High-dimensional Bayesian inference via the Unadjusted Langevin Algorithm

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Abstract

We consider in this paper the problem of sampling a high-dimensional probability distribution $\pi$ having a density w.r.t. the Lebesgue measure on $\mathbb{R}^d$, known up to a normalization factor $x \mapsto \pi(x) = e^{-U(x)} / \int_{\mathbb{R}^d} e^{-U(y)} \, dy$. Such problem naturally occurs for example in Bayesian inference and machine learning. Under the assumption that $U$ is continuously differentiable, $\nabla U$ is globally Lipschitz and $U$ is strongly convex, we obtain non-asymptotic bounds for the convergence to stationarity in Wasserstein distance of order 2 and total variation distance of the sampling method based on the Euler discretization of the Langevin stochastic differential equation, for both constant and decreasing step sizes. The dependence on the dimension of the state space of the obtained bounds is studied to demonstrate the applicability of this method. The convergence of an appropriately weighted empirical measure is also investigated and bounds for the mean square error and exponential deviation inequality are reported for functions which are measurable and bounded. An illustration to Bayesian inference for binary regression is presented.

1 Introduction

There has been recently an increasing interest in Bayesian inference applied to high-dimensional models often motivated by machine learning applications. Rather than

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obtaining a point estimate, Bayesian methods attempt to sample the full posterior distribution over the parameters and possibly latent variables which provides a way to assert uncertainty in the model and prevents from overfitting [28], [37].

The problem can be formulated as follows. We aim at sampling a posterior distribution $\pi$ on $\mathbb{R}^d$, $d \geq 1$, with density $x \mapsto e^{-U(x)} / \int_{\mathbb{R}^d} e^{-U(y)} dy$ w.r.t. the Lebesgue measure, where $U$ is continuously differentiable. The Langevin stochastic differential equation associated with $\pi$ is defined by:

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

where $(B_t)_{t \geq 0}$ is a $d$-dimensional Brownian motion defined on the filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0}, \mathbb{P})$, satisfying the usual conditions. Under mild technical conditions, the Langevin diffusion admits $\pi$ as its unique invariant distribution.

We study the sampling method based on the Euler-Maruyama discretization of (1). This scheme defines the (possibly) non-homogeneous, discrete-time Markov chain $(X_k)_{k \geq 0}$ given by

$$X_{k+1} = X_k - \gamma_{k+1} \nabla U(X_k) + \sqrt{2\gamma_{k+1}} Z_{k+1} ,$$

where $(Z_k)_{k \geq 1}$ is an i.i.d. sequence of $d$-dimensional standard Gaussian random variables and $(\gamma_k)_{k \geq 1}$ is a sequence of step sizes, which can either be held constant or be chosen to decrease to 0. This algorithm has been first proposed by [14] and [30] for molecular dynamics applications. Then it has been popularized in machine learning by [17], [18] and computational statistics by [28] and [32]. Following [32], in the sequel this method will be refer to as the unadjusted Langevin algorithm (ULA). When the step sizes are held constant, under appropriate conditions on $U$, the homogeneous Markov chain $(X_k)_{k \geq 0}$ has a unique stationary distribution $\pi_{\gamma}$, which in most of the cases differs from the distribution $\pi$. It has been proposed in [33] and [32] to use a Metropolis-Hastings step at each iteration to enforce reversibility w.r.t. $\pi$. This algorithm is referred to as the Metropolis adjusted Langevin algorithm (MALA).

The ULA algorithm has already been studied in depth for constant step sizes in [35], [32] and [27]. In particular, [35, Theorem 4] gives an asymptotic expansion for the weak error between $\pi$ and $\pi_{\gamma}$. For sequence of step sizes such that $\lim_{k \to +\infty} \gamma_k = 0$ and $\sum_{k=1}^{\infty} \gamma_k = \infty$, weak convergence of the weighted empirical distribution of the ULA algorithm has been established in [23], [24] and [25].

Contrary to these previously reported works, we focus in this paper on non-asymptotic results. More precisely, we obtain explicit bounds between the distribution of the $n$-th iterate of the Markov chain defined in (2) and the target distribution $\pi$ in Wasserstein and total variation distance for nonincreasing step sizes. When the sequence of step sizes is held constant $\gamma_k = \gamma$ for all $k \geq 0$, both fixed horizon (the total computational budget is fixed and the step size is chosen to minimize the upper bound on the Wasserstein or total variation distance) and fixed precision (for a fixed target precision, the number of iterations and the step size are optimized simultaneously to meet this constraint) strategies are studied. In addition, quantitative estimates between $\pi$ and $\pi_{\gamma}$ are obtained. When $\lim_{k \to +\infty} \gamma_k = 0$ and $\sum_{k=1}^{\infty} \gamma_k = \infty$, we show that the marginal distribution of
the non-homogeneous Markov chain \((X_k)_{k\geq0}\) converges to the target distribution \(\pi\) and provide explicit convergence bounds. A special attention is paid to the dependency of the proposed upper bounds on the dimension of the state space, since we are particularly interested in the application of these methods to sampling in high-dimension.

Compared to [10] and [11], our contribution is twofold. First, we report sharper convergence bounds for constant and non-increasing step sizes. In particular, it is shown that the number of iterations required to reach the target distribution \(\pi\) with a precision \(\epsilon > 0\) in total variation is upper bounded (up to logarithmic factors) by \((\epsilon d)^{-1}\), where \(d\) is the dimension, under appropriate regularity assumption (in [11], the upper bound was shown to be \(d^{-1}\epsilon^{-2}\)). We show that our result is optimal (up to logarithmic factors again) in the case of the standard \(d\)-dimensional Gaussian distribution, for which explicit computation can be done. Besides, we establish computable bound for the mean square error associated with ULA for measurable bounded functions, which is an important result in Bayesian statistics to estimate credibility regions. For that purpose, we study the convergence of the Euler-Maruyama discretization towards its stationary distribution in total variation using a discrete time version of reflection coupling introduced in [4].

The paper is organized as follows. In Section 2, we study the convergence in the Wasserstein distance of order 2 of the Euler discretization for constant and decreasing step sizes. In Section 3, we give non asymptotic bounds in total variation distance between the Euler discretization and \(\pi\). This study is completed in Section 4 by non-asymptotic bounds of convergence of the weighted empirical measure applied to bounded and measurable functions. Our claims are supported in a Bayesian inference for a binary regression model in Section 5. The proofs are given in Section 6. Finally in Section 8, some results of independent interest, used in the proofs, on functional autoregressive models are gathered. Some technical proofs and derivations are postponed and carried out in a supplementary paper [12].

Notations and conventions

Denote by \(B(\mathbb{R}^d)\) the Borel \(\sigma\)-field of \(\mathbb{R}^d\), \(\mathcal{F}(\mathbb{R}^d)\) the set of all Borel measurable functions on \(\mathbb{R}^d\) and for \(f \in \mathcal{F}(\mathbb{R}^d)\), \(\|f\|_{\infty} = \sup_{x \in \mathbb{R}^d} |f(x)|\). For \(\mu\) a probability measure on \((\mathbb{R}^d, B(\mathbb{R}^d))\) and \(f \in \mathcal{F}(\mathbb{R}^d)\) a \(\mu\)-integrable function, denote by \(\mu(f)\) the integral of \(f\) w.r.t. \(\mu\). We say that \(\zeta\) is a transference plan of \(\mu\) and \(\nu\) if it is a probability measure on \((\mathbb{R}^d \times \mathbb{R}^d, B(\mathbb{R}^d \times \mathbb{R}^d))\) such that for all measurable set \(A\) of \(\mathbb{R}^d\), \(\zeta(A \times \mathbb{R}^d) = \mu(A)\) and \(\zeta(\mathbb{R}^d \times A) = \nu(A)\). We denote by \(\Pi(\mu, \nu)\) the set of transference plans of \(\mu\) and \(\nu\). Furthermore, we say that a couple of \(\mathbb{R}^d\)-random variables \((X, Y)\) is a coupling of \(\mu\) and \(\nu\) if there exists \(\zeta \in \Pi(\mu, \nu)\) such that \((X, Y)\) are distributed according to \(\zeta\). For two probability measures \(\mu\) and \(\nu\), we define the Wasserstein distance of order \(p \geq 1\) as

\[
W_p(\mu, \nu) \overset{\text{def}}{=} \left(\inf_{\zeta \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^p \, d\zeta(x, y)\right)^{1/p}.
\]

By [36, Theorem 4.1], for all \(\mu, \nu\) probability measures on \(\mathbb{R}^d\), there exists a transference plan \(\zeta^* \in \Pi(\mu, \nu)\) such that for any coupling \((X, Y)\) distributed according to \(\zeta^*\),
The function $H_1$. Consider the following assumption on the potential $U$.

**H1.** The function $U$ is continuously differentiable on $\mathbb{R}^d$ and gradient Lipschitz: there exists $L \geq 0$ such that for all $x, y \in \mathbb{R}^d$, $\|\nabla U(x) - \nabla U(y)\| \leq L\|x - y\|$. 

2 Non-asymptotic bounds in Wasserstein distance of order 2 for ULA

Consider the following assumption on the potential $U$:

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a Lipschitz function, namely there exists $C \geq 0$ such that for all $x, y \in \mathbb{R}^d$, $|f(x) - f(y)| \leq C\|x - y\|$. Then we denote

$$\|f\|_{\text{Lip}} = \inf\{|f(x) - f(y)| \|x - y\|^{-1} | x, y \in \mathbb{R}^d, x \neq y\}.$$ 

The Monge-Kantorovich theorem (see [36, Theorem 5.9]) implies that for all $\mu, \nu$ probability measures on $\mathbb{R}^d$,

$$W_1(\mu, \nu) = \sup \left\{ \int_{\mathbb{R}^d} f(x)d\mu(x) - \int_{\mathbb{R}^d} f(x)d\nu(x) | f: \mathbb{R}^d \to \mathbb{R} ; \|f\|_{\text{Lip}} \leq 1 \right\}.$$ 

Denote by $\mathcal{F}_b(\mathbb{R}^d)$ the set of all bounded Borel measurable functions on $\mathbb{R}^d$. For $f \in \mathcal{F}_b(\mathbb{R}^d)$ set $\text{osc}(f) = \sup_{x,y \in \mathbb{R}^d} |f(x) - f(y)|$. For two probability measures $\mu$ and $\nu$ on $\mathbb{R}^d$, the total variation distance between $\mu$ and $\nu$ is defined by $\|\mu - \nu\|_{\text{TV}} = \sup_{A \in \mathcal{B}(\mathbb{R}^d)} |\mu(A) - \nu(A)|$. By the Monge-Kantorovich theorem the total variation distance between $\mu$ and $\nu$ can be written on the form:

$$\|\mu - \nu\|_{\text{TV}} = \inf_{\zeta \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} 1_{D_\zeta}(x,y)d\zeta(x,y),$$

where $D = \{(x,y) \in \mathbb{R}^d \times \mathbb{R}^d | x = y\}$. For all $x \in \mathbb{R}^d$ and $M > 0$, we denote by $B(x, M)$, the ball centered at $x$ of radius $M$. For a subset $A \subset \mathbb{R}^d$, denote by $A^c$ the complementary of $A$. Let $n \in \mathbb{N}^*$ and $M$ be an $n \times n$-matrix, then denote by $M^T$ the transpose of $M$ and $\|M\|$ the operator norm associated with $M$ defined by $\|M\| = \sup_{\|x\| = 1} \|Mx\|$. Define the Frobenius norm associated with $M$ by $\|M\|_F^2 = \text{Tr}(M^TM)$. Let $n, m \in \mathbb{N}^*$ and $F : \mathbb{R}^n \to \mathbb{R}^m$ be a twice continuously differentiable function. Denote by $\nabla F$ and $\nabla^2 F$ the Jacobian and the Hessian of $F$ respectively. Denote also by $\Delta F$ the vector Laplacian of $F$ defined by: for all $x \in \mathbb{R}^d$, $\Delta F(x)$ is the vector of $\mathbb{R}^m$ such that for all $i \in \{1, \cdots, m\}$, the $i$-th component of $\Delta F(x)$ is equals to $\sum_{j=1}^d (\partial^2 F_i/\partial x_j^2)(x)$. In the sequel, we take the convention that $\sum_{i}^n = 0$ and $\prod_{i}^n = 1$ for $n, p \in \mathbb{N}, n < p$. 

2 Non-asymptotic bounds in Wasserstein distance of order 2 for ULA

Consider the following assumption on the potential $U$:
Under \( \textbf{H1} \), for all \( x \in \mathbb{R}^d \) by [21, Theorem 2.5, Theorem 2.9 Chapter 5] there exists a unique strong solution \((Y_t)_{t \geq 0}\) to (1) with \( Y_0 = x \). Denote by \((P_t)_{t \geq 0}\) the semi-group associated with (1). It is well-known that \( \pi \) is its (unique) invariant probability. To get geometric convergence of \((P_t)_{t \geq 0}\) to \( \pi \) in Wasserstein distance of order 2, we make the following additional assumption on the potential \( U \).

\( \textbf{H2}. \ U \) is strongly convex, i.e. there exists \( m > 0 \) such that for all \( x, y \in \mathbb{R}^d \),

\[
U(y) \geq U(x) + \langle \nabla U(x), y - x \rangle + (m/2) \|x - y\|^2 .
\]

Under \( \textbf{H2} \), [29, Theorem 2.1.8] shows that \( U \) has a unique minimizer \( x^* \in \mathbb{R}^d \). If in addition \( \textbf{H1} \) holds, then [29, Theorem 2.1.12, Theorem 2.1.9] show that for all \( x, y \in \mathbb{R}^d \):

\[
\langle \nabla U(y) - \nabla U(x), y - x \rangle \geq \kappa \|y - x\|^2 + \frac{1}{m + L} \|\nabla U(y) - \nabla U(x)\|^2 ,
\]

where

\[
\kappa = \frac{2mL}{m + L} .
\]

We briefly summarize some background material on the stability and the convergence in \( W_2 \) of the overdamped Langevin diffusion under \( \textbf{H1} \) and \( \textbf{H2} \). Most of the statements in Proposition 1 are known and are recalled here for ease of references; see e.g. [6].

**Proposition 1.** Assume \( \textbf{H1} \) and \( \textbf{H2} \).

(i) For all \( t \geq 0 \) and \( x \in \mathbb{R}^d \),

\[
\int_{\mathbb{R}^d} \|y - x^*\|^2 P_t(x, dy) \leq \|x - x^*\|^2 e^{-2mt} + (d/m)(1 - e^{-2mt}) .
\]

(ii) The stationary distribution \( \pi \) satisfies \( \int_{\mathbb{R}^d} \|x - x^*\|^2 \pi(dx) \leq d/m \).

(iii) For any \( x, y \in \mathbb{R}^d \) and \( t > 0 \), \( W_2(\delta_x P_t, \delta_y P_t) \leq e^{-mt} \|x - y\| \).

(iv) For any \( x \in \mathbb{R}^d \) and \( t > 0 \), \( W_2(\delta_x P_t, \pi) \leq e^{-mt} \left\{ \|x - x^*\| + (d/m)^{1/2} \right\} \).

**Proof.** The proof is given in the supplementary document [12, Section 1.1]. \( \square \)

Note that the convergence rate in Proposition 1-(iv) is independent from the dimension. Let \((\gamma_k)_{k \geq 1}\) be a sequence of positive and non-increasing step sizes and for \( n, \ell \in \mathbb{N} \), denote by

\[
\Gamma_{n, \ell} \overset{\text{def}}{=} \sum_{k=n}^\ell \gamma_k , \quad \Gamma_n = \Gamma_{1, n} .
\]

For \( \gamma > 0 \), consider the Markov kernel \( R_\gamma \) given for all \( A \in \mathcal{B}(\mathbb{R}^d) \) and \( x \in \mathbb{R}^d \) by

\[
R_\gamma(x, A) = \int_A (4\pi \gamma)^{-d/2} \exp\left(-\frac{1}{4\gamma} \|y - x + \gamma \nabla U(x)\|^2\right) dy .
\]
The process \((X_k)_{k \geq 0}\) given in (2) is an inhomogeneous Markov chain with respect to the family of Markov kernels \((R_{\gamma_k})_{k \geq 1}\). For \(\ell, n \in \mathbb{N}^*, \ell \geq n\), define
\[
Q_{\gamma}^{n, \ell} = R_{\gamma_n} \cdots R_{\gamma_\ell}, \quad Q_{\gamma}^{n} = Q_{\gamma}^{1,n}
\] (7)
with the convention that for \(n, \ell \in \mathbb{N}, n < \ell\), \(Q_{\gamma}^{\ell,n}\) is the identity operator.

We first derive a Foster-Lyapunov drift condition for \(Q_{\gamma}^{n, \ell}\), \(\ell, n \in \mathbb{N}^*, \ell \geq n\).

**Proposition 2. Assume \(H1\) and \(H2\).**

(i) Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \(\gamma_1 \leq 2/(m + L)\). Let \(x^*\) be the unique minimizer of \(U\). Then for all \(x \in \mathbb{R}^d\) and \(n, \ell \in \mathbb{N}^*\),
\[
\int_{\mathbb{R}^d} \|y - x^*\|^2 Q_{\gamma}^{n, \ell}(x, dy) \leq \varrho_{n, \ell}(x),
\]
where \(\varrho_{n, \ell}(x)\) is given by
\[
\varrho_{n, \ell}(x) = \prod_{k=n}^\ell (1 - \kappa \gamma_k) \|x - x^*\|^2 + 2d\kappa^{-1}\left\{1 - \kappa^{-1} \prod_{i=n}^\ell (1 - \kappa \gamma_i)\right\}, \tag{8}
\]
and \(\kappa\) is defined in (4).

(ii) For any \(\gamma \in (0, 2/(m + L)]\), \(R_{\gamma}\) has a unique stationary distribution \(\pi_{\gamma}\) and
\[
\int_{\mathbb{R}^d} \|x - x^*\|^2 \pi_{\gamma}(dx) \leq 2d\kappa^{-1}.
\]

**Proof.** The proof is postponed to [12, Section 1.2]. □

We now proceed to establish the contraction property of the sequence \((Q_{\gamma}^{n})_{n \geq 1}\) in \(W_2\). This result implies the geometric convergence of the sequence \((\delta_x R_{\gamma}^{n})_{n \geq 1}\) to \(\pi_{\gamma}\) in \(W_2\) for all \(x \in \mathbb{R}^d\). Note that the convergence rate is again independent of the dimension.

**Proposition 3. Assume \(H1\) and \(H2\). Then,**

(i) Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \(\gamma_1 \leq 2/(m + L)\). For all \(x, y \in \mathbb{R}^d\) and \(\ell \geq n \geq 1\),
\[
W_2(\delta_x Q_{\gamma}^{n, \ell}, \delta_y Q_{\gamma}^{n, \ell}) \leq \left\{\prod_{k=n}^\ell (1 - \kappa \gamma_k) \|x - y\|^2\right\}^{1/2}.
\]

(ii) For any \(\gamma \in (0, 2/(m + L)]\), for all \(x \in \mathbb{R}^d\) and \(n \geq 1\),
\[
W_2(\delta_x R_{\gamma}^{n}, \pi_{\gamma}) \leq (1 - \kappa \gamma)^n/2 \left\{\|x - x^*\|^2 + 2\kappa^{-1}d\right\}^{1/2}.
\]
Proof. The proof is postponed to [12, Section 1.3].

Corollary 4. Assume H1 and H2. Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \(\gamma_1 \leq 2/(m + L)\). Then for all Lipschitz functions \(f : \mathbb{R}^d \rightarrow \mathbb{R}\) and \(\ell \geq n \geq 1\), \(Q^n_{\gamma_1} f\) is a Lipschitz function with \(\|Q^n_{\gamma_1} f\|_{\text{Lip}} \leq \prod_{k=n}^{\ell} (1 - \kappa \gamma_k)^{1/2} \|f\|_{\text{Lip}}\).

Proof. The proof follows from Proposition 3-(i) using

\[
\left| Q^n_{\gamma_1} f(y) - Q^n_{\gamma_1} f(z) \right| \leq \|f\|_{\text{Lip}} W_2(\delta_y Q^n_{\gamma_1}, \delta_z Q^n_{\gamma_1}) .
\]

\(\square\)

We now proceed to establish explicit bounds for \(W_2(\delta_k Q^n_{\gamma_1}, \pi)\), with \(x \in \mathbb{R}^d\). Since \(\pi\) is invariant for \(P_t\) for all \(t \geq 0\), it suffices to get some bounds on \(W_2(\delta_k Q^n_{\gamma_1}, \nu_0 P_{\Delta t})\), with \(\nu_0 \in \mathcal{P}_2(\mathbb{R}^d)\) and take \(\nu_0 = \pi\). To do so, we construct a coupling between the diffusion and the linear interpolation of the Euler discretization. An obvious candidate is the synchronous coupling \((Y_t, \overline{Y}_t)_{t \geq 0}\) defined for all \(n \geq 0\) and \(t \in [\Gamma_n, \Gamma_{n+1}]\) by

\[
\begin{align*}
Y_t &= Y_{\Gamma_n} - \int_{\Gamma_n}^t \nabla U(Y_s) ds + \sqrt{2}(B_t - B_{\Gamma_n}) \\
\overline{Y}_t &= \overline{Y}_{\Gamma_n} - \nabla U(\overline{Y}_{\Gamma_n})(t - \Gamma_n) + \sqrt{2}(B_t - B_{\Gamma_n}) ,
\end{align*}
\]

with \(Y_0\) is distributed according to \(\nu_0\), \(\overline{Y}_0 = x\) and \((\Gamma_n)_{n \geq 1}\) is given in (5). Therefore since for all \(n \geq 0\), \(W_2^2(\delta_k Q^n_{\gamma_1}, \nu_0 P_{\Delta t}) \leq \mathbb{E}[||Y_{\Gamma_n} - \overline{Y}_{\Gamma_n}||^2]\), taking \(\nu_0 = \pi\), we derive an explicit bound on the Wasserstein distance between the sequence of distributions \((\delta_k Q^n_{\gamma_1})_{k \geq 0}\) and the stationary measure \(\pi\) of the Langevin diffusion (1).

Theorem 5. Assume H1 and H2. Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \(\gamma_1 \leq 1/(m + L)\). Then for all \(x \in \mathbb{R}^d\) and \(n \geq 1\),

\[
W_2^2(\delta_k Q^n_{\gamma_1}, \pi) \leq u_n^{(1)}(\gamma) \left\{ \|x - x^*\|^2 + d/m \right\} + u_n^{(2)}(\gamma) ,
\]

where

\[
u_n^{(1)}(\gamma) = 2 \sum_{k=1}^{n} (1 - \kappa \gamma_k/2)
\]

\(\kappa\) is defined in (4) and

\[
u_n^{(2)}(\gamma) = L^2 \sum_{i=1}^{n} \left[ \gamma_k^2 \left\{ \kappa^{-1} + \gamma_i \right\} \left\{ 2d + \frac{dL^2 \gamma_i}{m} + \frac{dL^2 \gamma_i^2}{6} \right\} \prod_{k=i+1}^{n} (1 - \kappa \gamma_k/2) \right] .
\]

Proof. Let \(x \in \mathbb{R}^d\), \(n \geq 1\) and \(\zeta_0 = \pi \otimes \delta_x\). Let \((Y_t, \overline{Y}_t)_{t \geq 0}\) with \((Y_0, \overline{Y}_0)\) distributed according to \(\zeta_0\) and defined by (9). By definition of \(W_2\) and since for all \(t \geq 0\), \(\pi\) is invariant for \(P_t\), \(W_2^2(\mu_0 Q^n, \pi) \leq \mathbb{E}_{\zeta_0}[||Y_{\Gamma_n} - \overline{Y}_{\Gamma_n}||^2]\). Lemma 20 with \(\epsilon = \kappa/4\), Proposition 1-(ii) imply, using a straightforward induction, that for all \(n \geq 0\)

\[
\mathbb{E}_{\zeta_0}[||Y_{\Gamma_n} - \overline{Y}_{\Gamma_n}||^2] \leq \nu_n^{(1)}(\gamma) \int_{\mathbb{R}^d} ||y - x||^2 \pi(dy) + A_n(\gamma) ,
\]

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where \((u^{(1)}_n(\gamma))_{n \geq 1}\) is given by (10), and

\[
A_n(\gamma) \overset{\text{def}}{=} L^2 \sum_{i=1}^{n} \gamma_i^2 \{\kappa^{-1} + \gamma_i\} \left(2d + dL^2 \gamma_i^2 / 6\right) \prod_{k=i+1}^{n} (1 - \kappa \gamma_k / 2) \\
+ L^4 \sum_{i=1}^{n} \delta_i \gamma_i^3 \{\kappa^{-1} + \gamma_i\} \prod_{k=i+1}^{n} (1 - \kappa \gamma_k / 2) \tag{13}
\]

with

\[
\delta_i = e^{-2m\Gamma_{i-1}} \mathbb{E}_{\tilde{\omega}} \left[\|Y_0 - x^*\|^2\right] + (1 - e^{-2m\Gamma_{i-1}})(d/m) \leq d/m .
\]

Since \(Y_0\) is distributed according to \(\pi\), Proposition 1-(ii) shows that for all \(i \in \{1, \ldots , n\}\),

\[
\delta_i \leq d/m . \tag{14}
\]

In addition since for all \(y \in \mathbb{R}^d, \|x - y\|^2 \leq 2(\|x - x^*\|^2 + \|x^* - y\|^2)\), using Proposition 1-(ii), we get \(\int_{\mathbb{R}^d} \|y - x\|^2 \pi(dy) \leq \|x - x^*\|^2 + d/m\). Plugging this result, (14) and (13) in (12) completes the proof. \(\square\)

**Corollary 6.** Assume \(H 1\) and \(H 2\). Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \(\gamma_1 \leq 1/(m + L)\). Assume that \(\lim_{k \to \infty} \gamma_k = 0\) and \(\lim_{n \to +\infty} \Gamma_n = +\infty\). Then for all \(x \in \mathbb{R}^d\), \(\lim_{n \to +\infty} W_2(\delta_{\tilde{\omega}} Q^n_{\gamma}, \pi) = 0\).

We preface the proof by a technical lemma which is established in the supplementary document Section 2.1.

**Lemma 7.** Let \((\gamma_k)_{k \geq 1}\) be a sequence of nonincreasing real numbers, \(\varpi > 0\) and \(\gamma_1 < \varpi^{-1}\). Then for all \(n \geq 0\), \(j \geq 1\) and \(\ell \in \{1, \ldots , n + 1\}\),

\[
\sum_{i=1}^{n+1} \prod_{k=i+1}^{n} (1 - \varpi \gamma_k) \gamma_i^{\ell} \leq \prod_{k=\ell}^{n+1} (1 - \varpi \gamma_k) \sum_{i=1}^{\ell-1} \gamma_i^{\ell-1-j} + \frac{\gamma_{\ell}^{j-1}}{\varpi} .
\]

**Proof of Corollary 6.** By Theorem 5, it suffices to show that \(u^{(1)}_n(\gamma)\) and \(u^{(2)}_n(\gamma)\), defined by (10) and (11) respectively, goes to 0 as \(n \to +\infty\). Using the bound \(1 + t \leq e^t\) for \(t \in \mathbb{R}\), and \(\lim_{n \to +\infty} \Gamma_n = +\infty\), we have \(\lim_{n \to +\infty} u^{(1)}_n(\gamma) = 0\). Since \((\gamma_k)_{k \geq 0}\) is nonincreasing, note that to show that \(\lim_{n \to +\infty} u^{(2)}_n(\gamma) = 0\), it suffices to prove \(\lim_{n \to +\infty} \sum_{i=1}^{n} \prod_{k=i+1}^{n} (1 - \kappa \gamma_k / 2) \gamma_i^2 = 0\). But since \((\gamma_k)_{k \geq 1}\) is nonincreasing, there exists \(c \geq 0\) such that \(c \Gamma_n \leq n - 1\) and by Lemma 7 applied with \(\ell = \lfloor c \Gamma_n \rfloor\) the integer part of \(c \Gamma_n\),

\[
\sum_{i=1}^{n} \prod_{k=i+1}^{n} (1 - \kappa \gamma_k / 2) \gamma_i^2 \leq 2\kappa^{-1} \gamma_{\lfloor c \Gamma_n \rfloor} + \exp \left(-2^{-1}\kappa(\Gamma_n - \Gamma_{\lfloor c \Gamma_n \rfloor})\right) \sum_{i=1}^{\lfloor c \Gamma_n \rfloor-1} \gamma_i . \tag{15}
\]

Since \(\lim_{k \to +\infty} \gamma_k = 0\), by the Cesáro theorem, \(\lim_{n \to +\infty} n^{-1} \Gamma_n = 0\). Therefore since \(\lim_{n \to +\infty} \Gamma_n = +\infty\), \(\lim_{n \to +\infty} (\Gamma_n)^{-1} \Gamma_{\lfloor c \Gamma_n \rfloor} = 0\), and the conclusion follows from combining in (15), this limit, \(\lim_{k \to +\infty} \gamma_k = 0\), \(\lim_{n \to +\infty} \Gamma_n = +\infty\) and \(\sum_{i=1}^{\lfloor c \Gamma_n \rfloor-1} \gamma_i \leq c \gamma_1 \Gamma_n\). \(\square\)
In the case of constant step sizes \( \gamma_k = \gamma \) for all \( k \geq 1 \), we can deduce from Theorem 5, a bound between \( \pi \) and the stationary distribution \( \pi_\gamma \) of \( R_\gamma \).

**Corollary 8.** Assume \( H1 \) and \( H2 \). Let \((\gamma_k)_{k \geq 1}\) be a constant sequence \( \gamma_k = \gamma \) for all \( k \geq 1 \) with \( \gamma \leq 1/(m + L) \). Then

\[
W_2^2(\pi, \pi_\gamma) \leq 2\kappa^{-1}L^2\gamma \left\{ \kappa^{-1} + \gamma \right\} \left( 2d + dL^2\gamma/m + dL^2\gamma^2/6 \right).
\]

**Proof.** Since by Proposition 3, for all \( x, y \in \mathbb{R}^d \), \((\delta_x \gamma^n)_{n \geq 0}\) converges to \( \pi_\gamma \) as \( n \to \infty \) in \((\mathcal{P}_2(\mathbb{R}^d), W_2)\), the proof then follows from Theorem 5 and Lemma 7 applied with \( \ell = 1 \).

We can improve the bound provided by Theorem 5 under additional regularity assumptions on the potential \( U \).

**H3.** The potential \( U \) is three times continuously differentiable and there exists \( \bar{L} \) such that for all \( x, y \in \mathbb{R}^d \), \( \| \nabla^2 U(x) - \nabla^2 U(y) \| \leq \bar{L} \| x - y \| \).

Note that under \( H1 \) and \( H3 \), we have that for all \( x, y \in \mathbb{R}^d \),

\[
\left\| \nabla^2 U(x) y \right\| \leq \bar{L} \| y \| , \left\| \Delta(\nabla U)(x) \right\| ^2 \leq d^2 \bar{L}^2 .
\]

**Theorem 9.** Assume \( H1, H2 \) and \( H3 \). Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \( \gamma_1 \leq 1/(m + L) \). Then for all \( x \in \mathbb{R}^d \) and \( n \geq 1 \),

\[
W_2^2(\delta_x Q^n, \pi) \leq u_n^{(1)}(\gamma) \left\{ \| x - x^* \|^2 + d/m \right\} + u_n^{(3)}(\gamma) ,
\]

where \( u_n^{(1)} \) is given by (10), \( \kappa \) in (4) and

\[
u_n^{(3)}(\gamma) = \sum_{i=1}^n d_i^3 \left\{ 2L^2 + \kappa^{-1} \left( \frac{d\bar{L}^2}{3} + \gamma_i L^4 + \frac{4L^4}{3m} \right) + \gamma_i L^4 \left( \frac{\gamma_i}{6} + m^{-1} \right) \right\} \times \prod_{k=i+1}^n \left( 1 - \frac{\kappa \gamma_k}{2} \right) .
\]

**Proof.** The proof of is along the same lines than Theorem 5, using Lemma 21 in place of Lemma 20.

In the case of constant step sizes \( \gamma_k = \gamma \) for all \( k \geq 1 \), we can deduce from Theorem 9, a sharper bound between \( \pi \) and the stationary distribution \( \pi_\gamma \) of \( R_\gamma \).

**Corollary 10.** Assume \( H1, H2 \) and \( H3 \). Let \((\gamma_k)_{k \geq 1}\) be a constant sequence \( \gamma_k = \gamma \) for all \( k \geq 1 \) with \( \gamma \leq 1/(m + L) \). Then

\[
W_2^2(\pi, \pi_\gamma) \leq 2\kappa^{-1}d\gamma^2 \left\{ 2L^2 + \kappa^{-1} \left( \frac{d\bar{L}^2}{3} + \gamma L^4 + \frac{4L^4}{3m} \right) + \gamma L^4 \left( \gamma/6 + m^{-1} \right) \right\} .
\]
Proof. The proof follows the same line as the proof of Corollary 8 and is omitted. □

Using Proposition 3-(ii) and Corollary 6 or Corollary 10, given \( \varepsilon > 0 \), we determine the smallest number of iterations \( n_\varepsilon \) and an associated step-size \( \gamma_\varepsilon \) satisfying \( W_2(\delta_x, R_{\gamma_\varepsilon}^n, \pi) \leq \varepsilon \) for all \( n \geq n_\varepsilon \). The dependencies on the dimension \( d \) and the precision \( \varepsilon \) of \( n_\varepsilon \) based on Theorem 5 and Theorem 9 are reported in Table 1. Under \( H_1 \) and \( H_2 \), the complexity we get is the same as the one established in [11] for the total variation distance. However if in addition \( H_3 \) holds, we improve this complexity with respect to the precision parameter \( \varepsilon \) as well. Finally, in the case where \( \bar{L} = 0 \) (for example for non-degenerate \( d \)-dimensional Gaussian distributions), then the dependency on the dimension of the number of iterations \( n_\varepsilon \) given by Theorem 9 turns out to be only of order \( O(d^{1/2} \log(d)) \).

Details and further discussions are included in the supplementary paper [12, Sections 6 to 8]. In particular, the dependencies of the obtained bounds with respect to the constants \( m \) and \( L \) which appear in \( H_1, H_2 \) are evidenced.

In a recent work [9] (based on a previous version of this paper), an improvement of the proof of Theorem 5 has been proposed for constant step size. Whereas the constants are sharper, the dependence with respect to the dimension and the precision parameter \( \varepsilon > 0 \) is the same (first line of Table 1).

### Table 1: Dependencies of the number of iterations \( n_\varepsilon \) to get \( W_2(\delta_x, R_{\gamma_\varepsilon}^n, \pi) \leq \varepsilon \)

| Parameter | \( d \) | \( \varepsilon \) |
|-----------|---------|---------|
| Theorem 5 and Proposition 3-(ii) | \( O(d \log(d)) \) | \( O(\varepsilon^{-2} |\log(\varepsilon)|) \) |
| Theorem 9 and Proposition 3-(ii) | \( O(d \log(d)) \) | \( O(\varepsilon^{-1} |\log(\varepsilon)|) \) |

For simplicity, consider sequences \( (\gamma_k)_{k \geq 1} \) defined for all \( k \geq 1 \) by \( \gamma_k = \gamma_1 k^{-\alpha} \), for \( \gamma_1 < 1/(m + L) \) and \( \alpha \in (0, 1] \). Then for \( n \geq 1 \), \( u_n^{(1)} \leq O(e^{-n^{1/2}}), u_n^{(2)} \leq O(n^{-\alpha}) \) and \( u_n^{(3)} \leq d^2 O(n^{-2\alpha}) \) (see [12, Sections 6 to 8] for details). Based on these upper bounds, we can obtained the convergence rates provided by Theorem 5 and Theorem 9 for this particular setting, see Table 2.

### Table 2: Order of convergence of \( W_2^2(\delta_x, Q_\gamma^n, \pi) \) for \( \gamma_k = \gamma_1 k^{-\alpha} \)

| \( \alpha \in (0, 1) \) | \( \alpha = 1 \) |
|----------------|--------------|
| Theorem 5 | \( dO(n^{-\alpha}) \) \( dO(n^{-1}) \) for \( \gamma_1 > 2^{-1} \) see [12, Section 8] |
| Theorem 9 | \( d^2 O(n^{-2\alpha}) \) \( d^2 O(n^{-2}) \) |

### 3 Quantitative bounds in total variation distance

We deal in this section with quantitative bounds in total variation distance. For Bayesian inference application, total variation bounds are of importance for computing highest posterior density (HPD) credible regions and intervals. For computing such bounds we
will use the results of Section 2 combined with the regularizing property of the semigroup \((P_t)_{t \geq 0}\). Under H2, define \(\chi_m\) for all \(t \geq 0\) by

\[
\chi_m(t) = \sqrt{\frac{4}{m}}(e^{2mt} - 1).
\]

The first key result consists in upper-bounding the total variation distance \(\|\mu P_t - \nu P_t\|_{TV}\) for \(\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)\). To that purpose, we use the coupling by reflection; see [26] and [6, Example 3.7]. This coupling is defined as the unique solution \((X_t, Y_t)_{t \geq 0}\) of the SDE:

\[
\begin{cases}
\mathrm{d}X_t &= -\nabla U(X_t)\mathrm{d}t + \sqrt{2}\mathrm{d}B^d_t \\
\mathrm{d}Y_t &= -\nabla U(Y_t)\mathrm{d}t + \sqrt{2}(\mathrm{Id} - 2ee^T_t)\mathrm{d}B^d_t,
\end{cases}
\]

where \(e_t = e(X_t - Y_t)\)

with \(X_0 = x, Y_0 = y, e(z) = z/\|z\|\) for \(z \neq 0\) and \(e(0) = 0\) otherwise. Define the coupling time \(T_c = \inf\{s \geq 0 \mid X_s = Y_s\}\). By construction \(X_t = Y_t\) for \(t \geq T_c\). By Levy’s characterization, \(B^d_t = \int_0^t (\mathrm{Id} - 2ee^T_s)\mathrm{d}B^d_s\) is a \(d\)-dimensional Brownian motion, therefore \((X_t)_{t \geq 0}\) and \((Y_t)_{t \geq 0}\) are weak solutions to (1) started at \(x\) and \(y\) respectively. Then by Lindvall’s inequality, for all \(t > 0\) we have \(\|P_t(x, \cdot) - P_t(y, \cdot)\|_{TV} \leq \mathbb{P}(X_t \neq Y_t)\).

**Theorem 11.** Assume H1 and H2.

(i) For any \(x, y \in \mathbb{R}^d\) and \(t > 0\), it holds

\[
\|P_t(x, \cdot) - P_t(y, \cdot)\|_{TV} \leq 1 - 2\Phi\{\|x - y\|/\chi_m(t)\},
\]

where \(\Phi\) is the cumulative distribution function of the standard normal distribution.

(ii) For any \(\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)\) and \(t > 0\),

\[
\|\mu P_t - \nu P_t\|_{TV} \leq \frac{\mathcal{W}_1(\mu, \nu)}{\sqrt{(2\pi/m)(e^{2mt} - 1)}}.
\]

(iii) For any \(x \in \mathbb{R}^d\) and \(t \geq 0\),

\[
\|\pi - \delta_x P_t\|_{TV} \leq \frac{(d/m)^{1/2} + \|x - x^*\|}{\sqrt{(2\pi/m)(e^{2mt} - 1)}}.
\]

**Proof.** (i) We now bound for \(t > 0\), \(\mathbb{P}(X_t \neq Y_t)\). For \(t < T_c\), denoting by \(B^1_t = \int_0^t 1_{\{s < T_c\}} e^T_s \mathrm{d}B_s\), we get

\[
\mathrm{d}\{X_t - Y_t\} = -\{\nabla U(X_t) - \nabla U(Y_t)\}\mathrm{d}t + 2\sqrt{2}e_t\mathrm{d}B^1_t.
\]

By Itô’s formula and H2, we have for \(t < T_c\),

\[
\|X_t - Y_t\| = \|x - y\| - \int_0^t \langle \nabla U(X_s) - \nabla U(Y_s), e_s \rangle \mathrm{d}s + 2\sqrt{2}B^1_t
\]

\[
\leq \|x - y\| - m\int_0^t \|X_s - Y_s\| \mathrm{d}s + 2\sqrt{2}B^1_t.
\]

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By Grönwall’s inequality, we have
\[ \|X_t - Y_t\| \leq e^{-mt} \|x - y\| + 2\sqrt{2} \int_0^t B_s^1 e^{-m(t-s)} ds . \]

Therefore by integration by parts, \( \|X_t - Y_t\| \leq U_t \) where \((U_t)_{t \in (0, T_c)}\) is the one-dimensional Ornstein-Uhlenbeck process defined by
\[ U_t = e^{-mt} \|x - y\| + 2\sqrt{2} \int_0^t e^{m(s-t)} dB_s^1 = e^{-mt} \|x - y\| + \int_0^t e^{m(s-t)} dB_s^1 . \]

Therefore, for all \( x, y \in \mathbb{R}^d \) and \( t \geq 0 \), we get
\[ P(T_c > t) \leq P\left( \min_{0 \leq s \leq t} U_t > 0 \right) . \]

Finally the proof follows from \([2, \text{Formula 2.0.2, page 542}]\).

(ii) Let \( \mu, \nu \in \mathcal{P}_1(\mathbb{R}^d) \) and \( \xi \in \Pi(\mu, \nu) \) be an optimal transference plan for \((\mu, \nu)\) w.r.t. \( W_1 \). Since for all \( s > 0, 1/2 - \Phi(-s) \leq (2\pi)^{-1/2} s, \) (i) implies that for all \( x, y \in \mathbb{R}^d \) and \( t > 0 \),
\[ \|\mu P_t - \nu P_t\|_{TV} \leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{\|x - y\|}{\sqrt{(2\pi/m)(e^{2mt} - 1)}} d\xi(x, y) , \]
which is the desired result.

(iii) The proof is a straightforward consequence of (ii) and Proposition 1-(iv).



Since for all \( s > 0, s \leq e^s - 1 \), note that Theorem 11-(ii) implies that for all \( t > 0 \) and \( \mu, \nu \in \mathcal{P}_1(\mathbb{R}^d) \),
\[ \|\mu P_t - \nu P_t\|_{TV} \leq (4\pi t)^{-1/2} W_1(\mu, \nu) . \tag{18} \]
Therefore for all bounded measurable function \( f \), \( P_t f \) is a Lipschitz function for all \( t > 0 \) with Lipschitz constant
\[ \|P_t f\|_{Lip} \leq (4\pi t)^{-1/2} \text{osc}(f) . \tag{19} \]

For all \( n, \ell \geq 1, n < \ell \) and \((\gamma_k)_{k \geq 1} \) a nonincreasing sequence denote by
\[ \Lambda_{n,\ell}(\gamma) = \kappa^{-1} \left\{ \prod_{j=n}^\ell (1 - \kappa \gamma_j)^{-1} - 1 \right\} , \quad \Lambda_{\ell}(\gamma) = \Lambda_{1,\ell}(\gamma) . \tag{20} \]

We will now study the contraction of \( Q_{n,\ell}^{\gamma} \) in total variation for non-increasing sequences \((\gamma_k)_{k \geq 1} \). Strikingly, we are able to derive results which closely parallel Theorem 11. The proof is nevertheless completely different because the reflection coupling is no longer applicable in discrete time. We use a coupling construction inspired by the method of [4, Section 3.3] for Gaussian random walks. This construction has been used in [13] to establish convergence of homogeneous Markov chain in Wasserstein distances using different method of proof. To avoid disrupting the stream of the proof, this construction is introduced in Section 8.
Theorem 12. Assume $\mathbf{H1}$ and $\mathbf{H2}$.

(i) Let $(\gamma_k)_{k \geq 1}$ be a nonincreasing sequence satisfying $\gamma_1 \leq 2/(m+L)$. Then for all $x, y \in \mathbb{R}^d$ and $n, \ell \in \mathbb{N}^*$, $n < \ell$, we have

$$\|\delta_x Q^n_{\gamma_l} - \delta_y Q^n_{\gamma_l}\|_{TV} \leq 1 - 2\Phi\{-\|x - y\| / \{8\Lambda_{n,\ell}(\gamma)\}^{1/2}\} .$$

(ii) Let $(\gamma_k)_{k \geq 1}$ be a nonincreasing sequence satisfying $\gamma_1 \leq 2/(m+L)$. For all $\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)$ and $\ell, n \in \mathbb{N}^*$, $n < \ell$,

$$\|\mu Q^n_{\gamma_l} - \nu Q^n_{\gamma_l}\|_{TV} \leq \{4\pi\Lambda_{n,\ell}(\gamma)\}^{-1/2}W_1(\mu, \nu) .$$

(iii) Let $\gamma \in (0,2/(m + L)]$. Then for any $x \in \mathbb{R}^d$ and $n \geq 1$,

$$\|\pi - \delta_x R^n_{\gamma_l}\|_{TV} \leq \{4\pi\kappa(1 - (1 - \kappa\gamma)^{n/2})\}^{-1/2}(1 - \kappa\gamma)^{n/2}\left\{\|x - x^*\| + (2\kappa^{-1}d)^{1/2}\right\} .$$

Proof. (i) By (3) for all $x, y$ and $k \geq 1$, we have

$$\|x - \gamma_k \nabla U(x) - y + \gamma_k \nabla U(y)\| \leq (1 - \kappa\gamma_k)^{1/2}\|x - y\| .$$

Let $n, \ell \geq 1$, $n < \ell$, then applying Theorem 23 in Section 8, we get

$$\|\delta_x Q^n_{\gamma_l} - \delta_y Q^n_{\gamma_l}\|_{TV} \leq 1 - 2\Phi\{-\|x - y\| / \{8\Lambda_{n,\ell}(\gamma)\}^{1/2}\} ,$$

(ii) Let $f \in \mathcal{F}_b(\mathbb{R}^d)$ and $\ell > n \geq 1$. For all $x, y \in \mathbb{R}^d$ by definition of the total variation distance and (i), we have

$$\left|Q^n_{\gamma_l} f(x) - Q^n_{\gamma_l} f(y)\right| \leq \text{osc}(f)\|\delta_x Q^n_{\gamma_l} - \delta_y Q^n_{\gamma_l}\|_{TV}$$

$$\leq \text{osc}(f)\left\{1 - 2\Phi\{-\|x - y\| / \{8\Lambda_{n,\ell}(\gamma)\}^{1/2}\}\right\} ,$$

Using that for all $s > 0$, $1/2 - \Phi(-s) \leq (2\pi)^{-1/2}s$ concludes the proof.

(iii) The proof follows from (iii), the bound for all $s > 0$, $1/2 - \Phi(-s) \leq (2\pi)^{-1/2}s$ and Proposition 2-(ii).

\[\square\]

We can combine this result and Theorem 5 or Theorem 9 to get explicit bounds in total variation between the Euler-Maruyama discretization and the target distribution $\pi$. To that purpose, we use the following decomposition, for all nonincreasing sequence $(\gamma_k)_{k \geq 1}$, initial point $x \in \mathbb{R}^d$ and $\ell \geq 0$:

$$\|\pi - \delta_x Q^n_{\gamma_l}\|_{TV} \leq \|\pi - \delta_x P_{\gamma_l}\|_{TV} + \|\delta_x P_{\gamma_l} - \delta_x Q^n_{\gamma_l}\|_{TV} .$$

(21)
The first term is dealt with Theorem 11-(iii). It remains to bound the second term in (21). Since we will use Theorem 5 and Theorem 9, we have two different results depending on the assumptions on $U$ again. Define for all $x \in \mathbb{R}^d$ and $n, p \in \mathbb{N}$,

$$
\vartheta_{n,p}^{(1)}(x) = L^2 \sum_{i=1}^{n} \gamma_i^2 \prod_{k=i+1}^{n} (1 - \kappa \gamma_k/2) \left[ \left\{ \kappa^{-1} + \gamma_i \right\} (2d + dL^2 \gamma_i^2/6) \right. \\
+ L^2 \gamma_i \delta_{i,n,p}(x) \left( \kappa^{-1} + \gamma_i \right)
$$

(22)

$$
\vartheta_{n,p}^{(2)}(x) = \sum_{i=1}^{n} \gamma_i^3 \prod_{k=i+1}^{n} (1 - \kappa \gamma_k/2) \left[ L^4 \delta_{i,n,p}(x)(4\kappa^{-1}/3 + \gamma_{n+1}) \right. \\
+ d \left\{ 2L^2 + 4\kappa^{-1}(dL^2/12 + \gamma_{n+1}L^4/4) + \gamma_{n+1}^2 L^4/6 \right\} \right],
$$

where $g_{n,p}(x)$ is given by (8) and

$$
\delta_{i,n,p}(x) = e^{-2m\Gamma_{i-1}} g_{n,p}(x) + (1 - e^{-2m\Gamma_{i-1}})(d/m),
$$

Theorem 13. Assume $H1$ and $H2$. Let $(\gamma_k)_{k \geq 1}$ be a nonincreasing sequence with $\gamma_1 \leq 1/(m + L)$. Then for all $x \in \mathbb{R}^d$ and $\ell, n \in \mathbb{N}$, $\ell > n$,

$$
\| \delta_x P_{\Gamma_{\ell}} - \delta_x Q_\gamma^\ell \|_{TV} \leq (\vartheta_n(x)/(4\pi \Gamma_{n+1,\ell}))^{1/2} \\
+ 2^{-3/2} L \left( \sum_{k=n+1}^{\ell} \left\{ \gamma_k^3 L^2/3 \vartheta_{1,k-1}(x) + d\gamma_k^2 \right\} \right)^{1/2}.
$$

(24)

where $q_{1,n}(x)$ is defined by (8), $\vartheta_n(x)$ is equal to $\vartheta_{n,0}^{(2)}(x)$ given by (23), if $H3$ holds, and to $\vartheta_{n,0}^{(1)}(x)$ given by (22) otherwise.

Proof. Applying Lemma 20 or Lemma 21, we get that for all $x \in \mathbb{R}^d$

$$
W_1(\delta_x Q_\gamma^n, \delta_x P_{T_n}) \leq \{ \vartheta_n(x) \}^{1/2}, \vartheta_n(x) = \begin{cases} \\
\vartheta_{n,0}^{(1)}(x) & \text{ (H1, H2)}, \\
\vartheta_{n,0}^{(2)}(x) & \text{ (H1, H2, H3)},
\end{cases}
$$

(25)

By the triangle inequality, we get

$$
\| \delta_x P_{\Gamma_{\ell}} - \delta_x Q_\gamma^\ell \|_{TV} \leq \| \{ \delta_x P_{T_n} - \delta_x Q_\gamma^n \} P_{T_{n+1,\ell}} \|_{TV} \\
+ \| \delta_x Q_\gamma^n \{ Q_\gamma^{n+1,\ell} - P_{T_{n+1,\ell}} \} \|_{TV}.
$$

(26)

Using (18) and (25), we have

$$
\| \{ \delta_x P_{T_n} - \delta_x Q_\gamma^{1,n} \} P_{T_{n+1,\ell}} \|_{TV} \leq (\vartheta_n(x)/(4\pi \Gamma_{n+1,\ell}))^{1/2}.
$$

(27)
For the second term, by [10, Equation 11] (note that we have a different convention for the total variation distance) and the Pinsker inequality, we have
\[
\left\| \delta_x Q^{1,n}_\gamma \left\{ Q^{n+1,\ell}_\gamma - P_{T_{n+1,\ell}} \right\} \right\|_{TV}^2 \\
\leq 2^{-3} L^2 \sum_{k=n+1}^\ell \left\{ (\gamma_k^3/3) \int_{\mathbb{R}^d} \| \nabla U(z) - \nabla U(x^*) \|^2 Q^{-1}_\gamma(x,z) + d\gamma_k^2 \right\} .
\]

By H1 and Proposition 2, we get
\[
\left\| \delta_x Q^{1,n}_\gamma \left\{ Q^{n+1,\ell}_\gamma - P_{T_{n+1,\ell}} \right\} \right\|_{TV}^2 \\
\leq 2^{-3} L^2 \sum_{k=n+1}^\ell \left\{ (\gamma_k^3 L^2 / 3) q_{1,k-1} + d\gamma_k^2 \right\} .
\]

Combining the last inequality and (27) in (26) concludes the proof.

Consider the case of decreasing step sizes defined: \( \gamma_k = \gamma_1 k^{-\alpha} \) for \( k \geq 1 \) and \( \alpha \in (0,1) \). Under H1 and H2, choosing \( n = \ell - \lceil \epsilon / \alpha \rceil \) in the bound given by Theorem 13 and using Table 2 implies that \( \| \delta_x Q^\ell_\gamma - \pi \|_{TV} = d^{1/2} \mathcal{O}(\epsilon^{-\alpha/2}) \). Note that for \( \alpha = 1 \), this rate is true only for \( \gamma_1 > 2\kappa^{-1} \). If in addition H3 holds, choosing \( n = \ell - \lceil \epsilon/2 \rceil \) in the bound given by (24) and using Table 2, (21) and Theorem 11-(iii) implies that \( \| \delta_x Q^\ell_\gamma - \pi \|_{TV} = d\mathcal{O}(\epsilon^{-3/4}) \). Note that these rates are explicit compared to the ones obtained in [11, Proposition 4]. These conclusions and the dependency on the dimension are summarized in Table 3.

| \( \gamma_k = \gamma_1 k^{-\alpha}, \alpha \in (0,1) \) | H1, H2 | H1, H2 and H3 |
|---|---|---|
| \( d^{1/2} \mathcal{O}(\epsilon^{-\alpha/2}) \) | \( d\mathcal{O}(\epsilon^{-3/4}) \) |

Table 3: Order of convergence of \( \| \delta_x^\ell Q^\ell_\gamma - \pi \|_{TV} \) for \( \gamma_k = \gamma_1 k^{-\alpha} \) based on Theorem 13

When \( \gamma_k = \gamma \in (0,1/(m + L)) \) for all \( k \geq 1 \), under H1 and H2, for \( \ell > \lceil \gamma^{-1} \rceil \) choosing \( n = \ell - \lceil \gamma^{-1} \rceil \) implies that (see the supplementary document [12, Section 2.2])
\[
\| \delta_x R^\ell_\gamma - \delta_x P_{T_\gamma} \|_{TV} \leq (4\pi)^{-1/2} \left[ \gamma D_1(\gamma, d) + \gamma^3 D_2(\gamma) D_3(\gamma, d, x) \right]^{1/2} + D_4(\gamma, d, x) ,
\]

where
\[
D_1(\gamma, d) = 2L^2 \kappa^{-1} \left( \kappa^{-1} + \gamma \right) \left( 2d + L^2 \gamma^2 / 6 \right) , 
D_2(\gamma) = L^4 \left( \kappa^{-1} + \gamma \right) 
D_3(\gamma, d, x) = \left\{ (\ell - \lceil \gamma^{-1} \rceil) e^{-m\gamma(\ell - \lceil \gamma^{-1} \rceil - 1)} \| x - x^* \|^2 + 2d(\kappa \gamma m)^{-1} \right\} 
D_4(\gamma, d, x) = 2^{-3} L \left[ d\gamma(1 + \gamma) + (L^2 \gamma^3 / 3) \left\{ (1 + \gamma^{-1}) (1 - \kappa \gamma) \ell - \lceil \gamma^{-1} \rceil \| x - x^* \|^2 + 2(1 + \gamma) \kappa^{-1} d \right\} \right]^{1/2} .
\]

Using this bound and Theorem 11-(iii), the minimal number of iterations \( \ell_\varepsilon > 0 \) for a target precision \( \varepsilon > 0 \) to get \( \| \delta_x^\ell R^\ell_\gamma - \pi \|_{TV} \leq \varepsilon \) is of order \( d \log(d) \mathcal{O}(\lceil \log(\varepsilon) \rceil \varepsilon^{-2}) \) (the proper choice of the step size \( \gamma_\varepsilon \) is given in Table 5). In addition, letting \( \ell \) go to infinity in (28) we get the following result.

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Corollary 14. Assume $\textbf{H1}$ and $\textbf{H2}$. Let $\gamma \in (0, 1/(m + L)]$. Then it holds

$$\|\pi_\gamma - \pi\|_{TV} \leq 2^{-3/2} L \left[ d\gamma (1 + \gamma) + 2(L^2 \gamma^3/3)(1 + \gamma) \kappa^{-1} d \right]^{1/2} + (4\pi)^{-1/2} \left[ \gamma D_1(\gamma, d) + 2d\gamma^2 D_2(\gamma)(\kappa m)^{-1} \right]^{1/2},$$

where $D_1(\gamma)$ and $D_2(\gamma)$ are given in (29).

Note that the bound provided by Corollary 14 is of order $d^{1/2} O(\gamma^{1/2})$.

If in addition $\textbf{H3}$ holds, for constant step sizes, we can improve with respect to the step size $\gamma$, the bounds given by Corollary 14.

Theorem 15. Assume $\textbf{H1, H2}$ and $\textbf{H3}$. Let $\gamma \in (0, 1/(m + L)]$. Then it holds

$$\|\pi_\gamma - \pi\|_{TV} \leq (4\pi)^{-1/2} \left\{ \gamma^2 E_1(\gamma, d) + 2d\gamma^2 E_2(\gamma)/(\kappa m) \right\}^{1/2} + (4\pi)^{-1/2} \left[ \log (\gamma^{-1}) / \log (2) \right] \left\{ \gamma^2 E_1(\gamma, d) + \gamma^2 E_2(\gamma)(2\kappa^{-1} d + d/m) \right\}^{1/2} + 2^{-3/2} L \left\{ 2d\gamma^3 L^2/(3\kappa) + d\gamma^2 \right\}^{1/2},$$

where $E_1(\gamma, d)$ and $E_2(\gamma)$ are defined by

$$E_1(\gamma, d) = 2d\kappa^{-1} \left\{ 2L^2 + 4\kappa^{-1}(d\tilde{L}^2/12 + \gamma L^4/4) + \gamma^2 L^4/6 \right\}$$

$$E_2(\gamma) = L^4(4\kappa^{-1}/3 + \gamma).$$

Proof. The proof is postponed to Section 7. \qed

Note that the bound provided by Theorem 15 is of order $dO(\gamma |\log(\gamma)|)$, improving the dependency given by Corollary 14, with respect to the step size $\gamma$. Furthermore when $L = 0$, this bound given by Theorem 15 is of order $d^{1/2} O(\gamma |\log(\gamma)|)$ and is sharp up to a logarithmic factor. Indeed, assume that $\pi$ is the $d$-dimensional standard Gaussian distribution. In such case, the ULA sequence $(X_k)_{k \geq 0}$ is the autoregressive process given for all $k \geq 0$ by $X_{k+1} = (1 - \gamma)X_k + \sqrt{2\gamma} Z_{k+1}$. For $\gamma \in (0, 1)$, this sequence has a stationary distribution $\pi_\gamma$, which is a $d$-dimensional Gaussian distribution with zero-mean and covariance matrix $\sigma^2 \gamma^2 I_d$, with $\sigma^2 = (1 - \gamma/2)^{-1}$. Therefore, using [22, Lemma 4.9] (or the Pinsker inequality), we get the following upper bound: $\|\pi - \pi_\gamma\|_{TV} \leq C d^{1/2} |\sigma^2 \gamma - 1| = C d^{1/2}/\gamma/2$, where $C$ is a universal constant.

We can also for a precision target $\varepsilon > 0$ choose $\gamma_\varepsilon > 0$ and the number of iterations $n_\varepsilon > 0$ to get $\|\delta_x R_{\gamma_\varepsilon} - \pi\|_{TV} \leq \varepsilon$. By Theorem 11-(iii), Theorem 12-(iii) and Theorem 15, the minimal number of iterations $\ell_\varepsilon$ is of order $d \log^2(d) O(\varepsilon^{-1} \log^2(\varepsilon))$ for a well chosen step size $\gamma_\varepsilon$. This result improves the conclusion of [11] and 14 with respect to the precision parameter $\varepsilon$, which provides an upper bound of the number of iterations of order $d \log(d) O(\varepsilon^{-2} \log^2(\varepsilon))$. We can also compare our reported upper bound with the one obtained for the $d$-dimensional standard Gaussian distribution. If the initial distribution is the Dirac mass at zero (the minimum of the potential $U(x) = \|x\|^2/2$ and $\gamma \in (0, 1)$, the distribution of the ULA sequence after $n$ iterations is zero-mean Gaussian with
covariance \((1 - (1 - \gamma)^2(n+1))/(1 - \gamma/2) I_d\). If we use \cite[Lemma 4.9]{22} again, we get for \(\gamma \in (0, 1)\),

\[
\|\delta_n R^n \gamma - \pi\|_{TV} \leq C d^{1/2} \gamma |1 - 2 - (1 - \gamma)^2(n+1)|,
\]

where \(C\) is a universal constant. To get an \(\varepsilon\) precision we need to choose \(\gamma = d^{-1/2} \varepsilon/(2C)\) and then \(n_\varepsilon = [(1/2) \log(\gamma)/\log(1 - \gamma)] = d^{1/2} \log(d) O(\varepsilon^{-1} \log(\varepsilon))\). On the other hand since \(\bar{L} = 0\), based on the bound given by Theorem 15, the minimal number of iterations to get \(\|\delta_x R^n \gamma - \pi\|_{TV} \leq \varepsilon\) is of order \(d^{1/2} \log^2(d) O(\varepsilon^{-1} \log^2(\varepsilon))\). It follows that our upper bound for the stepsize and the optimal number of iterations is again sharp up to a logarithmic factor in the dimension and the precision. The discussions on the bounds for constant sequences of step sizes are summarized in Table 4 and Table 5.

|                  | H1, H2                           | H1, H2 and H3                   |
|------------------|----------------------------------|---------------------------------|
| \(\|\pi - \pi\gamma\|_{TV}\) | \(d^{1/2} \mathcal{O}(\varepsilon^{1/2})\) | \(d\mathcal{O}(\varepsilon \log(\varepsilon))\) |

Table 4: Order of the bound between \(\pi\) and \(\pi\gamma\) in total variation function of the step size \(\gamma = 0\) and the dimension \(d\).

| \(\gamma\)   | \(\varepsilon\) | \(n_\varepsilon\) |
|-------------|----------------|-----------------|
| \(d^{-1} \mathcal{O}(\varepsilon^d)\) | \(d^{-1} \mathcal{O}(\varepsilon \log^{-1}(\varepsilon))\) | \(d^{-1} \log^{-1}(d) \mathcal{O}(\varepsilon \log^{-1}(\varepsilon))\) |

Table 5: Order of the step size \(\gamma \varepsilon > 0\) and the number of iterations \(n_\varepsilon \in \mathbb{N}^*\) to get \(\|\delta_x R^n \gamma R^n \varepsilon - \pi\|_{TV} \leq \varepsilon\) for \(\varepsilon > 0\).

4 Mean square error and concentration for bounded measurable functions

The result of the previous section allows us to study the approximation of \(\int_{\mathbb{R}^d} f(y) \pi(dy)\) by the weighted average estimator \(\hat{\pi}_n^N(f)\) defined, for a measurable and bounded function \(f : \mathbb{R}^d \to \mathbb{R}\), \(N, n \in \mathbb{N}\), \(n \geq 1\) by

\[
\hat{\pi}_n^N(f) = \sum_{k=N+1}^{N+n} \omega_{k,n}^N f(X_k) , \quad \omega_{k,n}^N = \gamma_{k+1}^{-1} \Gamma_{N+1,N+n+1} \ .
\]

We derive a bound on the mean-square error, defined as \(\text{MSE}_{N,n}^f = \mathbb{E}_x \left[ |\hat{\pi}_n^N(f) - \pi(f)|^2 \right]\).

The \(\text{MSE}_{N,n}^f\) can be decomposed as the sum of the squared bias and variance:

\[
\text{MSE}_{N,n}^f = \left\{ \mathbb{E}_x[\hat{\pi}_n^N(f) - \pi(f)] \right\}^2 + \text{Var}_x \left\{ \hat{\pi}_n^N(f) \right\} \ .
\]
We first obtain a bound for the bias. By the Jensen inequality and because $f$ is bounded, we have:

$$\left( \mathbb{E}_x \left[ \hat{\pi}^N_n(f) - \pi(f) \right] \right)^2 \leq \text{osc}(f)^2 \sum_{k=N+1}^{N+n} \omega_{k,n}^N \| \delta_x Q_k^\gamma - \pi \|^2_{TV} :$$

Using the results of Section 3, we can deduce different bounds for the bias, depending on the assumptions on $U$ and the sequence of step sizes $(\gamma_k)_{k \geq 1}$. It is now required to derive a bound for the variance. Our main tool is the Gaussian Poincaré inequality [3, Theorem 3.20] which can be applied to $R_\gamma(y, \cdot)$ defined by (6), noticing that $R_\gamma(y, \cdot)$ is a Gaussian distribution with mean $y - \gamma \nabla U(y)$ and covariance matrix $2\gamma I_d$: for all Lipschitz function $g : \mathbb{R}^d \to \mathbb{R}$

$$R_\gamma \{ g(\cdot) - R_\gamma(y) \}^2 (y) \leq 2\gamma \| g \|^2_{\text{Lip}} .$$

Lemma 16. Assume $H1$ and $H2$. Let $(\gamma_k)_{k \geq 1}$ be a nonincreasing sequence with $\gamma_1 \leq 2/(m + L)$. Let $g : \mathbb{R}^d \to \mathbb{R}$ be a Lipschitz function. Then for all $n, p \geq 1$, $n \leq p$ and $y \in \mathbb{R}^d$

$$0 \leq \int_{\mathbb{R}^d} Q_{\gamma}^{n,p}(y, dz) \left\{ g(z) - Q_{\gamma}^{n,p}g(y) \right\}^2 \leq 2\kappa_1^{-1} \| g \|^2_{\text{Lip}} ,$$

where $Q_{\gamma}^{n,p}$ is given by (7).

Proof. By decomposing $g(X_p) - \mathbb{E} G_n^y[g(X_p)] = \sum_{k=n+1}^{p} \mathbb{E}^G_{y} [g(X_p) - \mathbb{E}^G_{y} [g(X_p)]]$, and using $\mathbb{E}^G_{y} [g(X_p)] = Q_{\gamma}^{k+1,p} g(X_k)$, we get

$$\text{Var} \gamma \{ g(X_p) \} = \sum_{k=n+1}^{p} \mathbb{E}^G_{y} \left[ \left( \mathbb{E}^G_{y} [g(X_p)] - \mathbb{E}^G_{y} [g(X_p)] \right)^2 \right]$$

$$= \sum_{k=n+1}^{p} \mathbb{E}^G_{y} \left[ R_{\gamma k} \left\{ Q_{\gamma}^{k+1,p} g(\cdot) - R_{\gamma k} Q_{\gamma}^{k+1,p} g(X_{k-1}) \right\}^2 (X_{k-1}) \right] .$$

Equation (31) implies $\text{Var} \gamma \{ g(X_p) \} \leq 2 \sum_{k=n+1}^{p} \gamma_k \| Q_{\gamma}^{k+1,p} g \|^2_{\text{Lip}}$. The proof follows from Corollary 4 and Lemma 7, using the bound $(1 - t)^{1/2} \leq 1 - t/2$ for $t \in [0, 1]$. □

Theorem 17. Assume $H1$ and $H2$. Let $(\gamma_k)_{k \geq 1}$ be a nonincreasing sequence with $\gamma_1 \leq 2/(m + L)$. Then for all $N \geq 0$, $n \geq 1$, $x \in \mathbb{R}^d$ and $f \in \mathcal{F}_0(\mathbb{R}^d)$, we get

$$\text{Var}_x \{ \hat{\pi}^N_N(x) \} \leq \text{osc}(f)^2 \left\{ 2\gamma_1 \Gamma_{N+2, N+n+1} + u^{(4)}_{N,n}(\gamma) \right\}$$

$$u^{(4)}_{N,n}(\gamma) = \sum_{k=N}^{N+n-1} \gamma_{k+1} \left\{ \sum_{i=k+2}^{N+n} \omega_{i,n}^N \left( \pi \Lambda_{k+2,i}(\gamma) \right) \right\}^{1/2} + \kappa^{-1} \left\{ \sum_{i=N+1}^{N+n} \omega_{i,n}^N \left( 4\pi \Lambda_{N+1,i}(\gamma) \right)^{1/2} \right\}^2 ,$$

for $n_1, n_2 \in \mathbb{N}$, $\Lambda_{n_1,n_2}(\gamma)$ is given by (20).
Proof. Let $N \geq 0$, $n \geq 1$, $x \in \mathbb{R}^d$ and $f \in \mathcal{F}_n(\mathbb{R}^d)$. We decompose $\hat{\pi}_n^N(f) - \mathbb{E}_x[\hat{\pi}_n^N(f)]$ as the sum of martingale increments, w.r.t. $(\mathcal{G}_n)_{n \geq 0}$, the natural filtration associated with Euler approximation $(X_n)_{n \geq 0}$, and we get

$$\text{Var}_x \{ \hat{\pi}_n^N(f) \} = \sum_{k=N}^{N+n-1} \mathbb{E}_x \left( \left( \mathbb{E}_{X_n}^k \left[ \hat{\pi}_n^N(f) \right] - \mathbb{E}_x^k \left[ \hat{\pi}_n^N(f) \right] \right)^2 \right)$$

$$+ \mathbb{E}_x \left( \left( \mathbb{E}_{X_n}^N \left[ \hat{\pi}_n^N(f) \right] - \mathbb{E}_x^N \left[ \hat{\pi}_n^N(f) \right] \right)^2 \right).$$  \hspace{1cm} (32)

The martingale increment $\mathbb{E}_{X_n}^{k+1} \left[ \hat{\pi}_n^N(f) \right] - \mathbb{E}_x^k \left[ \hat{\pi}_n^N(f) \right]$ has a simple expression. For $k = N + n - 1, \ldots, N + 1$, define (backward in time) the function

$$\Phi_{n,k}^N : x_k \mapsto \omega_{k,n}^N f(x_k) + R_{\gamma_{k+1}} \Phi_{n,k+1}^N(x_k),$$  \hspace{1cm} (33)

where $\Phi_{n,N+n}^N : x_{N+n} \mapsto \Phi_{n,N+n}^N(x_{N+n}) = \omega_{N+n}^N f(x_{N+n})$. Denote finally

$$\Psi_n^N : x_N \mapsto \sum_{k=N}^{N+n} \Phi_{\gamma_{k+1}}^N \Phi_{n,k+1}^N(x_N).$$  \hspace{1cm} (34)

Note that for $k \in \{N, \ldots, N + n - 1\}$, by the Markov property,

$$\Phi_{n,k+1}^N(X_{k+1}) - R_{\gamma_{k+1}} \Phi_{n,k+1}^N(X_k) = \mathbb{E}_{X_n}^{k+1} \left[ \hat{\pi}_n^N(f) \right] - \mathbb{E}_x^k \left[ \hat{\pi}_n^N(f) \right],$$  \hspace{1cm} (35)

and $\Psi_n^N(X_N) = \mathbb{E}_{X_n}^N \left[ \hat{\pi}_n^N(f) \right]$. With these notations, (32) may be equivalently expressed as

$$\text{Var}_x \{ \hat{\pi}_n^N(f) \} = \sum_{k=N}^{N+n-1} \mathbb{E}_x \left( \sum_{k=N}^{N+n} \left( R_{\gamma_{k+1}} \Phi_{n,k+1}^N(x_k) - R_{\gamma_{k+1}} \Phi_{n,k+1}^N(x_k) \right)^2 \right)$$

$$+ \mathbb{E}_x \left( \left( \mathbb{E}_{X_n}^N \left[ \hat{\pi}_n^N(f) \right] - \mathbb{E}_x^N \left[ \hat{\pi}_n^N(f) \right] \right)^2 \right).$$  \hspace{1cm} (36)

Let $k \in \{N, \ldots, N + n - 1\}$. We cannot directly apply the Poincaré inequality (31) since the function $\Phi_{n,k}^N$, defined in (33), is not Lipschitz. However, Theorem 12-(ii) shows that for all $\ell, n \in \mathbb{N}^*$, $n < \ell$, $Q_\gamma^{n,\ell} f$ is a Lipschitz function with

$$\left\| Q_\gamma^{n,\ell} f \right\|_{\text{Lip}} \leq \text{osc}(f) / \{4\pi \Lambda_{n,\ell}(\gamma)\}^{1/2}. \hspace{1cm} (37)$$

Using (33), we may decompose $\Phi_{n,k}^N = \omega_{k,n}^N f + \tilde{\Phi}_{n,k}^N$, where $\tilde{\Phi}_{n,k}^N = \sum_{i=k+2}^{N+n} \omega_{i,n}^N Q_\gamma^{i-k+2,\ell} f$ which is Lipschitz with constant

$$\left\| \tilde{\Phi}_{n,k}^N \right\|_{\text{Lip}} \leq \sum_{i=k+2}^{N+n} \omega_{i,n}^N \left\| Q_\gamma^{i-k+2,\ell} f \right\|_{\text{Lip}} \leq \text{osc}(f) \sum_{i=k+2}^{N+n} \omega_{i,n}^N / \{4\pi \Lambda_{k+2,\ell}(\gamma)\}^{1/2}.$$

Using the inequality $(a + b)^2 \leq 2a^2 + 2b^2$, (31), we finally get for any $y \in \mathbb{R}^d$

$$R_{\gamma_{k+1}} \left( \Phi_{n,k+1}^N(y) - R_{\gamma_{k+1}} \Phi_{n,k+1}^N(y) \right)^2 \leq 2(\omega_{k+1,n}^N)^2 \text{osc}(f)^2$$

$$+ \gamma_{k+1} \text{osc}(f)^2 \left( \sum_{i=k+2}^{N+n} \omega_{i,n}^N / \{4\pi \Lambda_{k+2,\ell}(\gamma)\}^{1/2} \right)^2. \hspace{1cm} (39)$$

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It remains to control \( \text{Var}_x \{ \Psi^N_n(X_N) \} \), where \( \Psi^N_n \) is defined in (34). Using (37), \( \Psi^N_n \) is a Lipschitz function with Lipschitz constant bounded by:

\[
\| \Psi^N_n \|_{\text{Lip}} \leq \sum_{i=N+1}^{N+n} \omega_{i,n}^N \| Q^{N+1,i}f \|_{\text{Lip}} \leq \text{osc}(f) \sum_{i=N+1}^{N+n} \omega_{i,n}^N / \left\{ 4 \pi A_{N+1,i}(\gamma) \right\}^{1/2} .
\] (40)

By Lemma 16, we have the following result which is the counterpart of Corollary 3: for all \( y \in \mathbb{R}^d \),

\[
\text{Var}_y \{ \Psi^N_n(X_N) \} \leq 2 \kappa^{-1} \| f \|_\infty^2 \left\{ \sum_{i=N+1}^{N+n} \omega_{i,n}^N / (\pi A_{N+1,i})^{1/2} \right\}^2 .
\] (41)

Finally, the proof follows from combining (39) and (41) in (36).

To illustrate the result Theorem 17, we study numerically the behaviour \( (u^{(4)}_{N,n})_{n \geq 1} \Gamma_n \) for \( \kappa = 1 \) \( N = 0 \), and four different non-increasing sequences of step-sizes \( (\gamma_k)_{k \geq 1} \), \( \gamma_k = (1 + k)^{-\alpha} \) for \( \alpha = 1/4, 1/2, 3/4 \) and \( \gamma_k = 1/2 \) for \( k \geq 1 \). These results are gathered in Figure 1, where it can be observed that \( (\Gamma_n u^{(4)}_{0,n}(\gamma))_{n \geq 1} \) converges to a limit as \( n \to +\infty \).

We now establish an exponential deviation inequality for \( \hat{\pi}^N_n(f) - E_x[\hat{\pi}^N_n(f)] \) given by (30) for a bounded measurable function \( f \).
Theorem 18. Assume H1 and H2. Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \(\gamma_1 \leq 2/(m+L)\). Let \((X_n)_{n \geq 0}\) be given by (2) and started at \(x \in \mathbb{R}^d\). Then for all \(N \geq 0\), \(n \geq 1\), \(r > 0\), and functions \(f \in \mathbb{F}_d(\mathbb{R}^d)\):

\[
\mathbb{P}_x \left[ \hat{p}_n^N(f) > \mathbb{E}_x[\hat{p}_n^N(f)] + r \right] \leq e^{-\{r-\text{osc}(f)\Gamma_{N+2,N+n+1}^{-1}\} / \{2\text{osc}(f)u_{N,n}^{(5)}(\gamma)\}},
\]

where

\[
u_N^{(5)}(\gamma) = \sum_{k=N}^{N+n-1} \gamma_{k+1} \left( \sum_{i=k+2}^{N+n} \frac{\omega_{i,n}^N}{(\pi \Lambda_{k+2,i})^{1/2}} \right)^2 + \kappa^{-1} \left( \sum_{i=N+1}^{N+n} \frac{\omega_{i,n}^N}{(\pi \Lambda_{N+1,i})^{1/2}} \right)^2.
\]

Proof. The proof is postponed in the supplementary document to Section 3.

5 Numerical experiments

Consider a binary regression set-up in which the binary observations (responses) \(\{Y_i\}_{i=1}^P\) are conditionally independent Bernoulli random variables with success probability \(\{g(\beta^T X_i)\}_{i=1}^P\), where \(g\) is the logistic function defined for \(z \in \mathbb{R}\) by \(g(z) = e^z / (1 + e^z)\) and \(\{X_i\}_{i=1}^P\) and \(\beta\) are \(d\) dimensional vectors of known covariates and unknown regression coefficients, respectively. The prior distribution for the parameter \(\beta\) is a zero-mean Gaussian distribution with covariance matrix \(\Sigma\). The density of the posterior distribution of \(\beta\) is up to a proportionality constant given by

\[
\pi_\beta(\beta|\{(X_i,Y_i)\}_{i=1}^P) \propto \exp \left( \sum_{i=1}^P \left( Y_i \beta^T X_i - \log(1 + e^{\beta^T X_i}) \right) - 2^{-1} \beta^T \Sigma^{-1} \beta \right).
\]

Bayesian inference for the logistic regression model has long been recognized as a numerically involved problem, due to the analytically inconvenient form of the likelihood function. Several algorithms have been proposed, trying to mimick the data-augmentation (DA) approach of [1] for probit regression; see [20], [15] and [16]. Recently, a very promising DA algorithm has been proposed in [31], using the Polya-Gamma distribution in the DA part. This algorithm has been shown to be uniformly ergodic for the total variation by [7, Proposition 1], which provides an explicit expression for the ergodicity constant. This constant is exponentially small in the dimension of the parameter space and the number of samples. Moreover, the complexity of the augmentation step is cubic in the dimension, which prevents from using this algorithm when the dimension of the regressor is large.

We apply ULA to sample from the posterior distribution \(\pi_\beta(\cdot|\{(X_i,Y_i)\}_{i=1}^P)\). The gradient of its log-density may be expressed as

\[
\nabla \log \{ \pi_\beta(\beta|\{(X_i,Y_i)\}_{i=1}^P) \} = \sum_{i=1}^P \left( Y_i X_i - \frac{X_i}{1 + e^{\beta^T X_i}} \right) - \Sigma^{-1} \beta,
\]
Therefore $- \log \pi_\beta(\{X_i, Y_i\}_{i=1}^p)$ is strongly convex $H_2$ with $m = \lambda_{\max}^{-1}(\Sigma_\beta)$ and satisfies $H_1$ with $L = (1/4) \sum_{i=1}^p X_i^T X_i + \lambda_{\min}^{-1}(\Sigma_\beta)$, where $\lambda_{\min}(\Sigma_\beta)$ and $\lambda_{\max}(\Sigma_\beta)$ denote the minimal and maximal eigenvalues of $\Sigma_\beta$, respectively. We first compare the histograms produced by ULA and the Pólya-Gamma Gibbs sampling from [31]. For that purpose, we take $d = 5$, $p = 100$, generate synthetic data $(Y_i)_{1 \leq i \leq p}$ and $(X_i)_{1 \leq i \leq p}$, and set $\Sigma_\beta^{-1} = (dp)^{-1} \sum_{i=1}^p X_i^T X_i I_d$. We produce $10^8$ samples from the Pólya-Gamma sampler using the R package BayesLogit [38]. Next, we make $10^3$ runs of the Euler approximation scheme with $n = 10^6$ effective iterations, with a constant sequence $(\gamma_k)_{k \geq 1}$, $\gamma_k = 10(n n^{1/2})^{-1}$ for all $k \geq 0$ and a burn-in period $N = n^{1/2}$. The histogram of the Pólya-Gamma Gibbs sampler for first component, the corresponding mean of the obtained histograms for ULA and the 0.95 quantiles are displayed in Figure 2. The same procedure is also applied with the decreasing step size sequence $(\gamma_k)_{k \geq 1}$ defined by $\gamma_k = \gamma_1 k^{-1/2}$, with $\gamma_1 = 10(n n^{1/2})^{-1}$ and for the burn in period $N = \log(n)$, see also Figure 2. In addition, we also compare MALA and ULA on five real data sets, which are summarized in Table 6. Note that for the Australian credit data set, the ordinal covariates have been stratified by dummy variables. Furthermore, we normalized the data sets and consider the Zellner prior setting $\Sigma^{-1} = (\pi^2 d/3) \Sigma_X^{-1}$ where $\Sigma_X = p^{-1} \sum_{i=1}^p X_i X_i^T$; see [34], [19] and the references therein. Also, we apply a pre-conditioned version of MALA and ULA, targeting the probability density $\tilde{\pi}_\beta(\cdot) \propto \pi_\beta(\Sigma_X^{1/2})$. Then, we obtain samples from $\tilde{\pi}_\beta$ by post-multiplying the obtained draws by $\Sigma_X^{1/2}$. We compare MALA and ULA for each data sets by estimating for each component $i \in \{1, \ldots, d\}$ the marginal accuracy between their $d$ marginal empirical distributions and the $d$ marginal posterior distributions, where the marginal accuracy between two probability measure $\mu, \nu$ on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ is defined by

$$MA(\mu, \nu) = 1 - (1/2)||\mu - \nu||_{TV}.$$  

This quantity has already been considered in [5] and [8] to compare approximate samplers. To estimate the $d$ marginal posterior distributions, we run $2 \cdot 10^7$ iterations of the Pólya-Gamma Gibbs sampler. Then 100 runs of MALA and ULA ($10^6$ iterations

Figure 2: Empirical distribution comparison between the Pólya-Gamma Gibbs Sampler and ULA. Left panel: constant step size $\gamma_k = \gamma_1$ for all $k \geq 1$; right panel: decreasing step size $\gamma_k = \gamma_1 k^{-1/2}$ for all $k \geq 1$.
### Table 6: Dimension of the data sets

| Data set                  | Observations $p$ | Covariates $d$ |
|---------------------------|------------------|----------------|
| German credit$^1$         | 1000             | 25             |
| Heart disease$^2$         | 270              | 14             |
| Australian credit$^3$     | 690              | 35             |
| Pima indian diabetes$^4$  | 768              | 9              |
| Musk$^5$                  | 476              | 167            |

Figure 3: Marginal accuracy across all the dimensions.

Upper left: German credit data set. Upper right: Australian credit data set. Lower left: Heart disease data set. Lower right: Pima Indian diabetes data set. At the bottom: Musk data set.

per run) have been performed. For MALA, the step-size is chosen so that the acceptance probability at stationarity is approximately equal to 0.5 for all the data sets. For ULA, we choose the same constant step-size than MALA. We display the boxplots of the mean of the estimated marginal accuracy across all the dimensions in Figure 3. These results all imply that ULA is an alternative to the Polya-Gibbs sampler and the MALA algorithm.

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1. [http://archive.ics.uci.edu/ml/datasets/Statlog+(German+Credit+Data)]
2. [http://archive.ics.uci.edu/ml/datasets/Statlog+(Heart)]
3. [http://archive.ics.uci.edu/ml/datasets/Statlog+(Australian+Credit+Approval)]
4. [http://archive.ics.uci.edu/ml/datasets/Pima+Indians+Diabetes]
5. [https://archive.ics.uci.edu/ml/datasets/Musk+(Version+1)]
6 Proofs

6.1 Proof of Theorem 5

We preface the proof by two technical Lemmata.

Lemma 19. Let $(Y_t)_{t \geq 0}$ be the solution of (1) started at $x \in \mathbb{R}^d$. For all $t \geq 0$ and $x \in \mathbb{R}^d$,
\[
\mathbb{E}_x \left[ \|Y_t - x\|^2 \right] \leq dt (2 + L^2 t^2 / 3) + (3/2) t^2 L^2 \|x - x^*\|^2 .
\]

Proof. Let $\mathcal{A}$ be the generator associated with $(P_t)_{t \geq 0}$ defined by (2). Denote for all $x, y \in \mathbb{R}^d$, $\tilde{V}_x(y) = \|y - x\|^2$. Note that the process $(\tilde{V}_x(Y_t) - \tilde{V}_x(x) - \int_0^t \mathcal{A}\tilde{V}_x(Y_s)ds)_{t \geq 0}$, is a $(\mathcal{F}_t)_{t \geq 0}$-martingale under $\mathbb{P}_x$. Denote for all $t \geq 0$ and $x \in \mathbb{R}^d$ by $\tilde{v}(t, x) = \tilde{P}_t \tilde{V}_x(x)$.

Then we get,
\[
\frac{\partial \tilde{v}(t, x)}{\partial t} = \tilde{P}_t \mathcal{A}\tilde{V}_x(x) .
\]

By H2, we have for all $y \in \mathbb{R}^d$, $\langle \nabla U(y) - \nabla U(x), y - x \rangle \geq m \|x - y\|^2$, which implies
\[
\mathcal{A}\tilde{V}_x(y) = 2 (-\langle \nabla U(y), y - x \rangle + d) \leq 2 \left( -m \tilde{V}_x(y) + d - \langle \nabla U(x), y - x \rangle \right) .
\]

Using (42), this inequality and that $\tilde{V}_x$ is positive, we get
\[
\frac{\partial \tilde{v}(t, x)}{\partial t} = \tilde{P}_t \mathcal{A}\tilde{V}_x(x) \leq 2 \left( d - \int_{\mathbb{R}^d} \langle \nabla U(x), y - x \rangle \tilde{P}_t(x, dy) \right) .
\]

By the Cauchy-Schwarz inequality, $\nabla U(x^*) = 0$, (1) and the Jensen inequality, we have,
\[
\left\| \mathbb{E}_x [ \langle \nabla U(x), Y_t - x \rangle ] \right\| \leq \|\nabla U(x)\| \left\| \mathbb{E}_x [ Y_t - x ] \right\|
\]
\[
\leq \|\nabla U(x)\| \left\| \mathbb{E}_x \left[ \int_0^t \{ \nabla U(Y_s) - \nabla U(x^*) \} ds \right] \right\|
\]
\[
\leq \sqrt{t} \|\nabla U(x) - \nabla U(x^*)\| \left( \int_0^t \mathbb{E}_x [ \|\nabla U(Y_s) - \nabla U(x^*)\|^2 ] ds \right)^{1/2} .
\]

Furthermore, by H1 and Proposition 1-(i), we have
\[
\left| \int_{\mathbb{R}^d} \langle \nabla U(x), y - x \rangle P_t(x, dy) \right| \leq \sqrt{t} L^2 \|x - x^*\| \left( \int_0^t \mathbb{E}_x [ \|Y_s - x^*\|^2 ] ds \right)^{1/2}
\]
\[
\leq \sqrt{t} L^2 \|x - x^*\| \left( \frac{1 - e^{-2mt}}{2m} \|x - x^*\|^2 + \frac{2tm + e^{-2mt} - 1}{2m} (d/m) \right)^{1/2}
\]
\[
\leq L^2 \|x - x^*\| \left( t \|x - x^*\| + t^{3/2} d^{1/2} \right) ,
\]

where we used for the last line that by the Taylor theorem with remainder term, for all $s \geq 0$, $(1 - e^{-2ms})/(2m) \leq s$ and $(2ms + e^{-2ms} - 1)/(2m) \leq ms^2$, and the inequality
\( \sqrt{a+b} \leq \sqrt{a} + \sqrt{b} \). Plugging this upper bound in (43), and since \( 2 \| x - x^* \| t^{3/2}d^{1/2} \leq t \| x - x^* \|^2 + t^2d \), we get
\[
\frac{\partial \tilde{v}(t, x)}{\partial t} \leq 2d + 3L^2t \| x - x^* \|^2 + L^2t^2d
\]
Since \( \tilde{v}(0, x) = 0 \), the proof is completed by integrating this result.

Let \((F_t)_{t \geq 0}\) be the filtration associated with \((B_t)_{t \geq 0}\) and \((Y_0, \overline{Y}_0)\).

Lemma 20. Assume \( H1 \) and \( H2 \). Let \((\gamma_k)_{k \geq 1}\) be a nonincreasing sequence with \( \gamma_1 \leq 1/(m + L) \). Let \( \zeta_0 \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d) \), \((Y_t, \overline{Y}_t)_{t \geq 0}\) such that \((Y_0, \overline{Y}_0)\) is distributed according to \( \zeta_0 \) and given by (9). Then almost surely for all \( n \geq 0 \) and \( \epsilon > 0 \),
\[
\| Y_{\Gamma_{n+1}} - \overline{Y}_{\Gamma_{n+1}} \|^2 \leq \{1 - \gamma_{n+1} (\kappa - 2\epsilon)\} \| Y_{\Gamma_n} - \overline{Y}_{\Gamma_n} \|^2 \\
+ (2\gamma_{n+1} + (2\epsilon)^{-1}) \int_{\Gamma_n}^{\Gamma_{n+1}} \| \nabla U(Y_s) - \nabla U(\overline{Y}_s) \|^2 \, ds,
\]
\[
\mathbb{E} \left[ \left\| Y_{\Gamma_{n+1}} - \overline{Y}_{\Gamma_{n+1}} \right\|^2 \right] \leq \{1 - \gamma_{n+1} (\kappa - 2\epsilon)\} \| Y_{\Gamma_n} - \overline{Y}_{\Gamma_n} \|^2 \\
+ L^2\gamma_{n+1}^2 (1/(4\epsilon) + \gamma_1) \left( 2d + L^2\gamma_{n+1} \| Y_n - x^* \|^2 + dL^2\gamma_{n+1}^2/6 \right).
\]

Proof. Let \( n \geq 0 \) and \( \epsilon > 0 \), and set \( \Theta_n = Y_{\Gamma_n} - \overline{Y}_{\Gamma_n} \). We first show (44). By definition we have:
\[
\| \Theta_{n+1} \|^2 = \| \Theta_n \|^2 + \left\| \int_{\Gamma_n}^{\Gamma_{n+1}} \{ \nabla U(Y_s) - \nabla U(\overline{Y}_s) \} \, ds \right\|^2 \\
- 2\gamma_{n+1} \langle \Theta_n, \nabla U(Y_{\Gamma_n}) - \nabla U(\overline{Y}_{\Gamma_n}) \rangle - 2 \int_{\Gamma_n}^{\Gamma_{n+1}} \langle \Theta_n, \{ \nabla U(Y_s) - \nabla U(\overline{Y}_s) \} \rangle \, ds.
\]
Young’s inequality and Jensen’s inequality imply
\[
\left\| \int_{\Gamma_n}^{\Gamma_{n+1}} \{ \nabla U(Y_s) - \nabla U(\overline{Y}_s) \} \, ds \right\|^2 \leq 2\gamma_{n+1}^2 \| \nabla U(Y_{\Gamma_n}) - \nabla U(\overline{Y}_{\Gamma_n}) \|^2 \\
+ 2\gamma_{n+1} \int_{\Gamma_n}^{\Gamma_{n+1}} \| \nabla U(Y_s) - \nabla U(\overline{Y}_s) \|^2 \, ds.
\]
Using (3), \( \gamma_1 \leq 1/(m + L) \) and \( (\gamma_k)_{k \geq 1}\) is nonincreasing, (46) becomes
\[
\| \Theta_{n+1} \|^2 \leq \{1 - \gamma_{n+1}\kappa\} \| \Theta_n \|^2 + 2\gamma_{n+1} \int_{\Gamma_n}^{\Gamma_{n+1}} \| \nabla U(Y_s) - \nabla U(\overline{Y}_s) \|^2 \, ds \\
- 2 \int_{\Gamma_n}^{\Gamma_{n+1}} \langle \Theta_n, \{ \nabla U(Y_s) - \nabla U(\overline{Y}_s) \} \rangle \, ds.
\]
Using the inequality \( |\langle a, b \rangle| \leq \epsilon \|a\|^2 + (4\epsilon)^{-1} \|b\|^2 \) concludes the proof of (44).
We now prove (45). Note that (44) implies that
\[
\mathbb{E}^{\mathcal{F}_{T_n}} \left[ \| \Theta_{n+1} \|^2 \right] \leq \left\{ 1 - \gamma_{n+1}(\kappa - 2\epsilon) \right\} \| \Theta_n \|^2 \\
+ (2\gamma_{n+1} + (2\epsilon)^{-1}) \int_{\Gamma_n}^{T_n} \mathbb{E}^{\mathcal{F}_{T_n}} \left[ \| \nabla U(Y_s) - \nabla U(Y_{T_n}) \|^2 \right] ds .
\]

By $\mathbf{H1}$, the Markov property of $(Y_t)_{t \geq 0}$ and Lemma 19, we have
\[
\int_{\Gamma_n}^{T_n} \mathbb{E}^{\mathcal{F}_{T_n}} \left[ \| \nabla U(Y_s) - \nabla U(Y_{T_n}) \|^2 \right] ds \\
\leq L^2 \left( d\gamma_{n+1}^2 + dL^2\gamma_{n+1}^4/2 + (1/2)L^2\gamma_{n+1}^3 \| Y_{T_n} - x^* \|^2 \right) .
\]
The proof is then concluded plugging this bound in (48).

6.2 Proofs of Theorem 9

Lemma 21. Assume $\mathbf{H1}$, $\mathbf{H2}$ and $\mathbf{H3}$. Let $(\gamma_k)_{k \geq 1}$ be a nonincreasing sequence with $\gamma_1 \leq 1/(m + L)$, and $\zeta_0 \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d)$. Let $(Y_t, Y^t)_{t \geq 0}$ be defined by (9) such that $(Y_0, Y^0)$ is distributed according to $\zeta_0$. Then for all $n \geq 0$ and $\epsilon > 0$, almost surely
\[
\mathbb{E}^{\mathcal{F}_{T_n}} \left[ \| Y_{T_n+1} - Y_{\Gamma_n} \|^2 \right] \leq \left\{ 1 - \gamma_{n+1}(\kappa - 2\epsilon) \right\} \| Y_{T_n} - Y_{\Gamma_n} \|^2 \\
+ \gamma_{n+1} \left\{ d(2L^2 + \epsilon^{-1}(dL^2/12 + \gamma_{n+1}L^4/4) + \gamma_{n+1}^2L^4/6) \\
+ L^4(\epsilon^{-1}/3 + \gamma_{n+1}) \| Y_{T_n} - x^* \|^2 \right\} .
\]

Proof. Let $n \geq 0$ and $\epsilon > 0$, and set $\Theta_n = Y_{T_n} - Y_{\Gamma_n}$. Using Itô’s formula, we have for all $s \in [\Gamma_n, T_n+1)$,
\[
\nabla U(Y_s) - \nabla U(Y_{T_n}) = \int_{\Gamma_n}^{s} \left\{ \nabla^2 U(Y_u) \nabla U(Y_u) + \bar{\Delta}(\nabla U)(Y_u) \right\} du \\
+ \sqrt{2} \int_{\Gamma_n}^{s} \nabla^2 U(Y_u) dB_u .
\]

Since $\Theta_n$ is $\mathcal{F}_{\Gamma_n}$-measurable and $(\int_0^s \nabla^2 U(Y_u) dB_u)_{s \in [0, T_n+1]}$ is a $(\mathcal{F}_s)_{s \in [0, T_n+1]}$-martingale under $\mathbf{H1}$, by (49) we have:
\[
\left| \mathbb{E}^{\mathcal{F}_{T_n}} \left| \langle \Theta_n, \nabla U(Y_s) - \nabla U(Y_{T_n}) \rangle \right| \right| \\
= \left| \left\langle \Theta_n, \mathbb{E}^{\mathcal{F}_{T_n}} \left[ \int_{\Gamma_n}^{s} \left\{ \nabla^2 U(Y_u) \nabla U(Y_u) + \bar{\Delta}(\nabla U)(Y_u) \right\} du \right] \right\rangle \right| .
\]

Combining this equality and $| \langle a, b \rangle | \leq \epsilon \| a \|^2 + (4\epsilon)^{-1} \| b \|^2$ in (47) we have
\[
\mathbb{E}^{\mathcal{F}_{T_n}} \left[ \| \Theta_{n+1} \|^2 \right] \leq \left\{ 1 - \gamma_{n+1}(\kappa - 2\epsilon) \right\} \| \Theta_n \|^2 \\
+ (2\epsilon)^{-1} A \\
2\gamma_{n+1} \mathbb{E}^{\mathcal{F}_{T_n}} \left[ \int_{\Gamma_n}^{T_n} \| \nabla U(Y_s) - \nabla U(Y_{T_n}) \|^2 ds \right] ,
\]

(50)
where
\[
A = \int_{\Gamma_n}^{\Gamma_{n+1}} \left\| \mathbb{E}^{\mathcal{F}_n} \left[ \int_{\Gamma_n}^{s} \nabla^2 U(Y_u) \nabla U(Y_u) + (1/2) \Delta (\nabla U)(Y_u) du \right] \right\|^2 ds .
\]

We now separately bound the two last terms of the right hand side. By H1, the Markov property of \((Y_t)_{t \geq 0}\) and Lemma 19, we have
\[
\int_{\Gamma_n}^{\Gamma_{n+1}} \mathbb{E}^{\mathcal{F}_n} \left[ \left\| \nabla U(Y_s) - \nabla U(Y_{\Gamma_n}) \right\|^2 \right] ds 
\leq L^2 \left( d \gamma_{n+1}^2 + dL^2 \gamma_{n+1}^4/12 + (1/2) L^2 \gamma_{n+1}^3 \|Y_{\Gamma_n} - x^*\|^2 \right) . \tag{51}
\]

We now bound \(A\). We get using Jensen’s inequality, Fubini’s theorem, \(\nabla U(x^*) = 0\) and (16)
\[
A \leq 2 \int_{\Gamma_n}^{\Gamma_{n+1}} \int_{\Gamma_n}^{s} \mathbb{E}^{\mathcal{F}_n} \left[ \left\| \nabla^2 U(Y_u) \nabla U(Y_u) \right\|^2 \right] du ds 
+ 2^{-1} \int_{\Gamma_n}^{\Gamma_{n+1}} \int_{\Gamma_n}^{s} \mathbb{E}^{\mathcal{F}_n} \left[ \left\| \Delta (\nabla U)(Y_u) \right\|^2 \right] du ds
\leq 2 \int_{\Gamma_n}^{\Gamma_{n+1}} (s - \Gamma_n)L^4 \int_{\Gamma_n}^{s} \mathbb{E}^{\mathcal{F}_n} \left[ \|Y_u - x^*\|^2 \right] du ds + \gamma_{n+1}^3 d^2 L^2 / 6 . \tag{52}
\]

By Lemma 19-(i), the Markov property and for all \(t \geq 0, 1 - e^{-t} \leq t\), we have for all \(s \in [\Gamma_n, \Gamma_{n+1}]\),
\[
\int_{\Gamma_n}^{s} \mathbb{E}^{\mathcal{F}_n} \left[ \|Y_u - x^*\|^2 \right] du \leq (2m)^{-1} (1 - e^{-2m(s - \Gamma_n)}) \|Y_{\Gamma_n} - x^*\|^2 + d(s - \Gamma_n)^2 .
\]

Using this inequality in (52) and for all \(t \geq 0, 1 - e^{-t} \leq t\), we get
\[
A \leq (2L^4 \gamma_{n+1}^3 / 3) \|Y_{\Gamma_n} - x^*\|^2 + L^4 \gamma_{n+1}^4 / 2 + \gamma_{n+1}^3 d^2 L^2 / 6 .
\]

Combining this bound and (51) in (50) concludes the proof. \(\square\)

7 Proof of Theorem 15

We preface the proof by a preliminary lemma. Define for all \(\gamma > 0\), the function \(n : \mathbb{R}_+^* \to \mathbb{N}\) by
\[
n(\gamma) = \left\lfloor \log (\gamma^{-1}) / \log(2) \right\rfloor . \tag{53}
\]

Lemma 22. Assume H1, H2 and H3. Let \(\gamma \in (0, 1/(m + L))\). Then for all \(x \in \mathbb{R}^d\) and \(\ell \in \mathbb{N}^*, \ell > 2^{n(\gamma)}\),
\[
\|\delta x P_{t\gamma} - \delta x R_{t\gamma}\|_{TV} \leq (\varphi^{(2)}_{t-2^{n(\gamma)+2}\gamma}(x)/\varphi^{(2)}_{t-2^{n(\gamma)+2}\gamma}(x)))^{1/2}
+ 2^{-3/2} L \left\{ \left( \gamma^3 L^2 / 3 \right) \varphi_{t-1}(x) + 2 \right\}^{1/2} + \sum_{k=1}^{n(\gamma)} (\varphi^{(2)}_{t-2^{k}\gamma}(x)/\varphi^{(2)}_{t-2^{k+1}\gamma}(x))^{1/2} .
\]

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where \( \vartheta_{1,\ell-1}(x) \) is defined by (8) and for all \( n_1, n_2 \in \mathbb{N}, \vartheta_{n_1,n_2}^{(2)} \) is given by (23).

**Proof.** Let \( \gamma \in (0,1/(m+L)) \) and \( \ell \in \mathbb{N}^* \). For ease of notation, let \( n = n(\gamma) \), and assume that \( \ell > 2^n \). Consider the following decomposition

\[
\| \delta_x P_{\ell \gamma} - \delta_x R_{\ell \gamma}^\ell \|_{TV} \leq \left\| \left\{ \delta_x P_{(\ell-2^n)\gamma} - \delta_x R_{\ell-2^n}^{\ell-2^n} \right\} P_{2^n \gamma} \right\|_{TV}
\]

\[
+ \| \delta_x R_{\ell-1} \{ P_{\gamma} - R_{\gamma} \} \|_{TV} + \sum_{k=1}^n \| \delta_x R_{\ell-2^k} \left\{ P_{2^k-1 \gamma} - R_{2^k-1 \gamma} \right\} P_{2^k-1 \gamma} \|_{TV}. \tag{54}
\]

We bound each term in the right hand side. First by (18) and Equation (25), we have

\[
\left\| \left\{ \delta_x P_{(\ell-2^n)\gamma} - \delta_x R_{\ell-2^n}^{\ell-2^n} \right\} P_{2^n \gamma} \right\|_{TV} \leq (\vartheta_{\ell-2^n,0}^{(2)}(x)/(\pi 2^{n+1}\gamma))^{1/2}, \tag{55}
\]

where \( \vartheta_{n,0}^{(2)}(x) \) is given by (23). Similarly but using in addition Proposition 2, we have for all \( k \in \{1, \ldots, n\} \),

\[
\left\| \delta_x R_{\ell-2^k} \left\{ P_{2^k-1 \gamma} - R_{2^k-1 \gamma} \right\} P_{2^k-1 \gamma} \right\|_{TV} \leq (\vartheta_{2^k-1,\ell-2^k}^{(2)}(x)/(\pi 2^{k+1}\gamma))^{1/2}, \tag{56}
\]

where \( \vartheta_{2^k-1,\ell-2^k}^{(2)}(x) \) is given by (23). For the last term, by [10, Equation 11] and the Pinsker inequality, we have

\[
\| \delta_x R_{\ell-2} \{ P_{\gamma} - R_{\gamma} \} \|_{TV}^2 \leq 2^{-3} L^2 \left\{ (\gamma^3/3) \int_{\mathbb{R}^d} \| \nabla U(z) \| R_{\ell-2}^{-1}(x,dz) + d\gamma^2 \right\}. \tag{57}
\]

By H1 and Proposition 2, we get

\[
\left\| \delta_x R_{\ell-1} \{ R_{\gamma} - P_{\gamma} \} \right\|_{TV}^2 \leq 2^{-3} L^2 \left\{ (\gamma^3 L^2/3) \vartheta_{1,\ell-1}(x) + d\gamma^2 \right\}. \tag{58}
\]

Combining (55), (56) and (57) in (54) concludes the proof. \( \square \)

**Proof of Theorem 15.** By Lemma 22, we get (see the supplementary document [12, Section 7] for the detailed calculation):

\[
\| \delta_x P_{\ell \gamma} - \delta_x R_{\gamma}^\ell \|_{TV} \leq 2^{-3/2} L \left\{ (\gamma^3 L^2/3) \left\{ (1 - \kappa \gamma)\ell^{-1} \| x - x^\ast \|^2 + 2\kappa^{-1} d \right\} + d\gamma^2 \right\}^{1/2}
\]

\[
+ (4\pi)^{-1/2} \left[ \gamma^2 E_1(\gamma,d) + \gamma^3 E_2(\gamma) E_3(\gamma,d,x) \right]^{1/2}
\]

\[
+ \kappa(\gamma)/(4\pi)^{-1/2} \left[ \gamma^2 E_1(\gamma,d) + \gamma^2 E_2(\gamma) E_4(\gamma,d,x) \right]^{1/2}, \tag{58}
\]

where

\[
E_3(\gamma,d,x) = (\ell - \gamma^{-1})e^{-m\gamma(\ell-2\gamma^{-1}-1)}\| x - x^\ast \|^2 + 2d/(\kappa \gamma m)
\]

\[
E_4(\gamma,d,x) = e^{-m\gamma(\ell-2\gamma^{-1}-1)}\| x - x^\ast \|^2 + 2\kappa^{-1} d + d/m.
\]

Letting \( \ell \) go to infinity, using Theorem 11-(iii) and Theorem 12-(iii), we get the desired conclusion. \( \square \)
8 Contraction in total variation for functional autoregressive models

In this section, we consider functional autoregressive models of the form: for all $k \geq 0$

$$X_{k+1} = h_{k+1}(X_k) + \sigma_{k+1}Z_{k+1},$$  

(59)

where $(Z_k)_{k \geq 1}$ is a sequence of i.i.d. $d$ dimensional standard Gaussian random variables, $(\sigma_k)_{k \geq 1}$ is a sequence of positive real numbers and $(h_k)_{k \geq 1}$ are a sequence of measurable map from $\mathbb{R}^d$ to $\mathbb{R}^d$ which satisfies the following assumption:

**AR1.** For all $k \geq 1$, there exists $\varpi_k \in \mathbb{R}$ such that $h_k$ is $1 - \varpi_k$-Lipschitz, i.e. for all $x, y \in \mathbb{R}^d$, $\|h_k(x) - h_k(y)\| \leq (1 - \varpi_k)\|x - y\|$.

The sequence $\{X_k, k \in \mathbb{N}\}$ defines an inhomogeneous Markov chain associated with the sequence of Markov kernel $(P_k)_{k \geq 1}$ on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$ given for all $x \in \mathbb{R}^d$ and $\mathbf{A} \in \mathbb{R}^d$ by

$$P_k(x, \mathbf{A}) = \frac{1}{(2\pi \sigma_k^2)^{d/2}} \int_{\mathbf{A}} \exp \left( -\|y - h_k(x)\|^2 / (2\sigma_k^2) \right) dy .$$  

(60)

We denote for all $n \geq 1$ by $Q^n$ the marginal laws of the sequence $(X_k)_{k \geq 1}$ and given by

$$Q^n = P_1 \cdots P_n .$$  

(61)

In this section we compute an upper bound of $\{\|\delta_x Q^n - \delta_y Q^n\|_{TV}, n \in \mathbb{N}\}$ which does not depend on the dimension $d$.

Let $x, y \in \mathbb{R}^d$. We consider for all $k \geq 1$ the following coupling $(X_1, Y_1)$ between $P_k(x, \cdot)$ and $P_k(y, \cdot)$. Define the function $E$ and $e$ from $\mathbb{R}^d \times \mathbb{R}^d$ to $\mathbb{R}^d$ by

$$E_k(x, y) = h_k(y) - h_k(x) , e_k(x, y) = \begin{cases} E_k(x, y) / \|E_k(x, y)\| & \text{if } E_k(x, y) \neq 0 \\ 0 & \text{otherwise} \end{cases} .$$  

(62)

For all $x, y, z \in \mathbb{R}^d$, $x \neq y$, define

$$F_k(x, y, z) = h_k(y) + (\text{Id} - 2e_k(x, y)e_k(x, y)^T) z \quad \text{and} \quad \alpha_k(x, y, z) = \frac{\varphi_{\sigma_k^2}(\|E_k(x, y)\| - \langle e_k(x, y), z \rangle)}{\varphi_{\sigma_k^2}(\|e_k(x, y)\|)} ,$$  

(63)

(64)

where $\varphi_{\sigma_k^2}$ is the probability density of a zero-mean gaussian variable with variance $\sigma_k^2$. Let $Z_1$ be a standard $d$-dimensional Gaussian random variable. Set $X_1 = h_k(x) + \sigma_k Z_1$ and

$$Y_1 = \begin{cases} h_k(y) + \sigma_k Z_1 & \text{if } E_k(x, y) = 0 \\ B_1 X_1 + (1 - B_1) F_k(x, y, Z_1) & \text{if } E_k(x, y) \neq 0 , \end{cases}$$

where $B_1$ is a Bernoulli random variable independent of $Z_1$ with success probability

$$p_k(x, y, z) = 1 \land \alpha_k(x, y, z) .$$

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The construction above defines for all \((x, y) \in \mathbb{R}^d \times \mathbb{R}^d\) the Markov kernel \(K_k\) on \((\mathbb{R}^d \times \mathbb{R}^d, \mathcal{B}(\mathbb{R}^d) \otimes \mathcal{B}(\mathbb{R}^d))\) given for all \((x, y) \in \mathbb{R}^d \times \mathbb{R}^d\) and \(\Lambda \in \mathcal{B}(\mathbb{R}^d) \otimes \mathcal{B}(\mathbb{R}^d)\) by

\[
K_k((x, y), \Lambda) = \frac{1}{(2\pi \sigma_k^2)^d/2} \int_{\mathbb{R}^d} I_\Lambda(\tilde{x}, x)e^{-\|\tau_k(\tilde{x}, x)\|^2/(2\sigma_k^2)}d\tilde{x} + \frac{1}{(2\pi \sigma_k^2)^d/2} \left[ \int_{\mathbb{R}^d} I_\Lambda(\tilde{x}, x)p_k(x, y, \tau_k(\tilde{x}, x))e^{-\|\tau_k(\tilde{x}, x)\|^2/(2\sigma_k^2)}d\tilde{x} \right],
\]

where for all \(\tilde{x} \in \mathbb{R}^d\), \(\tau_k(\tilde{x}, x) = \tilde{x} - h_k(x)\) and \(D = \{(\tilde{x}, \tilde{y}) \in \mathbb{R}^d \times \mathbb{R}^d \mid \tilde{x} = \tilde{y}\}\). It is shown in [4, Section 3.3] that for all \(x, y \in \mathbb{R}^d\) and \(k \geq 1\), \(K_k((x, y), \cdot)\) is a transference plan of \(P_k(x, \cdot)\) and \(P_k(y, \cdot)\). Furthermore, we have for all \(x, y \in \mathbb{R}^d\) and \(k \geq 1\)

\[
K_k((x, y), D) = 2\Phi\left(-\frac{\|E_k(x, y)\|}{2\sigma_k}\right).
\]

For all initial distribution \(\mu_0\) on \((\mathbb{R}^d \times \mathbb{R}^d, \mathcal{B}(\mathbb{R}^d) \otimes \mathcal{B}(\mathbb{R}^d))\), \(\tilde{P}_{\mu_0}\) and \(\widetilde{E}_{\mu_0}\) denote the probability and the expectation respectively, associated with the sequence of Markov kernels \(K_k\) defined in (65). It may be evaluated to \(\llbracket\delta_x Q^k - \delta_y Q^k\rrbracket_{\text{TV}}\), \(n \geq 1\) amounts to evaluate \(\tilde{P}_{(x,y)}(X_n = Y_n)\). It is the content of the proof of the main result of this section.

**Theorem 23.** Assume **AR1**. Then for all \(x, y \in \mathbb{R}^d\) and \(n \geq 1\),

\[
\llbracket\delta_x Q^n - \delta_y Q^n\rrbracket_{\text{TV}} \leq \llbracket D^c((x, y))\rrbracket \left\{ 1 - 2\Phi\left(-\frac{\|x - y\|}{2\Xi_n^{1/2}}\right) \right\},
\]

where \((\Xi_i)_{i \geq 1}\) is defined for all \(k \geq 1\) by \(\Xi_k = \sum_{i=1}^k \sigma_i^2\{\prod_{j=1}^i (1 - \omega_j)^{-2}\}^2\).

We preface the proof by a technical Lemma.

**Lemma 24.** For all \(\zeta, a > 0\) and \(t \in \mathbb{R}_+\), the following identity holds

\[
\frac{1}{t} \int_{\mathbb{R}} \varphi_{\zeta^2}(y) \left\{ 1 \wedge \frac{\varphi_{\zeta^2}(t - y)}{\varphi_{\zeta^2}(y)} \right\} \left\{ 1 - 2\Phi\left(-\frac{|2y - t|}{2a}\right) \right\}dy
\]

\[
= 1 - 2\Phi\left(-\frac{t}{2(\zeta^2 + a^2)^{1/2}}\right).
\]

**Proof.** The proof is postponed to [12, Section 4.2].
Proof of Theorem 23. Since for all $k \geq 1$, $(X_k, Y_k)$ is a coupling of $\delta_x Q^k$ and $\delta_y Q^k$, 
$$||\delta_x Q^k - \delta_y Q^k||_{TV} \leq \hat{P}_{(x,y)}(X_k \neq Y_k).$$
Define for all $k_1, k_2 \in \mathbb{N}^*$, $k_1 \leq k_2$, $\Xi_{k_1,k_2} = \sum_{i=k_1}^{k_2} \sigma_i^2 \{ \prod_{j=k_1}^{i-1} (1 - \omega_j)^{-2} \}$. Let $n \geq 1$.
We show by backward induction that for all $k \in \{0, \cdots, n-1\}$,

$$\hat{P}_{(x,y)}(X_n \neq Y_n) \leq \hat{E}_{(x,y)} \left[ \mathbbm{1}_{D^c}(X_k, Y_k) \left( 1 - 2\Phi \left\{ \frac{||X_k - Y_k||}{2 \Xi_{k+1,n}^{1/2}} \right\} \right) \right], \quad (67)$$

Note that the inequality for $k = 0$ will conclude the proof.

Since $X_n \neq Y_n$ implies that $X_{n-1} \neq Y_{n-1}$, the Markov property and (66) imply

$$\hat{P}_{(x,y)}(X_n \neq Y_n) = \hat{E}_{(x,y)} \left[ \mathbbm{1}_{D^c}(X_{n-1}, Y_{n-1}) \hat{E}_{(X_{n-1}, Y_{n-1})} \left[ \mathbbm{1}_{D^c}(X_1, Y_1) \right] \right] \leq \hat{E}_{(x,y)} \left[ \mathbbm{1}_{D^c}(X_{n-1}, Y_{n-1}) \left( 1 - 2\Phi \left\{ \frac{||E_n(X_{n-1}, Y_{n-1})||}{2 \sigma_n} \right\} \right) \right].$$

Using $\texttt{AR1}$ and (62), $||E_n(X_{n-1}, Y_{n-1})|| \leq (1 - \omega_n) ||X_{n-1} - Y_{n-1}||$, showing (67) holds for $k = n - 1$.

Assume that (67) holds for $k \in \{1, \cdots, n-1\}$. On $\{X_k \neq Y_k\}$, we have

$$||X_k - Y_k|| = -||E_k(X_{k-1}, Y_{k-1})|| + 2 \sigma_k e_k(X_{k-1}, Y_{k-1})^T Z_k,$$

which implies

$$\mathbbm{1}_{D^c}(X_k, Y_k) \left( 1 - 2\Phi \left\{ \frac{||X_k - Y_k||}{2 \Xi_{k+1,n}^{1/2}} \right\} \right) = \mathbbm{1}_{D^c}(X_k, Y_k) \left( 1 - 2\Phi \left\{ \frac{-2 \sigma_k e_k(X_{k-1}, Y_{k-1})^T Z_k - ||E_k(X_{k-1}, Y_{k-1})||}{2 \Xi_{k+1,n}^{1/2}} \right\} \right).$$

Since $Z_k$ is independent of $\hat{F}_{k-1}$, $\sigma_k e_k(X_{k-1}, Y_{k-1})^T Z_k$ is a real Gaussian random variable with zero mean and variance $\sigma_k^2$, therefore by Lemma 24, we get

$$\hat{P}_{(x,y)}(X_k \neq Y_k) \mathbbm{1}_{D^c}(X_k, Y_k) \left( 1 - 2\Phi \left\{ \frac{||X_k - Y_k||}{2 \Xi_{k+1,n}^{1/2}} \right\} \right) \leq \mathbbm{1}_{D^c}(X_{k-1}, Y_{k-1}) \left( 1 - 2\Phi \left\{ \frac{||E_k(X_{k-1}, Y_{k-1})||}{2 \left( \sigma_k^2 + \Xi_{k+1,n}^{1/2} \right)} \right\} \right).$$

Using by $\texttt{AR1}$ that $||E_k(X_{k-1}, Y_{k-1})|| \leq (1 - \omega_k) ||X_{k-1} - Y_{k-1}||$ concludes the induction. \qed
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