a fixed dimension free Lipschitz constant, then a step size of order $O(d^{-1/q})$ is required. This scenario is more common in applications in Bayesian statistics and machine learning [48, 3].

An alternative to ULA is the unadjusted Hamiltonian Monte Carlo algorithm (uHMC) [19, 45, 5, 7, 25] which is based on the Hamiltonian flow $(\psi_t)_{t \geq 0}$ associated to the unit mass Hamiltonian $H(q, p) = U(q) + |p|^2/2$, i.e., $\psi_T(q_0, p_0) = (q_T, p_T)$ where $(q_t, p_t)_{t \geq 0}$ is the solution of the ordinary differential equation $\frac{d}{dt}(q_t, p_t) = (p_t, -\nabla U(q_t))$ with initial value $(q_0, p_0)$. Fix $T > 0$, let $(G_k)_{k \geq 1}$ be a sequence of independent standard normal
random variables, and denote by \( \text{proj}_q : \mathbb{R}^{2d} \to \mathbb{R} \) the projection onto the first \( d \) components. Then the recursion \( Q_{k+1} = \text{proj}_q(\Psi_T(Q_k, G_{k+1})) \) defines a Markov chain for which \( \pi \) is invariant. This Markov chain corresponds to the exact Hamiltonian Monte Carlo (xHMC) algorithm. To be able to carry out numerical computations, the Hamiltonian flow is approximated using the Verlet scheme with a given time step size \( \gamma > 0 \), or an alternative integrator, see Section 2.2. The MCMC method using the Markov chain defined as above, but with the exact Hamiltonian flow \((\Psi_t)_{t \geq 0}\) replaced by its numerical approximation \((\tilde{\Psi}_t)_{t \geq 0}\), i.e., \( \tilde{Q}_{k+1} = \text{proj}_q(\tilde{\Psi}_T(\tilde{Q}_k, G_{k+1})) \), is referred to as the unadjusted Hamiltonian Monte Carlo (uHMC) algorithm. It can be shown under mild assumptions that the corresponding transition kernel \( K_{T,\gamma} \) has an invariant probability measure \( \pi_{T,\gamma} \) such that \( W_p(\pi_{T,\gamma}, \pi) \) is of order \( O(\gamma^2) \) for any \( p \in [1, 2] \). The improved order compared to ULA comes from the fact that the Verlet scheme is a higher order integrator. Once more, we are interested in the precise dependence of the corresponding bounds on the dimension and the step size. In the case where \( \pi \) is a product measure associated with \( U \) of the form (1), \( \pi_{T,\gamma} \) is also a \( d \)-fold product of the invariant measure \( \mu_{T,\gamma} \) associated with uHMC with target distribution \( \mu \). Thus following similar arguments as for ULA, we obtain

\[
W_2(\pi_{T,\gamma}, \pi) = W_2(\mu_{T,\gamma}, \mu) = d^{1/2} W_2(\mu_{T,\gamma}, \mu) \leq O(d^{1/2} \gamma^2),
\]

\[
W_{p,\ell_k}(\pi_{T,\gamma}, \pi) = W_{2,\ell_k}(\pi_{T,\gamma}, \pi) = d^{-1/2} W_2(\pi_{T,\gamma}, \pi) \leq O(\gamma^2),
\]

\[
W_{p,\ell_k}(\pi_{T,\gamma}, \pi) = d^{1/q} W_{p,\ell_k}(\pi_{T,\gamma}, \pi) \leq O(d^{1/q} \gamma^2).
\]

Again, these bounds are sharp if \( \mu \) is a Gaussian measure and \( q = 2 \), see Section 3.2. Thus in the product case, the situation is completely analogous for uHMC as for ULA, except that the dependence of the orders on \( \gamma \) is better for uHMC. In particular, for an accurate approximation of the invariant measure w.r.t. the \( W_{p,\ell_k} \) distance, the discretization step size \( \gamma \) in uHMC should be chosen of order \( O(d^{-1/(2q)}) \), whereas an accurate approximation in \( W_{p,\ell_k} \) can be achieved again with a step size that is independent of the dimension.

Our goal in this paper is to study under which assumptions results similar to the ones described above hold. For ULA as well as for unadjusted Hamiltonian Monte Carlo, we will see that in the general case where \( \pi \) admits a smooth density proportional to \( e^{-U} \) with respect to the Lebesgue measure, the dimension dependence enters in an explicit way through some key quantities depending on \( \nabla U \). In particular, \( |\Delta \nabla U|^2 \) turns out to be crucial for controlling the dimension dependence – see the discussion after Theorem 5 and Section 3.1. As a consequence, we can show that for a broad class of models, the dimension dependence is under appropriate assumptions of the same order as in the \textit{product case}. Besides product models, this class of \textit{“nice” models} includes finite range graphical models, mean-field models, and their perturbations (e.g., finite dimensional projections of measures on infinite dimensional spaces that are absolutely continuous w.r.t. a Gaussian reference measure), see Section 3.1. In particular, to the authors’ knowledge, the class of models that we identify seems to include essentially all models for which scaling limits of Metropolis-Hastings algorithms have been established; see for
example [50, 52, 59, 47, 4]. On the other hand, there is a more general class of models for which our bounds have a worse dimension dependence as in the product case. We expect that this is not a coincidence but that the dimension dependence of the asymptotic bias may be generically worse.

Our main results are stated in Section 2. In Section 3, we study the resulting dimension dependence for concrete classes of models, and we compare what is known for unadjusted and for Metropolis-adjusted methods. Most of the proofs of our results are gathered in Section 4.

Notation

If X is a topological space then we denote by \( \mathcal{B}(X) \) the corresponding Borel \( \sigma \)-field, and by \( \mathcal{P}(X) \) the set of probability measures on \( (X, \mathcal{B}(X)) \). The Euclidean inner product on \( \mathbb{R}^d \) are denoted by \( \langle \cdot, \cdot \rangle \) and \( \langle \cdot, \cdot \rangle \) respectively, and we set \( \mathcal{P}_\mu(\mathbb{R}^d) = \{ \mu \in \mathcal{P}(\mathbb{R}^d) : f_{\mathbb{R}^d} |x|^p \mu(dx) < +\infty \} \). We denote by \( C^k(\mathbb{R}^d, \mathbb{R}^m) \) the set of \( k \)-times continuously differentiable functions from \( \mathbb{R}^d \) to \( \mathbb{R}^m \), and \( C^k(\mathbb{R}^d, \mathbb{R}) \) stands for \( C^k(\mathbb{R}^d, \mathbb{R}) \). For \( f : \mathbb{R}^d \rightarrow \mathbb{R}^m \), denote by \( \nabla f : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m} \) the gradient of \( f \) and \( \Delta f \) the vector Laplacian of \( f \) if they exist. For any function \( f : \mathbb{R}^d \rightarrow \mathbb{R}^m \), \( \partial_i f \) denotes the partial derivative with respect to the \( i \)-th variable of \( f \) and \( Df \) is the differential of \( f \). \( \text{div} \) stands for the divergence operator defined by \( \text{div}(\psi) = \sum_{i=1}^d \partial_i \psi_i \), where \( \psi_i \) is the \( i \)-th component of \( \psi \). \( | \cdot | \) and \( \lfloor \cdot \rfloor \) stand for the upper and lower integer part, respectively. For any matrix \( A = (A_{i,j})_{i,j=1}^d \in \mathbb{R}^{d \times d} \), \( \text{Tr}(A) = \sum_{i=1}^d A_{i,i} \) denotes the trace of \( A \). Finally, we denote by \( \varphi_d(x) = (2\pi)^{-d/2} \exp(-|x|^2/2) \) the density of the \( d \)-dimensional standard normal distribution.

2 Main results

Before specializing to more specific settings, we start with some simple but important general observations that are the basis for all the results below. Let \( (X, \mathcal{X}) \) be a measurable space, and suppose that \( W : \mathcal{P}(X) \times \mathcal{P}(X) \rightarrow [0, +\infty] \) is a distance function on the space \( \mathcal{P}(X) \) consisting of all probability measures on \( (X, \mathcal{X}) \). Note that we allow the value infinity for the distance. The bounds on distances between invariant measures that we derive below are all based on the following lemma.

Lemma 1 (The triangle inequality trick). Let \( Q \) and \( S \) be Markov transition kernels on \( (X, \mathcal{X}) \) with invariant probability measures \( \pi_Q \) and \( \pi_S \), respectively. Suppose that there exist functions \( \varphi, \varepsilon : \mathbb{N} \rightarrow \mathbb{R}_+ \) with \( \inf_{n \in \mathbb{N}} \varphi(n) < 1 \) such that for any \( n \in \mathbb{N} \),

\[
W(\pi_S Q^n, \pi_Q) \leq \varphi(n) W(\pi_S, \pi_Q), \quad \text{and} \quad (4)
\]

\[
W(\pi_S S^n, \pi_S Q^n) \leq \varepsilon(n). \quad (5)
\]

Then,

\[
W(\pi_S, \pi_Q) \leq \inf \left\{ \frac{\varepsilon(n)}{1 - \varphi(n)} : n \in \mathbb{N} \text{ with } \varphi(n) < 1 \right\}. \quad (6)
\]
Proof. By the triangle inequality and the invariance of $\pi_Q$ and $\pi_S$ w.r.t. $Q$ and $S$, we get that for any $n \in \mathbb{N}$,

$$W(\pi_Q, \pi_S) \leq W(\pi_Q, \pi_S Q^n) + W(\pi_S Q^n, \pi_S) \leq \varphi(n) W(\pi_Q, \pi_S) + \varepsilon(n).$$

The conclusion follows by rearranging and minimizing over $n$. $\square$

Based on Lemma 1, if we have a bound $\varphi(n)$ quantifying the convergence to equilibrium for the Markov chain with transition kernel $Q$, then we can derive upper bounds on the distance $W(\pi_S, \pi_Q)$ by controlling the accuracy $\varepsilon(n)$ for the approximation of the stationary Markov chain with initial distribution $\pi_S$ and transition kernel $S$ by the Markov chain with the same initial distribution and transition kernel $Q$. This approach is not new and appears in variations at several places in the literature, see for example [42, Remark 6.3] and [34]. Of course, it can also be applied with the roles of $Q$ and $S$ interchanged, which yields different bounds.

**Example 2.** Suppose that there exist $A, B, c, \lambda, \gamma \in (0, +\infty)$ such that Conditions (4) and (5) are satisfied with

$$\varphi(n) = A \exp(-cn\gamma) \quad \text{and} \quad \varepsilon(n) = \gamma B \exp(\lambda n\gamma).$$

Then by choosing $n = \lceil (c\gamma)^{-1} \{ \log(A) + \log(1 + c/\lambda) \} \rceil$, we obtain the upper bound

$$W(\pi_S, \pi_Q) \leq \frac{\gamma B \exp(\lambda n\gamma)}{1 - A \exp(-cn\gamma)} \leq \gamma B e^{1+\lambda\gamma} A^{\lambda/c} \left( \frac{\lambda}{c} + 1 \right). \qquad (7)$$

In the applications we are interested in, typically $\gamma$ is a small constant (the discretization step size), and $c < \lambda$. Note that $A = 1$ can be guaranteed by choosing the distance $W$ in an adequate way, see the examples in Section 3.

More generally, we can also apply Lemma 1 if the distance to equilibrium of the Markov chain with transition kernel $Q$ decays subgeometrically:

**Example 3.** Suppose that there exist $B, \lambda, \gamma \in (0, +\infty)$ and a decreasing continuous function $\psi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ with $\lim_{t \rightarrow +\infty} \psi(t) = 0$ such that (4) and (5) are satisfied with

$$\varphi(n) = \psi(n\gamma) \quad \text{and} \quad \varepsilon(n) = \gamma B \exp(\lambda n\gamma).$$

Let $t_{\text{rel}} = \inf \{ t \geq 0 : \psi(t) \leq 1/2 \}$. Then, choosing $n = \lceil t_{\text{rel}}/\gamma \rceil$, we obtain

$$W(\pi_S, \pi_Q) \leq \frac{\gamma B \exp(\lambda n\gamma)}{1 - \psi(n\gamma)} \leq 2 \gamma B \exp(\lambda \cdot (t_{\text{rel}} + \gamma)). \qquad (8)$$

If $\psi$ is decaying exponentially then this bound is weaker than the one in (7).
In this work, our focus is on quantifying the dependence on the dimension of corresponding bounds for Markov processes on $\mathbb{R}^d$. As distance functions on $\mathcal{P}(\mathbb{R}^d)$ we consider $L^p$ Wasserstein distances $W = W_{p,d}$ where $p \in [1, 2]$ and $d : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_+$ is a lower semicontinuous distance function on $\mathbb{R}^d$. It is important to note that there is some flexibility in choosing the underlying metric $d$. It is this flexibility that will often enable us to satisfy the conditions in Example 2 with $A = 1$.

We assume that $d$ is upper bounded by the Euclidean distance:

**A1.** There exists $C_d \in (0, +\infty)$ such that for any $x, y \in \mathbb{R}^d$,

$$d(x, y) \leq C_d|x - y|.$$  

For example, if $d$ is the $\ell^q$ distance defined in (3) for some $q \in [1, 2]$, then A1 holds with $C_d = \|1 - \frac{1}{q}\|_2$, and if $d$ is the $\tilde{\ell}^q$ distance defined in (3), then $C_d = 1$.

Obtaining precise information on the dimension dependence of $W_{p,d}(\pi_S, \pi_Q)$ using Lemma 1 requires bounds as stated in (4) and (5) with explicit dimension dependence of $\varphi(n)$ and $\varepsilon(n)$. Regarding the former, in recent years, dimension free contractions in appropriate Wasserstein distances have been proven under different assumptions for various important classes of Markov processes including overdamped Langevin diffusions and more general Kolmogorov processes [27, 29], corresponding Euler discretizations [31, 14], second order Langevin diffusions [11], and both exact and unadjusted Hamiltonian Monte Carlo [41, 7, 8]. It is well-known that such contractions immediately imply upper bounds as assumed in (4) and (5). For the reader’s convenience, a short proof of this fact is included in Section 4.1.

Besides convergence bounds for the reference kernel, the second key ingredient for studying the dimension dependence of the distance between two invariant measures is an accuracy bound as in (5) that quantifies the distance between the laws at time $n$ of the corresponding Markov chains started with the same initial distribution. Such bounds depend on the approximation that is considered and can only be derived on a case-by-case basis. The precise dimension dependence of the function $\varepsilon(n)$ in these bounds in different situations is one of the main contributions of this work.

### 2.1 Euler-Maruyama discretizations of stochastic differential equations

Consider a diffusion process $(Y_t)_{t \geq 0}$ on $\mathbb{R}^d$ that solves a stochastic differential equation (SDE)

$$dY_t = b(Y_t) \, dt + \sqrt{2} \, dB_t,$$  

where $(B_t)_{t \geq 0}$ is a $d$-dimensional Brownian motion and $b : \mathbb{R}^d \to \mathbb{R}^d$ is a twice continuously differentiable function. We assume that (9) admits a unique non-explosive solution $(Y_t)_{t \geq 0}$ for every starting point $x \in \mathbb{R}^d$. Moreover, we impose the following assumption on the Markov semigroup $(P_t)_{t \geq 0}$ defined by $(Y_t)_{t \geq 0}$.

**E1.** $(P_t)_{t \geq 0}$ admits an invariant probability measure $\pi \in \mathcal{P}_2(\mathbb{R}^d)$.  

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In particular, the assumption is satisfied if \( \pi \) admits a density with respect to the Lebesgue measure of the form

\[
\pi(dx) = Z^{-1} e^{-U(x)} \, dx, \quad Z = \int e^{-U(x)} \, dx < +\infty,
\]

for a function \( U \in C^3(\mathbb{R}^d) \) satisfying \( \int_{\mathbb{R}^d} (1 + |x|^2) e^{-U(x)} \, dx < +\infty \), and if \( b = -\nabla U + \Xi \) for a \( C^2 \) vector field \( \Xi : \mathbb{R}^d \to \mathbb{R}^d \) such that \( \text{div}(e^{-U} \Xi) = 0 \) (e.g. \( \Xi = -J\nabla U \) for an antisymmetric matrix \( J \in \mathbb{R}^{d \times d} \)), see \cite{30}.

We consider Euler-Maruyama type discretization schemes for (9), i.e., the class of Markov chains \((X_k)_{k \geq 0}\) defined by the following recursion: for any integer \( k \geq 0 \),

\[
X_{k+1} = X_k + \gamma \tilde{b}_\gamma(X_k) + \sqrt{2\gamma} \Gamma_{k+1},
\]

where \( \gamma > 0 \) is the step size, \((G_k)_{k \in \mathbb{N}}\) is a sequence of independent zero-mean Gaussian random variables on \( \mathbb{R}^d \) with covariance matrix identity, and \( \{\tilde{b}_\gamma : \mathbb{R}^d \to \mathbb{R}^d : \gamma \in (0, \bar{\gamma}]\} \), with \( \bar{\gamma} > 0 \), is a family of approximate drift functions satisfying the following condition.

**E2.** There exists a function \( \Gamma : \mathbb{R}^d \to \mathbb{R}_+ \) such that for any \( \gamma > 0 \) and \( x \in \mathbb{R}^d \),

\[
\left| \tilde{b}_\gamma(x) - b(x) \right| \leq \gamma \Gamma(x).
\]

For the standard Euler-Maruyama scheme, \( \tilde{b}_\gamma = b \) for any \( \gamma \in (0, \bar{\gamma}] \), and therefore **E2** is satisfied with \( \Gamma = 0 \). In the case \( b = -\nabla U \), the Euler scheme corresponds to the standard Unadjusted Langevin Algorithm (ULA) \cite{51}, but as mentioned previously, \( b = -(I_d + J)\nabla U \) with an antisymmetric matrix \( J \in \mathbb{R}^{d \times d} \) is also an option to target \( \pi \) of the form (10). Moreover, our conditions also cover the tamed Euler-Maruyama discretization \cite{9} for which \( \tilde{b}_\gamma(x) = b(x)/(1 + \gamma |b(x)|) \). In this case, **E2** holds with \( \Gamma(x) = |b(x)| \).

The transition kernel of the Markov chain defined by the recursion (11) is

\[
R_\gamma(x, A) = (2\gamma)^{-d/2} \int_A \varphi_d \left( \frac{y - x - \gamma \tilde{b}_\gamma(x)}{\sqrt{2\gamma}} \right) \, dy.
\]

We assume the following condition on the family \( \{R_\gamma : \gamma \in (0, \bar{\gamma}]\} \).

**E3.** For every \( \gamma \in (0, \bar{\gamma}] \), \( R_\gamma \) has an invariant probability measure \( \pi_\gamma \in P_2(\mathbb{R}^d) \).

We aim at applying Lemma 1 in order to obtain explicit upper bounds on Wasserstein distances of the invariant measures \( \pi \) and \( \pi_\gamma \) for \( \gamma \in (0, \bar{\gamma}] \). This can be achieved by choosing either \( Q = R_\gamma \) and \( S = P_\gamma \) in Lemma 1, or, conversely, \( Q = P_\gamma \) and \( S = R_\gamma \). Both approaches lead to slightly different results that are not comparable to each other, see Theorems 5 and 7 below, respectively. In particular, one either requires a convergence bound on the approximate dynamics as assumed in (15), or a convergence bound on the exact dynamics as assumed in (18).
2.1.1 A first result

The first main result stated in Theorem 5 has a simple form and is relatively easy to derive but requires stronger assumptions. In particular, we assume a global Lipschitz condition on the approximate drift functions $\tilde{b}_\gamma$.

**E4.** There exists $L \in \mathbb{R}_+$ such that for any $x, y \in \mathbb{R}^d$ and $\gamma \in (0, \bar{\gamma}]$,

$$|\tilde{b}_\gamma(x) - \tilde{b}_\gamma(y)| \leq L|x - y|.$$  

We consider the extended generator of (9) given for $f \in C^2(\mathbb{R}^d)$ by

$$\mathcal{L}^L f = \langle b, \nabla f \rangle + \Delta f .$$  

(13)

For any twice continuously differentiable function $F : \mathbb{R}^d \to \mathbb{R}^n$, we define $\mathcal{L}^L F$ component-wise, i.e., $\mathcal{L}^L F$ is the function from $\mathbb{R}^d$ to $\mathbb{R}^n$ with $i$-th component given by $\mathcal{L}^L F_i$ where $F_i$ is the $i$-th component of $F$. Let $\|A\|_F$ denote the Frobenius (or Hilbert-Schmidt) norm of a matrix $A \in \mathbb{R}^{d \times d}$, i.e., $\|A\|^2_F = \sum_{i,j=1}^d A_{i,j}^2$.

**Proposition 4.** Assume E1, E2 and E4. Then for any $\gamma \in (0, \bar{\gamma}]$ and $n \in \mathbb{N}$,

$$W_2(\pi P_{n\gamma}, \pi R_{n\gamma}^n) \leq \gamma M_L^{1/2} e^{\lambda_L n \gamma},$$

where

$$\lambda_L = 1 + L^2 + 3L^2\bar{\gamma}/2,$$

$$M_L = \left(6^{-1} + 3\gamma/4\right) M_1 + 3M_2/2 + (1 + 3\gamma/2)M_3 ,$$

with

$$M_1 = \int |\mathcal{L}^L b|^2 d\pi, \quad M_2 = \int \|Db\|^2_F d\pi, \quad M_3 = \int \Gamma^2 d\pi .$$  

(14)

The proof of the proposition is given in Section 4.2. Of course, it is well-known that the Euler-Maruyama approximation is accurate of order $O(\gamma)$, see for example [54]. The point of Theorem 4 is however that the explicit form of the prefactor $M_L^{1/2}$ enables us to analyze precisely the dimension dependence for different classes of models, see Section 3.1 below.

Recall the definition of the constant $C_d$ from Assumption A1 above. By combining Proposition 4, Lemma 1, and Examples 2 and 3 we obtain our first main result.

**Theorem 5.** Assume E1, E2, E3 and E4, and fix $p \in [1, 2]$. Suppose that $d$ is a distance function on $\mathbb{R}^d$ satisfying A1, and assume that there exist $A \geq 0$ and $c > 0$ such that for any $\gamma \in (0, \bar{\gamma}]$ and $n \in \mathbb{N}$,

$$W_{p,d}(\pi_{\gamma}, \pi R_{n\gamma}^n) \leq Ae^{-c n \gamma} W_{p,d}(\pi_{\gamma}, \pi) .$$  

(15)

Let $\lambda_L$ and $M_L$ be defined as in Proposition 4. Then for any $\gamma \in (0, \bar{\gamma}]$,

$$W_{p,d}(\pi_{\gamma}, \pi) \leq \gamma C_d M_L^{1/2} e^{1+\lambda_L \gamma} A^{\lambda_L/c} (\lambda_L/c + 1) .$$  

(16)
More generally, suppose instead of (15) that there exists a decreasing continuous function
\( \psi : \mathbb{R}_+ \to \mathbb{R}_+ \) with \( \lim_{t \to +\infty} \psi(t) = 0 \) such that for any \( \gamma \in (0, \bar{\gamma}] \) and \( n \in \mathbb{N} \),
\[
W_{p,d}(\pi_\gamma, \pi R^n_\gamma) \leq \psi(n\gamma)W_{p,d}(\pi_\gamma, \pi).
\]
Let \( t_{rel} = \inf\{ t \geq 0 : \psi(t) \leq 1/2 \} \). Then for any \( \gamma \in (0, \bar{\gamma}] \),
\[
W_{p,d}(\pi_\gamma, \pi) \leq 2\gamma C_d M_L^{1\over 2} e^\lambda L \cdot (t_{rel} + \gamma).
\]

Theorem 5 is a direct consequence of Proposition 4 and the bounds in (7) and (8). In particular, if \( L, A, c, \lambda_L \) and \( \psi \) are independent of the dimension \( d \), then the dimension dependence of the upper bounds is determined completely by the key quantities \( C_d \) and \( M_L \). In Section 3.1, we will see that for ULA, the dimension dependence of \( M_L \) relies crucially on bounds for \( |\Delta b(x)|^2 \) and \( \|D^2 b(x)\|^2 \) where \( b = -\nabla U \), cf. (29) and (30). If these quantities are bounded uniformly of order \( O(d) \) then under appropriate assumptions, the resulting dimension dependence on upper bounds of the standard \( L^1 \) Wasserstein distance \( W_1(\pi_\gamma, \pi) \) is of order \( O(\gamma d^{1/2}) \). This is the case for models with a limited amount of interactions such as product models, mean-field models, finite range graphical models, and perturbations thereof. On the other hand, for general models where the second partial derivatives of \( b \) are bounded, one can only expect bounds on the above quantities of order \( O(d) \) and hence bounds on the asymptotic bias of order \( O(\gamma d) \).

2.1.2 An improved result

In our second main result stated in Theorem 7 below, we relax the assumptions substantially, see the comments below Theorem 7. In contrast to Theorem 5, we only assume a quantitative convergence bound for the diffusion process, and, more importantly, we replace the global Lipschitz condition in \( E_4 \) by the following one-sided Lipschitz condition on \( b \).

\( E_5 \). There exists \( \kappa > 0 \) such that for any \( x, y \in \mathbb{R}^d \),
\[
(b(x) - b(y), x - y) \leq \kappa \|x - y\|^2.
\]

For any \( f \in C^2(\mathbb{R}^d) \), we define \( \mathcal{L}^D f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \), for \( x, y \in \mathbb{R}^d \) by
\[
(\mathcal{L}^D f)(x, y) = (b(x), (\nabla f)(y)) + (\Delta f)(y).
\]

For any twice continuously differentiable function \( F : \mathbb{R}^d \to \mathbb{R}^n \), we define \( \mathcal{L}^D F \) component-wise, i.e., \( \mathcal{L}^D F \) is the function from \( \mathbb{R}^d \times \mathbb{R}^d \) to \( \mathbb{R}^n \) with \( i \)-th component given by \( \mathcal{L}^D F_i \) where \( F_i \) is the \( i \)-th component of \( F \).

**Proposition 6.** Assume \( E_1, E_2, E_3 \) and \( E_5 \). Then for any \( \gamma \in (0, \bar{\gamma}] \) and \( n \in \mathbb{N} \),
\[
W_2(\pi_\gamma P_{n\gamma}, \pi_P^n) \leq \gamma^{3/2}(n+1)^{1/2} M_L^{1/2} e^{(1+\kappa)n\gamma} \leq \gamma(1+\gamma)^{1/2} M_L^{1/2} e^{(1+\kappa)n\gamma},
\]
where

\[ \tilde{M}_L = \frac{1}{6} \tilde{M}_1 + \frac{1}{2} \gamma^{1/2} \tilde{M}_2^{1/2} \tilde{M}_3^{1/2} + \frac{1}{\sqrt{2}} \tilde{M}_2^{1/2} \tilde{M}_4^{1/2} + \frac{1}{2} \tilde{M}_5, \]

with

\[ \tilde{M}_1 = \sup_{u \in (0, \gamma]} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left| (\mathcal{L}^\gamma b)(x, x + u \tilde{b}_\gamma(x) + (2u)^{1/2} z) \right|^2 \varphi_d(z) \, dz \, \pi_\gamma(dx), \]

\[ \tilde{M}_2 = \sup_{u \in (0, \gamma]} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \| (\mathcal{D} b)(x + u \tilde{b}_\gamma(x) + (2u)^{1/2} z) \|_F^2 \varphi_d(z) \, dz \, \pi_\gamma(dx), \]

\[ \tilde{M}_3 = \sup_{t \in \mathbb{R}_+} \int |\mathcal{L}^\gamma b|^2 \, d(\pi_\gamma P_t), \quad \tilde{M}_4 = \sup_{t \in \mathbb{R}_+} \int \| D b \|^2_F \, d(\pi_\gamma P_t), \]

\[ \tilde{M}_5 = \int \Gamma^2 \, d\pi_\gamma. \]

The proof of the proposition is given in Section 4.3 below. By combining Proposition 6, Lemma 1, and Examples 2 and 3, we obtain our second main result.

**Theorem 7.** Assume **E1, E2, E3 and E5**, and fix \( p \in [1, 2] \). Suppose that \( d \) is a distance function on \( \mathbb{R}^d \) satisfying **A1**, and assume that there exist \( A \geq 0 \) and \( c > 0 \) such that for any \( t \geq 0 \) and any probability measure \( \nu \in \mathcal{P}(\mathbb{R}^d) \),

\[ W_{p, d}(\nu P_t, \pi) \leq A e^{-ct} W_{p, d}(\nu, \pi). \]  

(18)

Let \( \tilde{M}_L \) be defined as in Proposition 6. Then for any \( \gamma \in (0, \bar{\gamma}] \),

\[ W_{p, d}(\pi_\gamma, \pi) \leq \gamma C d \tilde{M}_L^{1/4} \exp\left[1 + (1 + \kappa) \frac{\gamma}{A(1 + \kappa)}\right] (1 + (1 + \kappa)/c). \]

More generally, suppose instead of (15) that there exists a decreasing continuous function \( \psi : \mathbb{R}_+ \to \mathbb{R}_+ \) with \( \lim_{t \to +\infty} \psi(t) = 0 \) such that for any \( t \geq 0 \) and any probability measure \( \nu \in \mathcal{P}(\mathbb{R}^d) \),

\[ W_{p, d}(\nu P_t, \pi) \leq \psi(t) W_{p, d}(\nu, \pi). \]

Let \( t_{rel} = \inf\{ t \geq 0 : \psi(t) \leq 1/2 \} \). Then for any \( \gamma \in (0, \bar{\gamma}] \),

\[ W_{p, d}(\pi_\gamma, \pi) \leq 2 \gamma C d \tilde{M}_L^{1/4} \exp(1 + \kappa) \Gamma(t_{rel} + \gamma). \]

A main feature of Theorem 7 is that the bounds depend on the one-sided Lipschitz constant \( \kappa \) of the unperturbed drift \( b \) and on the convergence to equilibrium of the diffusion process, whereas the bounds in Theorem 5 depend on the global Lipschitz constant \( L \) of the perturbed drift \( \tilde{b}_\gamma \) and on the convergence to equilibrium of the approximating process. In particular, if \( \kappa, A, c \) and \( \psi \) are independent of the dimension \( d \), then the dimension dependence of the upper bounds is determined completely by the quantities \( C_d \) and \( \tilde{M}_i, i = 1, 2, \ldots, 5 \). The price to pay is that these quantities take a more complicated form than the corresponding quantities \( M_1, M_2 \) and \( M_3 \) occurring in Theorem 5. It turns out that nevertheless, \( \tilde{M}_L \) can be bounded in applications similarly as \( M_L \), see the examples in Section 3.1.
We conclude this section by noting that Theorem 7 easily implies convergence guarantees for ULA, if it is combined with either convergence bounds in Wasserstein distance for the Langevin diffusion or its discretization as established in [14, 31, 26, 29]. To illustrate our point, assume under the conditions of Theorem 7 that (18) holds and $A, c, \kappa, C_d$ do not depend on the dimension. Suppose, moreover, that the Wasserstein distance $W_{p,d}(\mu_0, \pi)$ between the initial distribution $\mu_0$ and the target distribution $\pi$ is of order $O(d^\omega)$ with $\omega > 0$. Then, by Theorem 7 and the triangle inequality, the number of steps $n \varepsilon \in \mathbb{N}$ sufficient to achieve $W_{p,d}(\mu_{\varepsilon}, \pi) \leq \varepsilon$ for an expected precision $\varepsilon > 0$, is of order $O(\varepsilon^{-1}M_{\varepsilon}^{1/2})$ (up to logarithmic terms), and thus it is of order $O(\varepsilon^{-1}d)$ if $b$ has bounded second derivative (see Section 3).

### 2.1.3 Asymptotic bias in total variation

By combining the results of the previous sections with those in [14], we can also provide explicit bounds on $\|\pi_\gamma - \pi\|_{TV}$. We consider the following general conditions.

**E6.** (i) There exist $\lambda_{tv} > 0$ and $A_{tv} \geq 0$, such that for any $\gamma \in (0, \tilde{\gamma}]$ and $n \in \mathbb{N},$

$$W_1(\pi_\gamma P_{n\gamma}, \pi_\gamma R_{\gamma}^n) \leq A_{tv} \gamma (\gamma n)^{1/2} \exp (\gamma n \lambda_{tv}).$$

(ii) There exists $B_{tv} \geq 0$, such that for any $\gamma \in (0, \tilde{\gamma}]$, $W_1(\pi, \pi_\gamma) \leq B_{tv} \gamma$.

(iii) There exists $C_{tv} \geq 0$ such that for any $t \in [0, 2]$ and $x, y \in \mathbb{R}^d$,

$$\|\delta_x P_t - \delta_y P_t\|_{TV} \leq C_{tv} \|x - y\| t^{-1/2}.$$

Note that under appropriate assumptions, we can show that **E6**-(i)-(ii) holds by applying Proposition 6 and Theorem 7, respectively. In particular, the expression of $\lambda_{tv}$ provided by these results does not depend explicitly on the dimension $d$. Moreover, the results established in [14] allow us to verify the bound in **E6**-(iii) with some explicit constants. For example, we can show the following statement for which the proof is postponed to Section 4.4.

**Theorem 8.** Assume **E4**-**E5** and $\sup_{x \in \mathbb{R}^d} \langle b(x), x \rangle < +\infty$. Then **E6**-(iii) holds with $C_{tv} = \sqrt{\kappa/\pi} \sup_{u \in [0,2]} \{u/(1 - e^{-2\kappa u})^{1/2}\}$.

Note that the expression for $C_{tv}$ provided by Theorem 8 does not depend on the dimension $d$. It would be possible to relax the global Lipschitz assumption on $b$ to a local Lipschitz condition, but this would require to introduce many additional technical details in the resulting proof.

We now state the main result of this section. The proof is postponed to Section 4.4 and is adapted from the proof of [24, Corollary 12] which considers the case $b = -\nabla U$ with a strongly convex function $U$. 

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Theorem 9. Assume $E_1$, $E_3$ and $E_6$. Suppose in addition that $\bar{\gamma} < 1$. Then, for any $\gamma \in (0, \bar{\gamma}]$,

$$\|\pi - \pi_\gamma\|_{TV} \leq 2^{-3/2}L\gamma \left\{ d + \gamma \tilde{M}_6/3 \right\}^{1/2} + \gamma C_{tv}B_{tv} + \gamma \left[ \log(\gamma^{-1})/\log(2) \right] \tilde{M}_7,$$

where

$$\tilde{M}_6 = \int_{\mathbb{R}^d} ||b||^2 d\pi_\gamma, \quad \tilde{M}_7 = 4C_{tv}A_{tv} \exp(2\lambda_{tv}).$$

We end this section with the same remark as in the Wasserstein distance case regarding convergence guarantees for ULA implied by Theorem 9. By the same reasoning, this result combined with convergence bounds for the Langevin diffusion or its discretization as established in [14, 31] easily leads to complexity bounds for ULA in the total variation distance.

2.2 Unadjusted Hamiltonian Monte Carlo

In this section, we are interested in establishing non-asymptotic bounds between the invariant distributions of the exact Hamiltonian Monte Carlo algorithm (xHMC) and the unadjusted Hamiltonian Monte Carlo algorithm (uHMC). Let $b : \mathbb{R}^d \to \mathbb{R}^d$ be a twice continuously differentiable and Lipschitz continuous function, and fix $T \in (0, +\infty)$. We consider a Markov chain $(Q_k, P_k)_{k \geq 0}$ with state space $\mathbb{R}^d \times \mathbb{R}^d$ defined recursively by

$$(Q_{k+1}, P_{k+1}) = \psi_T(Q_k, G_{k+1}),$$

where $(G_k)_{k \in \mathbb{N}}$ is a sequence of i.i.d. $d$-dimensional zero-mean Gaussian random variables with covariance matrix identity, and $(\psi_t)_{t \geq 0}$ is the differentiable flow associated to the ordinary differential equation

$$\frac{d}{dt}(q_t, p_t) = (p_t, b(q_t)), \quad (20)$$

i.e., $\psi_T(q_0, p_0) = (q_T, p_T)$ where $(q_t, p_t)_{t \geq 0}$ is the solution of (20) with initial value $(q_0, p_0)$. In particular, in the case $b = -\nabla U$, $(\psi_t)_{t \geq 0}$ is the Hamiltonian flow associated to the unit mass Hamiltonian

$$H(q, p) = U(q) + |p|^2/2,$$

and correspondingly, $(Q_k, P_k)_{k \geq 0}$ is the Markov chain associated to the xHMC algorithm with complete momentum refreshment. The sequence $(Q_k)_{k \geq 0}$ is a Markov chain with state space $\mathbb{R}^d$ and transition kernel

$$K_T(q, A) = \int_{\mathbb{R}^d} 1_A \times \mathbb{R}^d (\psi_T(q, p_0)) \varphi_d(p_0) \, dp_0, \quad q \in \mathbb{R}^d, \quad A \in \mathcal{B}(\mathbb{R}^d).$$

Note that similarly to Section 2.1, we consider a general setup where $b$ is a vector field which is not assumed to be the gradient of a real-valued function. In addition, we assume the existence of a stationary distribution.
The Markov kernel $K_T$ admits an invariant probability measure $\pi \in \mathcal{P}_2(\mathbb{R}^d)$. 

In the case where $b = -\nabla U$ for some potential function $U : \mathbb{R}^d \to \mathbb{R}$ such that $\int_{\mathbb{R}^d} (1 + |q|^2) e^{-U(q)} dq < +\infty$, H1 is always satisfied with $\pi$ of the form (10), see e.g. [5, 45]. In practice, (20) can usually not be solved exactly, and therefore numerical schemes are used to get approximate solutions. In this paper, we consider discretization with the leapfrog (or Verlet) integrator. More generally, and analogously as above for the Euler-Maruyama discretization, we consider a family \{\tilde{b}_\gamma : \mathbb{R}^d \to \mathbb{R}^d : \gamma \in (0, \tilde{\gamma}]\}, $\tilde{\gamma} > 0$, of approximate drift functions satisfying the following condition.

There exists $\Lambda : \mathbb{R}^d \to \mathbb{R}_+$ such that for any $\gamma > 0$ and $q \in \mathbb{R}^d$,

$$|b(q) - \tilde{b}_\gamma(q)| \leq \gamma^2 \Lambda(q).$$

Then, the corresponding uHMC algorithm with discretization step size $\gamma > 0$ satisfying $T/\gamma \in \mathbb{N}$ is given by the Markov chain $(\tilde{Q}_k, \tilde{P}_k)_{k \geq 0}$ with state space $\mathbb{R}^d \times \mathbb{R}^d$ that is defined recursively by

$$(\tilde{Q}_{k+1}, \tilde{P}_{k+1}) = \tilde{\Psi}_T(\tilde{Q}_k, G_{k+1}),$$

with $\tilde{\Psi}_\gamma(q_0, p_0) = (q_\gamma, p_\gamma)$, where $(q_\gamma, p_\gamma)_{t \geq 0}$ is the (unique) solution of

$$\frac{d}{dt} (q_\gamma, p_\gamma) = \left(p_{[t/\gamma]} - (\gamma/2)\tilde{b}_\gamma(q_{[t/\gamma]}), (1/2)\{\tilde{b}_\gamma(q_{[t/\gamma]}) + \tilde{b}_\gamma(q_{[t/\gamma]})\}\right)$$

with initial value $(q_0, p_0)$. In particular, for any $n \in \mathbb{N}$, $\tilde{\Psi}_{n\gamma} = \tilde{\Psi}_{\gamma}^{o(n)}$ where $\tilde{\Psi}_\gamma : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is given by

$$\tilde{\Psi}_\gamma(q_0, p_0) = (q_\gamma, p_\gamma), \quad \begin{cases} q_\gamma = q_0 - (\gamma^2/2)\tilde{b}_\gamma(q_0) + \gamma p_0, \\ p_\gamma = p_0 - (\gamma/2)\{\tilde{b}_\gamma(q_0) + \tilde{b}_\gamma(q_\gamma)\}. \end{cases} \quad (21)$$

If $\tilde{b}_\gamma = b$ then the function $\tilde{\Psi}_\gamma$ corresponds to one step of the leapfrog (or Verlet) integrator. Again, $(\tilde{Q}_k)_{k \geq 0}$ is a Markov chain, and the transition kernel is

$$K_{T, \gamma}(q, A) = \int_{\mathbb{R}^d} \mathbb{1}_A(q, p) \tilde{\Phi}_\gamma(q_\gamma, p_\gamma) \varphi(p_0) dp_0, \quad q \in \mathbb{R}^d, \quad A \in B(\mathbb{R}^d).$$

Similarly as for xHMC, we also assume that the uHMC chain has an invariant probability measure if the step size $\gamma$ is small enough.

For every $\gamma \in [0, \tilde{\gamma}]$, the Markov kernel $K_{T, \gamma}$ has an invariant probability measure $\pi_{T, \gamma}$.

Finally, we assume that $b$ satisfies a global Lipschitz condition.

There exists $L \geq 0$ such that for any $q_1, q_2 \in \mathbb{R}^d$,

$$|b(q_1) - b(q_2)| \leq L |q_1 - q_2|.$$
2.2.1 Main results for unadjusted HMC

The Liouville operator, i.e., the infinitesimal generator of the deterministic dynamics (20), is given for any \( f \in C^1(\mathbb{R}^{2d}) \) and \( (q,p) \in \mathbb{R}^{2d} \) by

\[
\mathcal{L}^H f(q,p) = \langle p, \nabla_q f(q,p) \rangle + \langle b(q), \nabla_p f(q,p) \rangle.
\]

For a continuously differentiable function \( F : \mathbb{R}^d \to \mathbb{R}^n \), we define \( \mathcal{L}^H F \) component-wise as the function from \( \mathbb{R}^d \to \mathbb{R}^n \) such that the \( i \)-th component is \( \mathcal{L}^H F_i \) where \( F_i \) is the \( i \)-th component of \( F \). Note that if \( (q_t, p_t)_{t \geq 0} \) is a solution of (20), then \( t \mapsto F(q_t, p_t) \) is continuously differentiable on \( \mathbb{R}_+ \) and

\[
dF(q_t, p_t)/dt = (\mathcal{L}^H F)(q_t, p_t).
\]  

Remarkably, the Liouville operator is related to the generator \( \mathcal{L}^L \) defined in (13). In particular, applying \( \mathcal{L}^H \) twice to the function \( (q,p) \mapsto b(q) \) yields for \( (q,p) \in \mathbb{R}^{2d} \), \( \mathcal{L}^H b(q,p) = (p^T \nabla b)(q) \) and \((\mathcal{L}^H)^2 b(q,p) = \sum_{i=1}^d D^2 b_i(q) \{ p \otimes p \} e_i + (b^T \nabla b)(q)\), where \( (e_i)_{i=1}^d \) is the canonical basis of \( \mathbb{R}^d \) and \( b_i \) is the \( i \)-th component of \( b \). Thus a short computation shows that for any \( q \in \mathbb{R}^d \),

\[
\int \left| (\mathcal{L}^H b)(q,p) \right|^2 \phi_d(p) dp = \| \nabla b(q) \|_F^2 ,
\]

\[
\int \left| (\mathcal{L}^H)^2 b(q,p) \phi_d(p) dp = (\mathcal{L}^L b)(q) \right| ,
\]

\[
\int \left| (\mathcal{L}^H)^2 b(q,p) \phi_d(p) dp = \left| (\mathcal{L}^L b)(q) \right|^2 + 2 \left| D^2 b(q) \right|_F^2 ,
\]

where we set \( \| D^2 b(q) \|_F^2 = \sum_{i=1}^d \| D^2 b_i(q) \|_F^2 = \sum_{k,j,i=1}^d (\partial_{kj} b_i(q))^2 \) and used that for any matrix \( A = (A_{i,j})_{i,j=1}^d \in \mathbb{R}^{d \times d} \), denoting by \( 1_{d \times d} \) the \( d \times d \) matrix with all entries equal to 1,

\[
\int (p^T A p)^2 \phi_d(p) dp = \int \text{Tr}(A^T p^T pp^T p A) \phi_d(p) dp
\]

\[
= \text{Tr}(A^T \{ 2 I_d + 1_{d \times d} \} A) = 2 \| A \|_F^2 + \text{Tr}(A)^2 .
\]

It is a consequence of these identities that the same constants \( M_1 \) and \( M_2 \) as introduced in (14) above, are also relevant to quantify the accuracy of uHMC.

**Proposition 10** (One-step accuracy of uHMC). Assume \( H1, H2 \) and \( H4 \). Then for any \( T > 0 \) and \( \gamma \in (0, \gamma] \) with \( T/\gamma \in \mathbb{N} \), we have

\[
W_2(\pi_{KT}, \pi_{KT,\gamma}) \leq \gamma^2 L^{-1} e^{\lambda_H T} M_H^{1/2} , \text{ where } \lambda_H = L^{1/2} \left( 1 + \frac{\gamma L^{1/2}}{2} + \frac{\gamma^2 L}{4} \right) ,
\]

and

\[
M_H = M_1 + (1 + \gamma^2 L) L M_2 + 2 M_4 + ((2 + \gamma L/2)^2 + L) M_5 ,
\]

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with
\[
M_1 = \int |L^b|^2 \, d\pi, \quad M_2 = \int \|Db\|_F^2 \, d\pi, \quad M_4 = \int \|D^2b\|_F^2 \, d\pi, \quad (25)
\]
\[
M_5 = \sup_{t \in [0,T]} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} A \left( \text{proj}_q(\tilde{\psi}_t(q,p)) \right)^2 \varphi_d(p) \, dp \, \pi(dq). \quad (26)
\]

Here \(\text{proj}_q : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d\) denotes the projection onto the first \(d\) components.

The proof of the theorem is given in Section 4.5. It can also be extended easily to quantify the accuracy for multiple transition steps, but for the applications below, it turns out to be sufficient to consider only a single transition step of uHMC (which usually already involves many Verlet steps). Recall the definition of the constant \(C_d\) from Assumption A1 above.

**Theorem 11.** Assume \(H_1, H_2, H_3\) and \(H_4\), and fix \(T \in (0, +\infty)\) and \(p \in [1, 2]\). Suppose that \(d\) is a distance function on \(\mathbb{R}^d\) satisfying A1, and assume that there exists a constant \(c \in (0, 1]\) such that for any \(\gamma \in (0, \bar{\gamma}]\),
\[
W_{p,d}(\pi_{T,\gamma}K_{T,\gamma}, \pi_{K_{T,\gamma}}) \leq (1 - c)W_{p,d}(\pi_{T,\gamma}, \pi). \quad (27)
\]

Let \(\lambda_H\) and \(M_H\) be defined as in Proposition 10. Then for any \(\gamma \in (0, \bar{\gamma}]\) with \(T/\gamma \in \mathbb{N}\),
\[
W_{p,d}(\pi_{T,\gamma}, \pi) \leq \gamma^2 (cL)^{-1} e^{\lambda_H T} C_d M_H^{1/2}. \quad (28)
\]

**Proof.** By the triangle inequality, (27), A1, and Proposition 10,
\[
W_{p,d}(\pi_{T,\gamma}, \pi) \leq W_{p,d}(\pi_{T,\gamma}K_{T,\gamma}, \pi_{K_{T,\gamma}}) + W_{p,d}(\pi_{K_{T,\gamma}}, \pi_{K_T}) \\
\leq (1 - c)W_{p,d}(\pi_{T,\gamma}, \pi) + C_d\gamma^2 L^{-1} e^{\lambda_H T} M_H^{1/2}.
\]
The assertion follows by rearranging. \(\square\)

Theorem 11 is a counterpart to Theorem 5. It would also be possible to state a corresponding counterpart to Theorem 7. We do not consider such a result here since in contrast to the results for ULA, it does not seem to provide a substantial improvement compared to Theorem 11.

Similarly as in the results above, we see that if \(L\) and \(c\) are independent of the dimension \(d\), then the dimension dependence of the upper bounds is determined completely by the key quantities \(C_d\) and \(M_H\). In Section 3.1, we will show that under appropriate assumptions and depending on the structure of the model, the resulting dimension dependence for upper bounds of the standard \(L^1\) Wasserstein distance \(W_1(\pi_\gamma, \pi)\) is then either of order \(O(\gamma^2d^{1/2})\) or of order \(O(\gamma^2d)\).

We conclude this section by noting that, similar to Theorem 7 for ULA, Theorem 11 combined with the convergence of uHMC and xHMC obtained in [7], gives complexity bounds for uHMC to achieve a precision \(\varepsilon\) in Wasserstein distance.

**Remark 12** (Total variation bias for uHMC). Quantifying the TV bias for uHMC is more involved than for Euler-Maruyama discretizations. Corresponding results are derived in the paper [6] that has been prepared in parallel to this work.
3 Accuracy in high dimension: Examples and applications

We now analyze the dimension dependence of the bounds we obtain for ULA and uHMC when applied to a target probability measure with density with respect to the Lebesgue measure of the form (10). At the end of this section we also discuss the relation of our results for unadjusted MCMC methods to mixing time bounds for the corresponding methods with Metropolis adjustment.

Recall the definitions of the constants $C_d$ from $A_1$, $M_L$ from Proposition 4, $\tilde{M}_L$ from Proposition 6, and $M_H$ from Proposition 10.

3.1 Accuracy of ULA and uHMC

Suppose that $\tilde{b}_\gamma = b$ for all $\gamma \in (0, \bar{\gamma}]$, and assume that $b$ satisfies $E4$ and there exist $K, J \in (0, +\infty)$ such that for any $x \in \mathbb{R}^d$,

$$|\Delta b(x)|^2 = \sum_{i,j=1}^d \langle \partial^2_{ii} b(x), \partial^2_{jj} b(x) \rangle = \sum_{i,j,k=1}^d \partial^2_{ii} b_k(x) \partial^2_{jj} b_k(x) \leq K,$$  (29)

$$\|D^2 b(x)\|_F^2 = \sum_{i,j=1}^d \left| \partial^2_{ij} b(x) \right|^2 = \sum_{i,j,k=1}^d \left| \partial^2_{ij} b_k(x) \right|^2 \leq J.$$  (30)

Then, one easily verifies that $M_3 = M_5 = 0$,

$$M_1 \leq 2K + 4L^2 \left( |b(0)|^2 + L^2 \int |x|^2 \, d\pi \right), \quad M_2 \leq dL^2, \quad \text{and} \quad M_4 \leq J.$$

It is natural to assume that $|b(0)|^2$ and $\int |x|^2 \, d\pi$ are of order $O(d)$. Then, if for a family of models with varying dimension, the Lipschitz constant $L$ is of order $O(1)$ and the constants $K$ and $J$ are of order $O(d)$, then the constant $M_L$ in Theorem 5 and the constant $M_H$ in Theorem 11 are of order $O(d)$. If we assume additionally that $A, c, \psi$ and $C_d$ can be chosen independently of the dimension then the upper bounds in (16) and (17) are of order $O(d^{1/2}\gamma)$. Similarly, if we assume that $c$ and $C_d$ can be chosen independently of the dimension then the upper bound in (28) is of order $O(d^{1/2}\gamma^2)$. As remarked in the introduction, these orders are sharp even in the product case with $d(x, y) = |x - y|$. Similarly, one verifies that $\tilde{M}_5 = 0$,

$$\tilde{M}_1 \leq 2K + 4L^2 \left( |b(0)|^2 + \int |x|^2 \, d\pi \right), \quad \tilde{M}_2 \leq dL^2,$n

$$\tilde{M}_3 \leq 2K + 4L^2 \left( |b(0)|^2 + \sup_{t \geq 0} \int |x|^2 \, d(\pi_t \gamma) \right), \quad \tilde{M}_4 \leq dL^2,$n

$$\tilde{M}_6 \leq 2L^2 \left( |b(0)|^2 + \int |x|^2 \, d\pi \right).$$
Again, it can be verified under weak assumptions that these constants, and hence $\tilde{M}_L$ in Theorem 7 are of order $O(d)$ if $L$ is of order $O(1)$ and $K$ is of order $O(d)$, see Remark 13 below.

The main constraint for corresponding bounds with optimal dimension dependence is the assumption that $K$ is of order $O(d)$. Note that this assumption is trivially satisfied in the Gaussian case (i.e., $b$ is linear), and also in the product case (i.e., $b(x) = (b_1(x_1), \ldots, b_d(x_d))$, provided a uniform bound on the components holds. More generally, it holds in several important classes of models that are frequently studied in applications, including the following:

(i) **Finite-range graphical models [35].** Suppose that for $d \in \mathbb{N}$, there exists a graph $(V_d, E_d)$ with vertex set $V_d = \{1, 2, \ldots, d\}$ and maximal degree $n \in \mathbb{N}$ such that $\partial^2_{ij}b_k = 0$ whenever $i \neq k$ and $\{i, k\} \notin E_d$. Then $\langle \partial^2_{ij}b, \partial^2_{ij}b \rangle$ and $\partial^2_{ij}b$ vanish if $i$ and $j$ do not have a common neighbour, and thus (29) and (30) are satisfied with

$$K = dn^2 \sup_{i,x} |\partial^2_{ij}b(x)|^2 \quad \text{and} \quad J = dn^2 \sup_{i,j,x} |\partial^2_{ij}b(x)|^2.$$ 

(ii) **Mean-field interactions [8].** Suppose that there exists a finite constant $C$ such that $|\partial^2_{ii}b_i(x)| \leq C$ for all $i$, and $|\partial^2_{ij}b_k(x)| \leq C/d$ for all $i, j, k$ such that $k \neq i$. Then (29) and (30) are satisfied with $K = J = 2C^2d$.

(iii) **Perturbations and composition.** If (29) and (30) are satisfied with constants $K_1$, $J_1$, and $K_2$, $J_2$ of order $O(d)$ for two drift functions $b_1$ and $b_2$, then a corresponding condition holds for $b = b_1 + b_2$.

It is also possible to verify a corresponding dimension dependence of $K$ and $L$ under locally uniform bounds on the derivatives of $b$, combined with an appropriate drift condition. However, although bounds with optimal dimension dependence hold for many important models, in general, assuming that the first two partial derivatives of $b$ are uniformly bounded, one can only ensure that $K$, $J$, $M_L$, $\tilde{M}_L$ and $M_H$ are of order $O(d^2)$. In this general case, the order of the upper bounds in Theorems 5, 7 and 11 differs from the one in the product case by a factor $d^{1/2}$.

**Remark 13.** We briefly comment on how to obtain bounds on the constants $\tilde{M}_i$, $i = 1, 2, \ldots, 5$, in Proposition 6 and Theorem 7 in the case where the derivatives of $b$ are not uniformly bounded. In this case, one requires upper bounds on $\int W d\pi_\gamma$ uniformly in $\gamma \in (0, \tilde{\gamma}]$ and on $\int W d(\pi_\gamma P_t) = \int P_t W d\pi_\gamma$ uniformly in $\gamma \in (0, \tilde{\gamma}]$ and $t \geq 0$ for $W: \mathbb{R}^d \to \mathbb{R}_+$. Such upper bounds can be established if $W$ satisfies Lyapunov conditions for the transition kernels $R_\gamma$, $\gamma \in (0, \tilde{\gamma}]$ and the generator $\mathcal{L}_L$. More specifically, assume that there exist $a \in [0, 1)$ and $b \geq 0$ such that for any $\gamma \in (0, \tilde{\gamma}]$ and $x \in \mathbb{R}^d$,

$$R_\gamma W(x) \leq a^\gamma W(x) + b \gamma.$$ 

Then by [22, Lemma 1], we obtain that for any $\gamma \in (0, \tilde{\gamma}]$,

$$R_\gamma^{[1/\gamma]} W(x) \leq a W(x) + ba^{-\gamma}/\log(1/a),$$

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and therefore by [18, Theorem 19.4.1],
\[
\int W \, d\pi_\gamma \leq ba^{-\bar{\gamma}}/(\{(1-a) \log(1/a)\}.
\]
(31)

Similarly, if \( W \) is twice continuously differentiable, and there exist \( \alpha \in (0, +\infty) \) and \( \beta \in [0, +\infty) \) such that for any \( x \in \mathbb{R}^d \),
\[
\mathcal{L}^L W(x) \leq -\alpha W(x) + \beta,
\]
then by Itô’s formula it holds that for any \( t \geq 0 \) and \( x \in \mathbb{R}^d \),
\[
P_t W(x) \leq e^{-\alpha t} W(x) + (1 - e^{-\alpha t})\beta/\alpha.
\]
(32)

Combining (31) and (32) implies upper bounds for \( \int P_t W \, d\pi_\gamma \).

**Example 14** (Euler scheme for asymptotically contractive drifts). Suppose in addition to the assumptions made above that there exists \( \mathcal{K}, \mathcal{R} \in (0, +\infty) \) such that for any \( x, y \in \mathbb{R}^d \) with \( |x - y| \geq \mathcal{R} \),
\[
\langle b(x) - b(y), x - y \rangle \leq -\mathcal{K}|x - y|^2.
\]
(33)

Then as a consequence of [27, Corollary 2], as well as [31, Theorem 2.12] and Lemma 21, respectively, there exists an explicit distance function \( d \) on \( \mathbb{R}^d \) and explicit constants \( c, m, \bar{\gamma} \in (0, +\infty) \) that depend only on \( L, \mathcal{K} \) and \( \mathcal{R} \) but not on the dimension \( d \) such that for \( p = 1 \), Conditions (18) and (15) are satisfied with \( A = 1 \) for all \( \gamma \in (0, \bar{\gamma}] \), and for all \( x, y \in \mathbb{R}^d \),
\[
m|x - y| \leq d(x, y) \leq |x - y|.
\]
(34)

Hence in this case, Theorems 5 and 7 show that
\[
W_1(\pi, \pi) \leq m^{-1}W_1, d(\pi, \pi) \leq \gamma e^{1+\lambda \gamma} \left( \frac{\lambda}{c} + 1 \right) m^{-1} \bar{M}_L^{1/2},
\]
\[
W_1(\pi, \pi) \leq m^{-1}W_1, d(\pi, \pi) \leq \gamma e^{1+(1+\kappa)\gamma} \left( \frac{1+\kappa}{c} + 1 \right) m^{-1} \bar{M}_L^{1/2},
\]
respectively. Since for fixed values of \( L, \mathcal{K} \) and \( \mathcal{R} \), all the other constants are dimension-free, the dimension dependence of these bounds is completely determined by \( \bar{M}_L^{1/2} \) and \( \bar{M}_L^{1/2} \). As pointed out above, the resulting bounds are of order \( \mathcal{O}(\gamma d^{1/2}) \) for models of type (i), (ii) or (iii), but only of order \( \mathcal{O}(\gamma d) \) for general models. Consequently, in order to achieve a given bound on the asymptotic bias for general Lipschitz continuous functions, the step size \( \gamma \) in the unadjusted Langevin algorithm has to be chosen of order \( \mathcal{O}(d^{-1/2}) \) for “nice” models, and of order \( \mathcal{O}(d^{-1}) \) for general models. Regarding the total variation bounds established in Theorem 9, we get bounds of order \( \mathcal{O}(\gamma \log(\gamma^{-1})d^{1/2}) \) for models of type (i), (ii) or (iii), but only of order \( \mathcal{O}(\gamma \log(\gamma^{-1})d) \) for general models.

**Remark 15** (\( W_2 \) bounds). In the globally contractive case where the conditions in Example 14 are satisfied with \( \mathcal{R} = 0 \), one also obtains corresponding bounds for \( p = 2 \) and \( d(x, y) = |x - y| \) and we get back [24, Corollary 9].
Example 16 (Unadjusted HMC for asymptotically contractive drifts). Suppose again that there exist $K, \mathcal{R} \in (0, +\infty)$ such that Condition (33) is satisfied for all $x, y \in \mathbb{R}^d$ with $|x - y| \geq \mathcal{R}$. Then by [8, Theorem 2] and Lemma 21, there exist an explicit distance function $d$ on $\mathbb{R}^d$ and explicit constants $c, \bar{m}, \bar{\gamma} \in (0, +\infty)$ that depend only on $L, K$ and $\mathcal{R}$ but not on the dimension $d$ such that (34) holds, and Condition (27) is satisfied for $p = 1$ and all $\gamma \in (0, \bar{\gamma}]$. Hence by Theorem 11,

$$W_1(\pi_\gamma, \pi) \leq m^{-1} W_{1,d}(\pi_\gamma, \pi) \leq \gamma^2 c^{-1} L^{-1} e^{\mu^T} m^{-1} M_{\mathbf{H}}^{1/2}.$$

For fixed values of $L, K$ and $\mathcal{R}$, the dimension dependence of this bound is completely determined by $M_{\mathbf{H}}^{1/2}$. As shown above, the resulting bound is of order $O(\gamma^2 d^{1/2})$ for models of type (i), (ii) or (iii), but only of order $O(\gamma^2 d)$ for general models. Consequently, in order to achieve a given bound on the asymptotic bias for general Lipschitz continuous functions, the step size $\gamma$ in unadjusted HMC has to be chosen of order $O(d^{-1/4})$ for “nice” models, and of order $O(d^{-1/2})$ for general models.

Example 17 (Euler scheme for weakly interacting systems). Another class of models for which dimension-free bounds for convergence to equilibrium are available are mean-field models and more general interacting systems with weak interactions, see [27]. Suppose that $d = nk$ with $n, k \in \mathbb{N}$, and assume that there exist twice continuously differentiable functions $b_0 : \mathbb{R}^k \to \mathbb{R}^k$ and $\gamma : \mathbb{R}^d \to \mathbb{R}^k$ such that for $x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^{nk}$,

$$b(x) = (b_1(x), b_2(x), \ldots, b_n(x)) \quad \text{with} \quad b_i(x) = b^0(x_i) + \gamma_i(x).$$

We assume that $b^0$ satisfies corresponding conditions as $b$ in Example 14 with constants $\mathcal{R}, L$ and $K$, and we consider the $\ell_1$ metric

$$d(x, y) = \sum_{i=1}^{n} d_0(x_i, y_i)$$

where the distance function $d_0$ on $\mathbb{R}^k$ is chosen as in Example 14 (but for $b^0$ instead of $b$). Then by [27, Theorem 7], there exist $c, \epsilon > 0$ that depend only on $\mathcal{R}, L$ and $K$ such that Condition (18) is satisfied with $A = 1$ whenever

$$\sum_{i=1}^{n} |\gamma_i(x) - \gamma_i(y)| \leq \epsilon \sum_{i=1}^{n} |x_i - y_i| \quad \text{for all } x, y \in \mathbb{R}^d.$$

Since $d(x, y) \leq \sum_{i=1}^{n} |x_i - y_i| \leq n^{1/2} |x - y|$, Theorem 7 implies the bound

$$W_{1,\ell_1}(\pi_\gamma, \pi) \leq m^{-1} W_{1,d}(\pi_\gamma, \pi) \leq \gamma e^{1+(1+\kappa)\gamma} \left( \frac{1+\kappa}{c} + 1 \right) m^{-1} n^{1/2} M_{\mathbf{L}}^{1/2},$$

where $\kappa$ is the constant in $E5$. If we assume that $\kappa$ does not depend on the number $n$ of components, then the upper bound for $W_{1,\ell_1}(\pi_\gamma, \pi)$ depends on $n$ only through $M_{\mathbf{L}}^{1/2}$. If we assume additionally that there exists a finite constant $C$ such that $|\Delta b_i| \leq C$ for all $i \in \{1, 2, \ldots, n\}$ then Condition (29) is satisfied with $K = C^2n$, and hence the upper
bound for $W_{1,\ell}(\pi_\gamma, \pi)$ is of order $O(\gamma n)$. This is the optimal order in the product case where $\gamma \equiv 0$. However, the assumptions above are satisfied in more general situations, including for example mean-field models of McKean-Vlasov type with weak interactions where $b_i(x) = -\nabla V(x_i) + \delta_n^{-1} \sum_{j \neq i} \nabla W(x_j - x_i)$ for sufficiently regular confinement and interaction potentials $V$ and $W$ and a sufficiently small coupling parameter $\delta$. On the other hand, for large $\delta$, these models can exhibit phase transitions. In that case, because of the non-uniqueness of invariant measures for the limiting McKean-Vlasov equation, $W_{1,\ell}(\pi_\gamma, \pi)$ will usually degenerate rapidly in high dimensions.

Example 18 (Unadjusted HMC for mean-field systems). Corresponding statements as in Example 17 also hold for unadjusted Hamiltonian Monte Carlo applied to mean-field models, except that the order in $\gamma$ improves from $O(\gamma)$ to $O(\gamma^2)$. We refer to Bou-Rabee and Schuh [8] for a detailed analysis of this setup.

3.2 The Gaussian case

For a standard normal target distribution $\pi(dx) = (2\pi)^{-d/2} \exp(-U(x)) dx$ with $U(x) = |x|^2/2$, the asymptotic Wasserstein bias of ULA and uHMC can be computed explicitly. The result serves as a benchmark for the general case.

Example 19 (ULA with standard normal target distribution). In this case, for any $x \in \mathbb{R}^d$, $\tilde{b}_\gamma(x) = -x$. It is easy to show that for $\gamma \in (0, 2)$, $E 3$ is satisfied and the measure $\pi_\gamma$ is the zero-mean Gaussian distribution with covariance matrix $(1-\gamma/2)^{-1} I_d$. Moreover, it can be shown that the synchronous coupling given by $(G, (1-\gamma/2)^{-1/2} G)$ where $G$ is a $d$-dimensional zero-mean Gaussian random variable with covariance matrix $I_d$, is an optimal coupling of the centered normal distributions $\pi$ and $\pi_\gamma$ w.r.t. $W_p$ for every $p \in [1, +\infty)$. Indeed, by rotational symmetry, this follows from the results in the one-dimensional case [43], noting that for any coupling, the average $L^p$ distances are lower bounded by corresponding Wasserstein distances of the one-dimensional marginal distributions of the radial parts; see also [32] for the case $p = 2$. Hence

$$W_p(\pi_\gamma, \pi) = \mathbb{E} \left[ \left| (1 - \frac{\gamma}{2})^{-1/2} G - G \right|^p \right]^{1/p} = \left| (1 - \frac{\gamma}{2})^{-1/2} - 1 \right| \mathbb{E} \left[ |G|^p \right]^{1/p} \geq C \gamma d^{1/2},$$

for some constant $C > 0$ independent of $\gamma$ and $d$.

Example 20 (uHMC with standard normal target distribution). If $U(q) = |q|^2/2$, then a step of the Verlet integrator is given by $\psi(q,p) = (q', p')$, where

$$q' = \left( 1 - \frac{\gamma^2}{2} \right) q + \gamma p, \quad p' = \left( 1 - \frac{\gamma^2}{2} \right) p - \gamma \left( 1 - \frac{\gamma^2}{4} \right) q.$$  

It can be easily verified that for $\gamma \in (0, 2)$, this map preserves the modified Hamiltonian

$$H_\gamma(q,p) = \frac{1}{2} \left( 1 - \frac{\gamma^2}{4} \right) |q|^2 + \frac{1}{2} |p|^2.$$
i.e.,  \( H_\gamma \circ \tilde{\Psi}_\gamma = H_\gamma \). Since \( \tilde{\Psi}_\gamma \) also preserves the Lebesgue measure on \( \mathbb{R}^{2d} \), we see that the probability measure with density proportional to \( \exp(-H_\gamma(q,p)) \) is preserved under \( \tilde{\Psi}_\gamma \), and also under momentum randomizations. The unique invariant probability measure \( \pi_{T,\gamma} \) of uHMC in position space is the first marginal of this measure, i.e., for every \( T > 0 \), \( \pi_{T,\gamma} \) is the \( d \)-dimensional zero-mean Gaussian measure with covariance matrix \( (1 - \gamma^2/4)^{-1/2} \). Therefore, similarly as in Example 19, we obtain

\[
W_p(\pi_{T,\gamma}, \pi) = \left| (1 - \gamma^2/4)^{-1/2} - 1 \right| \mathbb{E} \left[ \|G\|^p \right]^{1/p} \geq C\gamma^2 d^{1/q}.
\]

for some constant \( C \geq 0 \) independent of \( \gamma \) and \( d \).

3.3 Comparison of unadjusted and Metropolis-adjusted MCMC methods

As an alternative to applying unadjusted MCMC methods, it is very common to use Metropolis-Hastings (MH) methods where the transition steps of unadjusted MCMC methods can be used as proposals, [49, 51, 45].

An obvious advantage of the Metropolis-adjustment is that one obtains a Markov chain that exactly preserves the target distribution, i.e., the asymptotic bias vanishes. Consequently, one can at least in principle approximate the target distribution with arbitrary precision by running the MH Markov chain for a sufficiently long time. Moreover, the number of steps required to achieve a given accuracy \( \epsilon > 0 \) is of order \( \log(\epsilon^{-1}) \), while for inexact schemes, the step size \( \gamma \) has to be adjusted to the desired accuracy, resulting in a complexity of order \( \epsilon^{-\alpha} \) where \( \alpha = 1 \) for ULA and \( \alpha = 1/2 \) for uHMC. On the other hand, a disadvantage of MH adjustment is that a high rejection rate can lead to slow mixing of the Metropolis-adjusted Markov chain, while the mixing properties of the unadjusted Markov chain usually remain stable even for larger step sizes (at the cost of introducing an asymptotic bias in the estimates). Moreover, the non-smooth dependence of the trajectories of Metropolis-adjusted chains on parameters or initial data can cause problems for both the theoretical analysis and practical applications such as the estimation of sensitivities.

To compare Metropolis-adjusted and unadjusted MCMC methods it is useful to distinguish two regimes:

(i) If the acceptance rate of the Metropolis-adjusted scheme is “sufficiently high” then one might expect that the adjusted chain has as good mixing properties as the unadjusted chain. However, no proof of such a general fact is known, and moreover, the acceptance rate may vary considerably in different regions of the state space. So far, mixing properties for MALA with a step size \( \gamma \) of order \( O(d^{-1/2}) \) have been proven only for strongly log-concave distributions and for a warm start, i.e., when the initial distribution already has a relative density w.r.t. the target distribution that is bounded by a fixed constant [12, 58]. It is not known how such a warm start can be generated in practice, and the best available bounds for a cold or feasible start require a step size \( \gamma \) of order \( O(d^{-1}) \) [37, 10]. Indeed, it can be shown that this
order cannot be improved in general [38], although a better dimension dependence may hold for subclasses of nice models. The existing rigorous upper bounds for HMC with Metropolis-adjustment are even less satisfactory [7, 10].

(ii) If, on the other hand, the acceptance rate of the Metropolis-adjusted scheme degenerates then it can be easily shown by a conductance argument that the mixing properties and even the relaxation time also degenerate [30]. Nevertheless, the unadjusted chain will often have good mixing properties even for large step sizes. Our results show that in this case, approximate samples produced by the unadjusted chain can sometimes still provide useful information. In particular, for nice models, the asymptotic Wasserstein bias of unadjusted HMC is well behaved for step sizes $\gamma$ of order $O(d^{-1/4})$, but it is known that for adjusted HMC, the acceptance probability can degenerate in this case, unless a warm start condition is assumed [30]. Moreover, Wasserstein distances are not scale invariant, and the bias in estimating integrals $\int f \, d\pi$ by inexact MCMC methods depends on the regularity of the function $f$. Therefore, even if the Wasserstein bias in a certain metric grows with the dimension, it may be possible to obtain good approximations for integrals of well-behaved observables. Indeed, we have already seen in the introduction that for example for intensive quantities in molecular dynamics simulations, approximations are sometimes possible even for step sizes that do not depend on the dimension at all. This shows another important difference between unadjusted and Metropolis-adjusted schemes: whereas the latter seem to either degenerate or work well, unadjusted schemes with large step sizes can still produce a good approximation for nice observables.

In practice, it is usually not known how to adjust the step size to obtain reliable estimates. One possibility, arising from the above discussion, might be to run an unadjusted chain with a large step size at the beginning of the simulation, and then reduce the step size until sufficiently high acceptance probabilities for the Metropolis-adjustment are achieved (this could be tested empirically), so that the chain can be run with Metropolis-adjustment from now on to fine tune the estimates. An important question for future research might be to clarify more precisely what “sufficiently high” means and to rigorously analyze if unadjusted schemes are indeed able to generate good initial distributions for Metropolis-adjusted methods.

4 Proofs

This section contains the proofs of the main results. In all cases, the main idea is to apply the triangle inequality trick from Lemma 1. Then, assuming convergence bounds in Wasserstein distance for the exact (respectively approximate) dynamics, the asymptotic bias can be quantified if we can control the Wasserstein distance between the dynamics and the stationary distribution of the scheme (respectively the iterates of the discretization scheme and the target). To this end, we compare the $L^2$ distance between the exact and approximate dynamics driven by the same noise. While this is standard in
the analysis of numerical schemes for SDE [36], we carefully analyze how discretization errors propagate along the iterations of the scheme to obtain precise bounds with the correct dependence on dimension.

After briefly reviewing basic facts on Wasserstein bounds, we first prove the main results for ULA (Theorems 5 and 5) and then the main result for uHMC (Theorem 11).

4.1 Wasserstein bounds for transition kernels

For the reader’s convenience, we recall the proof of the following well-known result.

**Lemma 21.** Suppose that $d : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_+$ is a lower semicontinuous distance function, and $P$ is a Markov transition kernel on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$. Let $p \in [1, +\infty)$. If there exists $\alpha \geq 0$ such that for all $x, y \in \mathbb{R}^d$,

$$W_{p,d}(\delta_x P, \delta_y P) \leq \alpha d(x, y),$$

then for all $n \in \mathbb{N}$ and all probability measures $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$,

$$W_{p,d}(\mu P^n, \nu P^n) \leq \alpha^n W_{p,d}(\mu, \nu).$$

Lemma 21 is an immediate consequence of the following lemma.

**Lemma 22.** Let $X$ be a Polish space with Borel $\sigma$-field $\mathcal{X}$, $p \in [1, +\infty)$, and suppose that $d : \mathcal{X}^2 \to \mathbb{R}_+$ is a lower semicontinuous distance function on $X$. Consider two Markov kernels $Q_1$ and $Q_2$ on $X \times X$, and suppose that there exists a measurable function $\Psi : X \times X \to \mathbb{R}_+$ such that for any $x, y \in X$,

$$W_{p,d}(\delta_x Q_1, \delta_y Q_2) \leq \Psi(x, y). \quad (35)$$

Then for any $\mu_1, \mu_2 \in \mathcal{P}_{p,d}(X)$, and for any coupling $\zeta \in \Gamma(\mu_1, \mu_2)$,

$$W_{p,d}(\mu_1 Q_1, \mu_2 Q_2) \leq \left\{ \int_{X \times X} \Psi(x, y)^p \zeta(d(x, y)) \right\}^{1/p}. \quad (36)$$

In particular if $\Psi = \alpha d$ for $\alpha \geq 0$, then $W_{p,d}(\mu_1 Q_1, \mu_2 Q_2) \leq \alpha W_{p,d}(\mu_1, \mu_2)$.

**Proof.** Let $\mu_1, \mu_2 \in \mathcal{P}_{p,d}(X)$ and $\zeta \in \Gamma(\mu_1, \mu_2)$. By [56, Corollary 5.22], there exists a Markov kernel $K$ on $(X \times X) \times (X \otimes X)$ such that for any $x, y \in X$, the probability measure $K((x, y), d(w, z))$ is an optimal coupling of $Q_1(x, dw)$ and $Q_2(x, dz)$, i.e.,

$$W_{p,d}(\delta_x Q_1, \delta_y Q_2) = \left\{ \int_{X \times X} d(w, z)^p K((x, y), d(w, z)) \right\}^{1/p}. \quad (37)$$

By Fubini’s theorem, the probability measure $\zeta K$ is a coupling of $\mu_1 Q_1$ and $\mu_2 Q_2$. Therefore, by definition of $W_{p,d}$, Fubini’s theorem, and (35),

$$W_{p,d}(\mu_1 Q_1, \mu_2 Q_2) \leq \left\{ \int_{X \times X} \int_{X \times X} d(w, z)^p K((x, y), d(w, z)) \zeta(d(x, y)) \right\}^{1/p} \leq \left\{ \int_{X \times X} \Psi(x, y)^p \zeta(d(x, y)) \right\}^{1/p}. \quad (38)$$

The last statement follows by taking the infimum over $\zeta \in \Gamma(\mu_1, \mu_2)$.
Proof of Lemma 21. Applying Lemma 22 with $Q_1 = Q_2 = P$, $\mu_1 = \mu$ and $\mu_2 = \nu$ yields $W_{p,d}(\mu P, \nu P) \leq \alpha W_{p,d}(\mu, \nu)$. The claim then follows by induction.  

4.2 Proofs of Proposition 4 and Theorem 5

We consider a synchronous coupling between the diffusion process (9) and its discretization (11). Let $W_0$ be an $\mathbb{R}^d$-valued random variable with $\mathbb{E}[|W_0|^2] < +\infty$ that is independent of the $d$-dimensional Brownian motion $(B_t)_{t \geq 0}$. We define processes $(Y_t)_{t \geq 0}$ and $(\bar{Y}_t)_{t \geq 0}$ by $Y_0 = \bar{Y}_0 = W_0$,

$$Y_t = Y_0 + \int_0^t b(Y_s)ds + \sqrt{2}B_t,$$

$$\bar{Y}_t = Y_0 + \int_0^t \bar{b}_n(\bar{Y}_{\lfloor s/\gamma \rfloor})ds + \sqrt{2}B_t. \tag{36}$$

Then $(Y_t)_{t \geq 0}$ is the unique strong solution of the SDE (9) with initial condition $W_0$, and $(\bar{Y}_t)_{t \geq 0}$ is the linear interpolation of the Euler-Maruyama type discretization in the sense that for every $n \in \mathbb{N}$, $X_n = bY_n$ satisfies the recursion (11) with independent standard normal random variables $G_k$ given by $G_{k+1} = (B_{(k+1)\gamma} - B_{k\gamma})/\sqrt{\gamma}$. In particular, for any $n \in \mathbb{N}$ and $\gamma \in (0, \bar{\gamma}]$, $(Y_n\gamma, \bar{Y}_n\gamma)$ is a coupling of the probability measures $\nu P_{n\gamma}$ and $\nu R^n_\gamma$, where $\nu$ is the law of the initial value $W_0$ and therefore

$$W_2\left(\nu P_{n\gamma}, \nu R^n_\gamma\right) \leq \mathbb{E}^{1/2}\left[|Y_{n\gamma} - \bar{Y}_{n\gamma}|^2\right]. \tag{37}$$

Finally, note that if $\nu = \pi$, then by E1, $(Y_t)_{t \geq 0}$ is a stationary process and for any $t \geq 0$, $Y_t$ has distribution $\pi$.

Proof of Proposition 4. We apply (37) with $\nu = \pi$. By Lemma 23 below, and a straightforward induction, we obtain that for any $\gamma \in (0, \bar{\gamma}]$ and $n \in \mathbb{N},$

$$W_2^2\left(\pi P_{n\gamma}, \pi R^n_\gamma\right) \leq \mathbb{E}\left[|Y_{n\gamma} - \bar{Y}_{n\gamma}|^2\right]$$

$$\leq \gamma^3 \left[(2 + 9\gamma)M_1/6 + 3M_2 + (2 + 3\gamma)M_3\right] \sum_{k=1}^n (1 + 2\lambda_L\gamma)^{n-k}$$

$$\leq \frac{\gamma^2}{2\lambda_L} \left[(2 + 9\gamma)M_1/6 + 3M_2 + (2 + 3\gamma)M_3\right] (1 + 2\lambda_L\gamma)^n.$$

The proof is concluded using that for any $t \geq 0$, $1 + t \leq e^t$ and $\lambda_L \geq 1$. 

Lemma 23. Assume E1, E2, E3 and E4. Then for any $\gamma \in (0, \bar{\gamma}]$ and $n \in \mathbb{N},$

$$\mathbb{E}\left[|Y_{(n+1)\gamma} - \bar{Y}_{(n+1)\gamma}|^2\right] \leq (1 + 2\lambda_L\gamma)\mathbb{E}\left[|Y_{n\gamma} - \bar{Y}_{n\gamma}|^2\right]$$

$$+ \gamma^3 \left[(2 + 9\gamma)M_1/6 + 3M_2 + (2 + 3\gamma)M_3\right],$$

$$+ \gamma^3 \left[(2 + 9\gamma)M_1/6 + 3M_2 + (2 + 3\gamma)M_3\right],$$

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where
\[ \lambda_{\gamma} = 1 + L^2 + 3\gamma L^2 / 2 , \]

\((Y_t, \tilde{Y}_t)_{t \geq 0}\) is defined by (36) with \(W_0\) distributed according to \(\pi\), and \(M_1, M_2, M_3\) are given by (14).

**Proof.** For any \(k \in \mathbb{N}\), define \(Z_k = Y_{k\gamma} - \tilde{Y}_{k\gamma}\) and let \(n \in \mathbb{N}, \gamma \in (0, \tilde{\gamma}]\). Then by (36) and using the decomposition \(b(Y_s) - \tilde{b}_\gamma(Y_{n\gamma}) = b(Y_s) - b(Y_{n\gamma} + b(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma})\), we get

\[
\mathbb{E} \left[ |Z_{n+1}|^2 \right] = \mathbb{E} \left[ |Z_n|^2 \right] + \int_{n\gamma}^{(n+1)\gamma} 2\mathbb{E} \left[ \langle Z_n, b(Y_s) - b(Y_{n\gamma}) \rangle \right] \, ds \\
+ 2\gamma \mathbb{E} \left[ \langle Z_n, b(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma}) \rangle \right] + \mathbb{E} \left[ \int_{n\gamma}^{(n+1)\gamma} \left\{ b(Y_s) - \tilde{b}_\gamma(Y_{n\gamma}) \right\} \, ds \right]^2.
\]

We now bound the terms on the right hand side. First, by Itô’s formula, for any \(s \geq n\gamma\),

\[
b(Y_s) - b(Y_{n\gamma}) = \int_{n\gamma}^{s} \mathcal{L} b(Y_u) \, du + \int_{n\gamma}^{s} \langle \nabla b(Y_u), dB_u \rangle.
\]

Denote by \((\mathcal{F}_t^B)_{t \geq 0}\) the filtration associated with \((B_t)_{t \geq 0}\). Since \(M_2 < +\infty\), the process \((\int_0^s \langle \nabla b(Y_u), dB_u \rangle)_{s \geq 0}\) is a \((\mathcal{F}_t^B)_{t \geq 0}\)-martingale. Using that \((Z_t)_{t \geq 0}\) is \((\mathcal{F}_t^B)_{t \geq 0}\)-adapted and for any \(t \geq 0\), \(Y_t\) has distribution \(\pi\), and we get by the Cauchy-Schwarz inequality

\[
2\mathbb{E} \left[ \langle Z_n, b(Y_s) - b(Y_{n\gamma}) \rangle \right] = 2\mathbb{E} \left[ \left\langle Z_n, \int_{n\gamma}^{s} \mathcal{L} b(Y_u) \, du \right\rangle \right] \\
\leq \mathbb{E} \left[ |Z_n|^2 \right] + \mathbb{E} \left[ \left| \int_{n\gamma}^{s} \mathcal{L} b(Y_u) \, du \right|^2 \right] \\
\leq \mathbb{E} \left[ |Z_n|^2 \right] + (s - n\gamma)^2 M_1.
\]

Therefore, we get

\[
\int_{n\gamma}^{(n+1)\gamma} 2\mathbb{E} \left[ \langle Z_n, b(Y_s) - b(Y_{n\gamma}) \rangle \right] \, ds \leq \gamma \mathbb{E} \left[ |Z_n|^2 \right] + \gamma^3 M_1 / 3.
\]

Furthermore, using the decomposition \(b(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma}) = b(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma}) + \tilde{b}_\gamma(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma})\), as well as \(\mathbf{E}2\) and \(\mathbf{E}4\), we have

\[
2\mathbb{E} \left[ \langle Z_n, b(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma}) \rangle \right] \leq \mathbb{E} \left[ |Z_n|^2 \right] + \mathbb{E} \left[ |b(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma})|^2 \right] \\
\leq \mathbb{E} \left[ |Z_n|^2 \right] + 2\gamma^2 M_3 + 2L^2 \mathbb{E} \left[ |Z_n|^2 \right],
\]

where \(M_3\) is defined in (14). Using \(b(Y_s) - \tilde{b}_\gamma(Y_{n\gamma}) = b(Y_s) - b(Y_{n\gamma}) + b(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma}) + \tilde{b}_\gamma(Y_{n\gamma}) - \tilde{b}_\gamma(Y_{n\gamma})\),
\( \bar{b}_\gamma(Y_{n\gamma}) - \bar{b}_\gamma(\bar{Y}_{n\gamma}) \) and (39), we get that

\[
\mathbb{E} \left[ \left( \int_{n\gamma}^{(n+1)\gamma} \left\{ b(Y_s) - \bar{b}_\gamma(Y_{n\gamma}) \right\} ds \right)^2 \right] \leq 3\mathbb{E} \left[ \left( \int_{n\gamma}^{(n+1)\gamma} \left\{ b(Y_s) - b(Y_{n\gamma}) \right\} ds \right)^2 \right] + 3\gamma^2 \mathbb{E} \left[ \left| b(Y_{n\gamma}) - \bar{b}_\gamma(Y_{n\gamma}) \right|^2 \right]
\]

\[
\leq 6\mathbb{E} \left[ \int_{n\gamma}^{(n+1)\gamma} \int_{n\gamma}^s \mathcal{L}b(Y_u) duds \right]^2 + \left( \int_{n\gamma}^{(n+1)\gamma} \int_{n\gamma}^s \langle \nabla b(Y_u), dB_u \rangle ds \right)^2
\]

\[
+ 3\gamma^4 M_3 + 3\gamma^2 L^2 \mathbb{E} \left[ |Z_n|^2 \right].
\]

Using the Cauchy-Schwarz inequality and that for any \( t \geq 0 \), \( Y_t \) has distribution \( \pi \), we have

\[
\mathbb{E} \left[ \left( \int_{n\gamma}^{(n+1)\gamma} \int_{n\gamma}^s \mathcal{L}b(Y_u) dud\gamma \right)^2 \right] \leq \left\{ \int_{n\gamma}^{(n+1)\gamma} \int_{n\gamma}^s dud\gamma \right\} M_1 = \frac{\gamma^4}{4} M_1.
\]

Similarly, using the Cauchy-Schwarz inequality and Itô’s isometry, we obtain

\[
\mathbb{E} \left[ \int_{n\gamma}^{(n+1)\gamma} \int_{n\gamma}^s \langle \nabla b(Y_u), dB_u \rangle ds \right]^2 \leq \gamma \int_{n\gamma}^{(n+1)\gamma} \int_{n\gamma}^s \mathbb{E} \left[ \text{Tr} \left( \nabla b(Y_u) \nabla b(Y_u)^T \right) \right] duds = \frac{\gamma^3}{2} M_2.
\]

The proof then follows from combining (40), (41), (42) and (43) in (38). \( \square \)

**Remark 24.** An alternative way to arrive at bounds as in Lemma 23 is through stochastic interpolation formulae [17, 16]. These provide exact expressions for the difference of two stochastic flows. In the simple scenario considered here, they seem to lead to similar bounds as above. However, the interpolation approach might be helpful in analyzing discretizations of stochastic differential equations with non-constant diffusion coefficients.

**Proof of Theorem 5.** The result is a direct consequence of Proposition 4 and the inequalities in (7) and (8). \( \square \)

### 4.3 Proofs of Proposition 6 and Theorem 7

Similarly as above, we consider \((Y_t, \bar{Y}_t)_{t \geq 0}\) defined by (36), but now with \(W_0\) distributed according to \( \pi_\gamma \). Then since \( \pi_\gamma \) is invariant for \( R_\gamma \) by E3, the process \((X_n = bY_{n\gamma})_{n \in \mathbb{N}}\) is stationary and for any \( n \in \mathbb{N} \) and \( \gamma \in (0, \bar{\gamma}) \), \( \bar{Y}_{n\gamma} \) has distribution \( \pi_\gamma \).

**Proof of Proposition 6.** By Lemma 26 below and since \( Y_0 = \bar{Y}_0 \), we have by a straightforward induction that for any \( \gamma \in (0, \bar{\gamma}) \) and \( n \in \mathbb{N} \),

\[
\mathbb{E} \left[ \left| Y_{n\gamma} - \bar{Y}_{n\gamma} \right|^2 \right] \leq (1 + 2\kappa) \int_0^{n\gamma} \mathbb{E} \left[ \left| Y_s - \bar{Y}_s \right|^2 \right] ds + n\gamma^3 M_L.
\]
Therefore, we get for any \( t \geq 0 \), using Lemma 26 again,
\[
\mathbb{E} \left[ |Y_t - \bar{Y}_t|^2 \right] \leq (1 + 2\kappa) \int_0^t \mathbb{E} \left[ |Y_s - \bar{Y}_s|^2 \right] \, ds + (t\gamma^2 + \gamma^3) \bar{M}_L.
\]
By Grönwall’s inequality, and since \( s \leq e^s \), we obtain that for any \( t \geq 0 \),
\[
\mathbb{E} \left[ |Y_t - \bar{Y}_t|^2 \right] \leq e^{1+2\kappa t}\gamma^2(t + \gamma)\bar{M}_L \leq e^{2(1+\kappa)t}\gamma^2(1 + \gamma)\bar{M}_L.
\]
The proof is then completed using (37).

We preface the proof of Lemma 26 by a technical result.

**Lemma 25.** Assume \( E3 \) and let \( f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_+ \) be a measurable function. Let \((\bar{Y}_t)_{t \geq 0}\) be defined by (36) with \( W_0 \) distributed according to \( \pi_{\gamma} \). Then for any \( n \in \mathbb{N}, \gamma \in (0, \bar{\gamma}] \) and \( u \in [0, \gamma] \),
\[
\mathbb{E} \left[ f(\bar{Y}_{n\gamma}, \bar{Y}_{n\gamma} + u) \right] = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(x, x + \tilde{u}_{\gamma}(x) + (2u)\gamma z) \varphi_d(z) \, dz \, \pi_{\gamma}(dx).
\]

**Proof.** Let \( n \in \mathbb{N}, \gamma \in (0, \bar{\gamma}] \) and \( u \in [0, \gamma] \). By definition, \( \bar{Y}_{n\gamma} = Y_{n\gamma} + \tilde{u}_{\gamma}(Y_{n\gamma}) + \sqrt{2}(B_{n\gamma} - B_{n\gamma}) \). Then, since \( \bar{Y}_{n\gamma} \) is \((\mathcal{F}_{t}^{B})_{t \leq n\gamma}\)-measurable, where \((\mathcal{F}_{t}^{B})_{t \leq n\gamma}\) is the filtration generated by \((B_t)_{t \geq 0}\). By the Markov property of the Brownian motion, the increment \( B_{n\gamma} - B_{n\gamma} \) is independent of \( \bar{Y}_{n\gamma} \) and therefore, we get
\[
\mathbb{E} \left[ f(\bar{Y}_{n\gamma}, \bar{Y}_{n\gamma} + u) \right] = \int_{\mathbb{R}^d} f(\bar{Y}_{n\gamma}, \bar{Y}_{n\gamma} + u) \varphi_d(z) \, dz.
\]
The proof is then completed using that \( \bar{Y}_{n\gamma} \) has distribution \( \pi_{\gamma} \).

**Lemma 26.** Assume \( E1, E2, E3 \) and \( E5 \). Let \((Y_t, \bar{Y}_t)_{t \geq 0}\) be defined by (36) with \( W_0 \) distributed according to \( \pi_{\gamma} \). Then for any \( \gamma \in (0, \bar{\gamma}] \), \( n \in \mathbb{N}, t \in [n\gamma, (n + 1)\gamma) \),
\[
\mathbb{E} \left[ |Y_t - \bar{Y}_t|^2 \right] \leq \mathbb{E} \left[ |Y_{n\gamma} - \bar{Y}_{n\gamma}|^2 \right] + (1 + 2\kappa) \int_{n\gamma}^t \mathbb{E} \left[ |Y_s - \bar{Y}_s|^2 \right] \, ds
\]
\[
+ \gamma^3 \left( \frac{1}{6} \bar{M}_1 + \frac{1}{2} \gamma^{1/2} \bar{M}_2^{1/2} \bar{M}_3^{1/2} + \frac{1}{\sqrt{2}} \bar{M}_2^{1/2} \bar{M}_4^{1/2} + \frac{1}{2} \bar{M}_5 \right),
\]
where \( \bar{M}_i, i \in \{1, \ldots, 5\} \), are defined in Proposition 6.

**Proof.** Let \( \gamma \in (0, \bar{\gamma}] \) and \( n \in \mathbb{N} \) and for any \( t \geq 0 \), \( Z_t = Y_t - \bar{Y}_t \). By (36), almost surely it holds
\[
dZ_t/dt = b(Y_t) - \tilde{b}_{\gamma}(\bar{Y}_{n\gamma}) \quad \text{for } t \in [n\gamma, (n + 1)\gamma).
\]
Therefore and by \( E5 \), we have for any \( t \in [n\gamma, (n + 1)\gamma) \),
\[
|Z_t|^2 = |Z_{n\gamma}|^2 + 2 \int_{n\gamma}^t \left\langle Z_s, b(Y_s) - \tilde{b}_{\gamma}(\bar{Y}_{n\gamma}) \right\rangle \, ds
\]
\[
= |Z_{n\gamma}|^2 + 2 \int_{n\gamma}^t \left\langle Z_s, b(Y_s) - \tilde{b}_{\gamma}(\bar{Y}_{n\gamma}) - b(Y_s) - b(\bar{Y}_{n\gamma}) \right\rangle \, ds
\]
\[
\leq |Z_{n\gamma}|^2 + 2\kappa \int_{n\gamma}^t |Z_s|^2 \, ds + B_1 + B_2,
\]
where
\[
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\]
We now bound $E[B_1]$ and $E[B_2]$. Let $s \in [n\gamma, (n+1)\gamma]$. We first give a bound on $E[(b(Y_s) - b(Y_{n\gamma}))^2]$. By (36) and Itô’s formula,

$$b(Y_s) - b(Y_{n\gamma}) = \int_{n\gamma}^{s} \mathcal{L}^b(Y_{n\gamma}, Y_u) du + \int_{n\gamma}^{s} \langle \nabla b(Y_u), dB_u \rangle.$$  

(47)

Therefore, we obtain using the Cauchy-Schwarz inequality and Itô’s isometry,

$$E \left[ (b(Y_s) - b(Y_{n\gamma}))^2 \right] \leq 2 \left\{ E \left[ \int_{n\gamma}^{s} \mathcal{L}^b(Y_{n\gamma}, Y_u) du \right]^2 + E \left[ \int_{n\gamma}^{s} \langle \nabla b(Y_u), dB_u \rangle \right]^2 \right\} \leq 2 \left\{ E \left[ (s-n\gamma) \int_{n\gamma}^{s} \mathcal{L}^b(Y_{n\gamma}, Y_u) du \right]^2 + E \left[ \int_{n\gamma}^{s} \text{Tr} \left( \nabla b \nabla b^T \right) (Y_u) du \right] \right\}.$$  

By Lemma 25, for any $u \in [n\gamma, (n+1)\gamma]$,  

$$E \left[ \mathcal{L}^b(Y_{n\gamma}, Y_u) \right]^2 \leq \bar{M}_1, \quad \text{and} \quad E \left[ \text{Tr} \left( \nabla b \nabla b^T \right) (Y_u) \right] \leq \bar{M}_2.$$  

(48)

Therefore, we get

$$E \left[ (b(Y_s) - b(Y_{n\gamma}))^2 \right] \leq 2(s-n\gamma)^2 \bar{M}_1 + 2(s-n\gamma)\bar{M}_2.$$  

We can now bound $E[B_1]$. Let $t \in [n\gamma, (n+1)\gamma]$ and define

$$B_{11} = E \left[ \int_{n\gamma}^{t} \left\langle Z_s, \int_{n\gamma}^{s} \langle \nabla b(Y_u), dB_u \rangle \right\rangle ds \right].$$  

By (46), (47), the Cauchy-Schwarz inequality and (48),

$$E[B_1] \leq \frac{1}{2} E \left[ \int_{n\gamma}^{t} |Z_s|^2 ds \right] + \frac{1}{2} E \left[ \int_{n\gamma}^{t} \int_{n\gamma}^{u} \mathcal{L}^b(Y_{n\gamma}, Y_u) du \right]^2 ds \right] + B_{11} \leq \frac{1}{2} \int_{n\gamma}^{t} E \left[ |Z_s|^2 \right] ds + \frac{1}{6} \gamma^3 \bar{M}_1 + B_{11}.$$  

(49)

We now bound $|B_{11}|$. Denote by $(\mathcal{F}_t^B)_{t \geq 0}$ the filtration associated with $(B_t)_{t \geq 0}$. Note that since $(\int_{0}^{t} \nabla b(Y_s) dB_s)_{t \geq 0}$ is a $(\mathcal{F}_t^B)_{t \geq 0}$-martingale and using that $(Y_t, Y_{\tilde{t}})_{t \geq 0}$ is $(\mathcal{F}_t^B)_{t \geq 0}$-adapted, we have for any $t \in [n\gamma, (n+1)\gamma]$, and $u \in [0,n\gamma]$, $E[(b(Y_u) - b_\gamma(Y_u), \int_{n\gamma}^{t} \nabla b(Y_s) dB_s)] = 0$ and $E[(Z_u, \int_{n\gamma}^{t} \nabla b(Y_s) dB_s)] = 0$. Therefore, by Fubini’s
theorem, (44) and the Cauchy-Schwarz inequality, we obtain for any \( t \in [n\gamma, (n+1)\gamma] \),

\[
B_{11} = \int_{n\gamma}^{t} \mathbb{E} \left[ \left\langle Z_s - Z_{n\gamma}, \int_{n\gamma}^{s} (\nabla b(Y_u), dB_u) \right\rangle \right] ds
\]

\[
= \int_{n\gamma}^{t} \mathbb{E} \left[ \left\langle \int_{n\gamma}^{s} \{b(Y_u) - \tilde{b}_{\gamma}(Y_{n\gamma})\} du, \int_{n\gamma}^{s} (\nabla b(Y_u), dB_u) \right\rangle \right] ds
\]

\[
= \int_{n\gamma}^{t} \mathbb{E} \left[ \left\langle \int_{n\gamma}^{s} \{b(Y_u) - b(Y_{n\gamma})\} du, \int_{n\gamma}^{s} (\nabla b(Y_u), dB_u) \right\rangle \right] ds
\]

\[
\leq \int_{n\gamma}^{t} \mathbb{E} \left[ \left\{ \int_{n\gamma}^{s} \{|b(Y_u) - b(Y_{n\gamma})|\} du \right\}^2 \right] ds^{1/2} \left( \frac{\gamma^2}{2} M_2 \right)^{1/2},
\]  \tag{50}

where we have used in the last step that by Itô's isometry,

\[
\int_{n\gamma}^{t} \mathbb{E} \left[ \left\{ \int_{n\gamma}^{s} (\nabla b(Y_u), dB_u) \right\}^2 \right] ds = \int_{n\gamma}^{t} \mathbb{E} \left[ \text{Tr}(\nabla b \nabla b^T)(Y_u) \right] du ds \leq \frac{\gamma^2}{2} M_2.
\]

Moreover, analogously as in (41), (42) and (43), we obtain

\[
\mathbb{E} \left[ \left\{ \int_{n\gamma}^{s} \{|b(Y_u) - b(Y_{n\gamma})|\} du \right\}^2 \right] ds \leq \frac{\gamma^4}{4} \tilde{M}_3 + \gamma^3 \tilde{M}_4.
\]  \tag{51}

The only difference to the argument used above is that now the law of \( Y_u \) is \( \pi_{\gamma} P_u \) instead of \( \pi \), and therefore the constants \( M_1 \) and \( M_2 \) appearing in (42) and (43) are replaced by \( \tilde{M}_3 \) and \( \tilde{M}_4 \), respectively.

By combining (49), (50) and (51), we conclude that

\[
\mathbb{E}[B_1] \leq \frac{1}{2} \int_{n\gamma}^{t} \mathbb{E} \left[ |Z_s|^2 \right] ds + \frac{1}{6} \gamma^3 \tilde{M}_1 + \frac{1}{2} \gamma^{7/2} \tilde{M}_2^{1/2} \tilde{M}_3^{1/2} + \frac{1}{2} \sqrt{\gamma^3} \tilde{M}_2^{1/2} \tilde{M}_4^{1/2}.
\]

Finally, by Cauchy-Schwarz, \( \mathbb{E}2 \) and since \( Y_{n\gamma} \) has distribution \( \pi_{\gamma} \),

\[
\mathbb{E}[B_2] \leq \frac{1}{2} \int_{n\gamma}^{t} \mathbb{E} \left[ |Z_s|^2 \right] ds + \frac{\gamma^2}{2} \int_{n\gamma}^{t} \mathbb{E} \left[ \Gamma^2(Y_{n\gamma}) \right] ds \leq \frac{1}{2} \int_{n\gamma}^{t} \mathbb{E} \left[ |Z_s|^2 \right] ds + \frac{\gamma^3}{2} \tilde{M}_5.
\]

Taking expectations in (45) and inserting the bounds completes the proof. \( \square \)

**Proof of Theorem 7.** The result is a direct consequence of Proposition 6 and the inequalities in (7) and (8). \( \square \)

### 4.4 Proofs of Theorem 8 and Theorem 9

Define for all \( \gamma > 0 \), the function \( n : (0, +\infty) \to \mathbb{N} \) by

\[
n(\gamma) = \lfloor \log(\gamma^{-1}) / \log(2) \rfloor.
\]  \tag{52}
Proof of Theorem 8. Under E4-E5 and \( \sup_{x \in \mathbb{R}^d} \langle b(x), x \rangle < +\infty \), [14, Theorem 19] shows that for any \( t \geq 0 \),

\[
\|\delta_x P_t - \delta_y P_t\|_{TV} \leq \limsup_{k \to +\infty} \|\delta_x R^k_{t/k} - R^k_{t/k}\|_{TV}, \tag{53}
\]

where \( R^k_{t/k} \) is given by (12) with \( \tilde{b}_{t/k} \equiv b \). Note that by E4 and E5, for any \( x, y \in \mathbb{R}^d \) and \( \gamma \in (0, \bar{\gamma}] \), \( \|x + \gamma b(x) - (y + \gamma b(y))\|^2 \leq (1 + \gamma \kappa(\gamma))\|x - y\|^2 \), with \( \kappa(\gamma) = 2\kappa + L^2 \gamma \). Therefore, by [24, Theorem 19], for any \( \gamma \in (0, \bar{\gamma}] \) and \( k \in \mathbb{N} \),

\[
\|\delta_x R^k_{\gamma} - \delta_y R^k_{\gamma}\|_{TV} \leq 1 - 2\Phi \left( -\{\kappa(\gamma)\}^{1/2} \frac{\|x - y\|}{\sqrt{1 - (1 + \kappa(\gamma)\gamma)^{k+1}}} \right),
\]

where \( \Phi \) is the cumulative distribution function of the standard one-dimensional Gaussian distribution. Combining this result with (53) completes the proof upon using that \( 1 - 2\Phi(-u) \leq u \sqrt{2/\pi} \) for any \( u \geq 0 \).

Proof of Theorem 9. Let \( \gamma \in (0, \bar{\gamma}] \) and set \( t_\gamma = \gamma2^{n(\gamma)} \) with \( n(\gamma) \) defined in (52). We consider the following decomposition

\[
\|\pi - \pi_\gamma\|_{TV} \leq \|\pi P_{t_\gamma} - \pi_\gamma P_{t_\gamma}\|_{TV} + \|\pi_\gamma P_{t_\gamma} - \pi_\gamma\|_{TV}. \tag{54}
\]

First by E6-(ii) and Lemma 27, we get using \( 2^{n(\gamma)} \gamma \geq 1 \)

\[
\|\pi P_{t_\gamma} - \pi_\gamma P_{t_\gamma}\|_{TV} \leq C_{TV} B_{TV}(1) \gamma.
\]

It remains to bound the second term in (54) for which we apply Lemma 28 and the bound

\[
\sum_{k=1}^{n(\gamma)} C_{TV} A_{TV}(\gamma^{2k-1})\gamma^{3}\gamma^{k-1} \frac{1}{2} \exp(\lambda_{TV} \gamma^{2k-1}) \leq 4n(\gamma) \gamma C_{TV} A_{TV} \bar{\gamma} \exp(\lambda_{TV} \gamma),
\]

where we have used \( 2^{n(\gamma)} \gamma \leq 4 \).

Lemma 27. Assume E1 and E6-(iii). Then, for any probability measure \( \mu, \nu \in \mathcal{P}_1(\mathbb{R}^d) \) and \( t > 0 \), we get

\[
\|\mu P_t - \nu P_t\|_{TV} \leq C_{TV} \chi(t) W_1(\mu, \nu).
\]

Proof. Let \( \mu, \nu \in \mathcal{P}_1(\mathbb{R}^d) \) and \( t > 0 \). First, for any coupling \( \xi \) of \( \mu \) and \( \nu \), we easily get using \( \|\mu' - \nu'\|_{TV} = (1/2) \sup\{| \int f d\mu' - \int f d\nu'| : |f| \leq 1\} \),

\[
\|\mu P_t - \nu P_t\|_{TV} \leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \xi(dx, dy) \|\delta_x P_t - \delta_y P_t\|_{TV}.
\]

Using E6-(iii) and taking for \( \xi \) the optimal coupling between \( \mu \) and \( \nu \) for \( W_1 \) complete the proof.
Lemma 28. Assume \( E1, E3, E4 \) and \( E6 \). Suppose in addition that \( \bar{\gamma} < 1 \). Then for any \( \gamma \in (0, \bar{\gamma}] \), \( \ell \in \mathbb{N}, \ell \geq 2^{n(\gamma)} \),

\[
\| \pi_\gamma P_{\ell \gamma} - \pi_\gamma \|_{TV} \leq C_{TV} A_{TV} \chi(2^n \gamma)[\gamma^3(\ell - 2^n(\gamma))]^{1/2} \exp(\lambda_{TV}(\ell - 2^n(\gamma))\gamma) \\
+ 2^{-3/2} L \left\{ \gamma^3 \bar{M_6}/3 + d\gamma^2 \right\}^{1/2} + \sum_{k=1}^{n(\gamma)} C_{TV} A_{TV} \chi(2^{k-1} \gamma)[\gamma^3 2^{k-1}]^{1/2} \exp(\lambda_{TV} 2^{k-1} \gamma),
\]

where \( \bar{M_6} \) is defined in (19).

Proof. For ease of notation, denote \( n = n(\gamma) \) for \( \gamma \in (0, \bar{\gamma}] \). Let \( \ell \in \mathbb{N} \) such that \( \ell \geq 2^n \).

Consider the following decomposition

\[
\| \pi_\gamma P_{\ell \gamma} - \pi_\gamma \|_{TV} = \| \pi_\gamma P_{\ell \gamma} - \pi_\gamma R_{\gamma}^\ell \|_{TV} \leq \left\| \left\{ \pi_\gamma P_{(\ell - 2^n) \gamma} - \pi_\gamma R_{\gamma}^{\ell - 2^n} \right\} P_{2^n \gamma} \right\|_{TV} \\
+ \left\| \left\{ \pi_\gamma R_{\gamma}^{\ell - 1} \{ P_\gamma - R_\gamma \} \right\} \right\|_{TV} + \sum_{k=1}^{n} \left\| \pi_\gamma R_{\gamma}^{\ell - 2^k} \left\{ P_{2^{k-1} \gamma} - R_{\gamma}^{2^{k-1}} \right\} P_{2^{k-1} \gamma} \right\|_{TV}.
\]

(55)

We bound each term in the right hand side. First by Lemma 27 and \( E6-(i) \), we have

\[
\left\| \left\{ \pi_\gamma P_{(\ell - 2^n) \gamma} - \pi_\gamma R_{\gamma}^{\ell - 2^n} \right\} P_{2^n \gamma} \right\|_{TV} \leq C_{TV} A_{TV} \chi(2^n \gamma)[\gamma^3(\ell - 2^n)]^{1/2} \exp(\lambda_{TV}(\ell - 2^n)\gamma). \tag{56}
\]

Similarly we get for all \( k \in \{1, \cdots, 2^n\}, \)

\[
\left\| \left\{ \pi_\gamma R_{\gamma}^{\ell - 2^k} \left\{ P_{2^{k-1} \gamma} - R_{\gamma}^{2^{k-1}} \right\} P_{2^{k-1} \gamma} \right\} \right\|_{TV} \leq C_{TV} A_{TV} \chi(2^{k-1} \gamma)[\gamma^3 2^{k-1}]^{1/2} \exp(\lambda_{TV} 2^{k-1} \gamma). \tag{57}
\]

For the last term, adapting the proof of [22, Proposition 2] to a general drift \( b \) in place of \( \nabla U \), we have

\[
\left\| \pi_\gamma R_{\gamma}^{\ell - 1} \{ P_\gamma - R_\gamma \} \right\|_{TV}^2 \leq 2^{-3} L^2 \left\{ \gamma^3 \bar{M_6}/3 + d\gamma^2 \right\}.
\]

Combining this inequality, (56), (57) in (55) concludes the proof.

4.5 Postponed proofs of Section 2.2.1

Lemma 29. Let \( f \in C^2([a, b], \mathbb{R}^d) \) for \( a, b \in \mathbb{R}, a < b \). Then for any \( t \in [a, b], \)

\[
\int_a^b \{ f(t) - (f(b) + f(a))/2 \} dt = -(1/2) \int_a^b f''(t)(b-t)(t-a) dt. \tag{58}
\]
Proof. For any $t \in [a, b]$, since $f \in C^2([a, b], \mathbb{R}^d)$, we have using integration by parts twice

$$f(t) - \frac{(b-t)f(a) + (t-a)f(b)}{b-a} = \left[ \frac{(b-t)}{b-a} \int_a^t f'(s)ds - \frac{(t-a)}{b-a} \int_t^b f'(s)ds \right]$$

$$= \frac{(b-t)}{b-a} \left\{ (t-a)f'(t) - \int_a^t f''(s)(s-a)ds \right\}$$

$$+ \frac{(t-a)}{b-a} \left\{ (t-b)f'(t) - \int_t^b f''(s)(s-b)ds \right\} ,$$

which implies

$$(b-a)f(t) = (b-t)f(a) + (t-a)f(b) + \frac{(b-t)}{b-a} \int_a^t f''(s)(s-a)ds$$

$$- \frac{(t-a)}{b-a} \int_t^b f''(s)(s-b)ds ,$$

Now integrating this identity over $[a, b]$, we obtain

$$\int_a^b f(t)dt = \frac{(f(b) + f(a))}{2} + \int_a^b \frac{(s-a)f''(s)}{b-a} \int_a^s (b-t)dt ds$$

$$- \int_a^b \frac{(b-s)f''(s)}{b-a} \int_s^b (a-t)dt ds ,$$

which implies (58). \qed

**Lemma 30.** Assume $H1$, $H2$ and $H4$ and let $\gamma \in (0, \bar{\gamma})$. Let $\tilde{\pi} \in \mathcal{P}_2(\mathbb{R}^d)$, and let $G, Q$ be $\mathbb{R}^d$-valued random variables such that $G$ is normally distributed with zero-mean and covariance matrix identity, $Q$ has distribution $\pi$ and is independent of $G$. Define $(X_k, V_k)_{k \geq 0}$ and $(\tilde{X}_k, \tilde{V}_k)_{k \geq 0}$ recursively by $X_0 = \tilde{X}_0 = Q$, $V_0 = \tilde{V}_0 = G$, and for any $k \in \mathbb{N},$

$$(X_{k+1}, V_{k+1}) = \Psi_\gamma(X_k, V_k), \quad (\tilde{X}_{k+1}, \tilde{V}_{k+1}) = \tilde{\Psi}_\gamma(\tilde{X}_k, \tilde{V}_k),$$

where $\Psi_\gamma$ and $\tilde{\Psi}_\gamma$ are defined by (20) and (21). Then for any integer $k \geq 0,$

$$\mathbb{E}^{1/2} \left[ X_{k+1} - \tilde{X}_{k+1} \right]^2 \leq \gamma^3((M_2/12)^{1/2} + M_5^{1/2}/2)$$

$$+ \left(1 + \frac{\gamma^2L}{2} \right) \mathbb{E}^{1/2} \left[ X_k - \tilde{X}_k \right]^2 + \gamma \mathbb{E}^{1/2} \left[ V_k - \tilde{V}_k \right]^2 , \quad \text{(59)}$$

$$\mathbb{E}^{1/2} \left[ V_{k+1} - \tilde{V}_{k+1} \right]^2 \leq \frac{\gamma^3}{2} \left( 2 + \frac{\gamma L}{2} \right) M_5^{1/2} + \frac{\gamma LM_2^{1/2}}{2\sqrt{12}} + \frac{(M_1 + 2M_4)^{1/2}}{15^{1/2}}$$

$$+ \left( \gamma L + \frac{\gamma^3 L^2}{4} \right) \mathbb{E}^{1/2} \left[ X_k - \tilde{X}_k \right]^2 + \left(1 + \frac{\gamma^2 L}{2} \right) \mathbb{E}^{1/2} \left| V_k - \tilde{V}_k \right|^2 \quad \text{(60)}$$

where $M_1, M_2, M_4$ and $M_5$ are given by (25) and (26).
Proof. For any $s \geq 0$ let $(X_s, V_s) = \psi_s(Q, G)$. Note that since $(\psi_s)_{s \in \mathbb{R}^+}$ is the flow associated with (20), we have by definition that for any $k \in \mathbb{N}$, $(X_k, V_k) = (X_{k\gamma}, V_{k\gamma})$, and for any $t, s \geq 0$ with $s \leq t$,

$$X_t = X_s + \int_s^t V_u \, du, \quad V_t = V_s + \int_s^t b(X_u) \, du.$$ 

Therefore for any $k \in \mathbb{N}$, using (21), we have that

$$X_{k+1} - \bar{X}_{k+1} = X_k + \int_{k\gamma}^{(k+1)\gamma} Y_s \, ds - \bar{X}_k - \gamma^2 \bar{b}_\gamma(\bar{X}_k)/2 - \gamma \bar{Y}_k$$

$$= X_k - \bar{X}_k + \int_{k\gamma}^{(k+1)\gamma} (b(X_u) - \bar{b}_\gamma(\bar{X}_k)) \, du + \gamma (Y_k - \bar{Y}_k), \quad (61)$$

$$Y_{k+1} - \bar{Y}_{k+1} = Y_k - \bar{Y}_k + \int_{k\gamma}^{(k+1)\gamma} b(X_s) \, ds - \gamma (\bar{b}_\gamma(\bar{X}_{k+1}) + \bar{b}_\gamma(\bar{X}_k))/2. \quad (62)$$

In addition, since $(X_0, Y_0)$ has distribution $\pi \otimes \mu_{0,1d}$, then by H1, for any $s \geq 0$ and $k \in \mathbb{N}$, $(X_s, V_s)$ and $(X_k, Y_k)$ have distribution $\pi \otimes \mu_{0,1d}$. We first establish (59). By (61), the Minkowski inequality, H2 and since $\bar{X}_k = \Phi_{\bar{h}}(Q, Z)$, we have that

$$\mathbb{E}^{1/2} \left[ \left| X_{k+1} - \bar{X}_{k+1} \right|^2 \right] \leq \mathbb{E}^{1/2} \left[ \left| X_k - \bar{X}_k \right|^2 \right] + \gamma \mathbb{E}^{1/2} \left[ \left| Y_k - \bar{Y}_k \right|^2 \right]$$

$$+ \left( \gamma^2/2 \right) \mathbb{E}^{1/2} \left[ \left| \bar{b}_\gamma(\bar{X}_k) - b(\bar{X}_k) \right|^2 \right] + \mathbb{E}^{1/2} \left[ \left| \int_{k\gamma}^{(k+1)\gamma} \{b(X_u) - \bar{b}_\gamma(\bar{X}_k)\} \, du \right|^2 \right] \quad (63)$$

Now using the Minkowski and Cauchy-Schwarz inequalities, we obtain that

$$\mathbb{E}^{1/2} \left[ \left| \int_{k\gamma}^{(k+1)\gamma} \{b(X_u) - b(\bar{X}_k)\} \, du \right|^2 \right] \leq \left( \gamma^2/2 \right) \mathbb{E}^{1/2} \left[ \left| b(X_k) - b(\bar{X}_k) \right|^2 \right]$$

$$+ \gamma^{1/2} \mathbb{E}^{1/2} \left[ \int_{k\gamma}^{(k+1)\gamma} (s-k\gamma) \int_{k\gamma}^{s} |b(X_u) - b(X_{k\gamma})|^2 \, du \, ds \right]$$

$$\leq \left( \gamma^2/2 \right) \mathbb{E}^{1/2} \left[ \left| b(X_k) - b(\bar{X}_k) \right|^2 \right]$$

$$+ \gamma^{1/2} \mathbb{E}^{1/2} \left[ \int_{k\gamma}^{(k+1)\gamma} (s-k\gamma) \int_{k\gamma}^{s} (u-k\gamma) \int_{k\gamma}^{u} \mathcal{L}^{\mathbf{H}} b(X_v, Y_v) \, dv \, du \right],$$

where we used the Cauchy-Schwarz inequality again for the last upper bound. We obtain by H4 and (23) that

$$\mathbb{E}^{1/2} \left[ \left| \int_{k\gamma}^{(k+1)\gamma} \{b(X_u) - b(\bar{X}_k)\} \, du \right|^2 \right]$$

$$\leq \left( \gamma^2 L/2 \right) \mathbb{E}^{1/2} \left[ \left| X_k - \bar{X}_k \right|^2 \right] + \gamma^3 (M_2/12)^{1/2}.$$
Plugging this result in (63) and using H2 and the definition of $M_5$ (26), we obtain (59).

We now turn to showing (60). By (62), the Minkowski and Cauchy-Schwarz inequalities, we have

$$
E^{1/2} \left( |Y_{k+1} - \bar{Y}_{k+1}|^2 \right) = E^{1/2} \left( |Y_k - \bar{Y}_k|^2 \right) + (\gamma/2)A + B ,
$$

where

$$
A = E^{1/2} \left[ (b(X_{k+1}) + b(X_k)) - (\bar{b}_\gamma(X_{k+1}) + \bar{b}_\gamma(X_k)) \right]^2 \, ,
$$

$$
B = E^{1/2} \left[ \int_{k\gamma}^{(k+1)\gamma} b(X_s) ds - \gamma(b(X_{k+1}) + b(X_k)) \right]^2 .
$$

We bound $A$ and $B$ separately. By the Minkowski inequality, H2 and H4, we have

$$
A \leq E^{1/2} \left[ (b(\bar{X}_{k+1}) + b(\bar{X}_k)) - (\bar{b}_\gamma(\bar{X}_{k+1}) + \bar{b}_\gamma(\bar{X}_k)) \right]^2 + E^{1/2} \left[ (b(X_{k+1}) + b(X_k)) - (b(\bar{X}_{k+1}) + b(\bar{X}_k)) \right]^2 \\
\leq 2\gamma^2 M_5^{1/2} + L \left\{ E^{1/2} \left( |X_{k+1} - \bar{X}_{k+1}|^2 \right) + E^{1/2} \left( |X_k - \bar{X}_k|^2 \right) \right\} .
$$

Then using (59), we get that

$$
A \leq 2\gamma^2 M_5^{1/2} + L \left\{ \gamma E^{1/2} \left( |Y_k - \bar{Y}_k|^2 \right) + (2 + \gamma^2 L/2) E^{1/2} \left( |X_k - \bar{X}_k|^2 \right) \right\} + L \left\{ \gamma^3 M_5^{1/2} + \gamma^3 (M_2/12)^{1/2} \right\} .
$$

Using (22), Lemma 29 and the Cauchy-Schwarz inequality, we obtain that

$$
2B = E^{1/2} \left[ \int_{k\gamma}^{(k+1)\gamma} (\mathcal{L}^H)^2 b(X_s, Y_s) \{(s - k\gamma)((k+1)\gamma - s)\} ds \right]^2 \\
\leq \gamma^{1/2} E^{1/2} \left[ \int_{k\gamma}^{(k+1)\gamma} \left| (\mathcal{L}^H)^2 b(X_s, Y_s) \right|^2 \{(s - k\gamma)((k+1)\gamma - s)\}^2 ds \right]^2 \\
= \gamma^3 15^{-1/2} \{M_1 + 2M_4\}^{1/2}
$$

where we used for the last equality that for any $s \geq 0$, $(X_s, V_s)$ has distribution $\pi \otimes \mu_{0,1_d}$ and by (24),

$$
E \left[ \left( (\mathcal{L}^H)^2 b \right)^2 (X_s, V_s) \right] = \int \int \left( (\mathcal{L}^H)^2 b \right)^2 (q, p) \varphi_d(p) dp \pi(dq) = M_1 + 2M_4 .
$$

Combining (65)-(66) in (64) concludes the proof of (60).

\[\square\]
Proof of Proposition 10. Let \( n = T/\gamma \), and let \((X_k, V_k)_{k \geq 0}\) and \((\bar{X}_k, \bar{V}_k)_{k \geq 0}\) be defined as in Lemma 30. Then by definition of the transition kernels, \( X_n \) and \( \bar{X}_n \) have law \( \pi_{K_T} \) and \( \pi_{K_{T,\gamma}} \), respectively, and thus

\[
W_2 (\pi_{K_T}, \pi_{K_{T,\gamma}}) \leq \mathbb{E}^{1/2} \left[ |X_n - \bar{X}_n|^2 \right]. \tag{67}
\]

Now consider the sequence in \( \mathbb{R}^2 \) defined by

\[
z_k = \left( \mathbb{E}^{1/2}[|X_k - \bar{X}_k|^2], L^{-1/2}\mathbb{E}^{1/2}[|V_k - \bar{V}_k|^2] \right)^T, \quad k \geq 0. \tag{68}
\]

By Lemma 30, for any \( k \geq 0 \), we have

\[
z_{k+1} \leq A z_k + \frac{1}{12} \gamma^3 \tilde{M}, \tag{69}
\]

where \( \leq_2 \) is the partial order on \( \mathbb{R}^2 \) defined by \((u, v)^T \leq_2 (\bar{u}, \bar{v})^T\) if and only if \( u \leq \bar{u} \) and \( v \leq \bar{v} \),

\[
A = \begin{pmatrix}
1 + \gamma^2 L/2 & \gamma L^{1/2} + \gamma^3 L^{3/2}/4 \\
\gamma L^{1/2} + \gamma^3 L^{3/2}/4 & 1 + \gamma^2 L/2
\end{pmatrix},
\]

\[
\tilde{M} = \begin{pmatrix}
(M_2/12)^{1/2} + M_5^{1/2}/2 \\
2 + \frac{\gamma L}{2} & M_5^{1/2} + \frac{\gamma^2 M_2^{1/2}}{2\sqrt{2}} + \frac{M_3 M_6^{1/2}}{15^{1/2}}
\end{pmatrix}. \tag{70}
\]

Since \( A \) has positive entries, application of \( A \) preserves the partial order on \( \mathbb{R}^2 \). Noting that \( z_0 = 0 \), a straightforward induction based on (69) shows that for any integer \( k \geq 0 \),

\[
z_k \leq 2 \gamma^3 \sum_{i=0}^{k-1} A^i \tilde{M}. \tag{71}
\]

Since \( A \) is symmetric with maximal eigenvalue

\[
\lambda_A = 1 + \gamma L^{1/2} + \gamma^2 L/2 + \gamma^3 L^{3/2}/4, \tag{72}
\]

by (71)-(68) and the triangle inequality, we have

\[
\mathbb{E}^{1/2} \left[ |X_n - \bar{X}_n|^2 \right] \leq |z_n| \leq \frac{1}{12} \gamma^3 \sum_{k=0}^{n-1} \lambda_A^k |\tilde{M}| = \gamma^3 \frac{\lambda_A^n - 1}{\lambda_A - 1} |\tilde{M}|.
\]

The assertion follows from this bound and (67), because by (72), \( \lambda - 1 \geq \gamma L^{1/2} \) and \( \lambda^n \leq \exp (n \gamma \lambda_H) \), and by (70), \( |\tilde{M}|^2 \leq L^{-1} M_H^2 \). \( \square \)
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